Materials Capability Review

Los Alamos National Laboratory
April 29-May 2, 2012

On the cover: Details of the electronic structure of the Hidden Order system URu$_2$Si$_2$ as measured by Angle-resolved Photoelectron Spectroscopy.”

Contents

2012 Materials Review Committee

Gary S. Was, Chair
University of Michigan
gsw@umich.edu

Barbara Jones, Vice Chair
IBM Research - Almaden
bajones@almaden.ibm.com

Dimitri Basov
University of California, San Diego
dbasov@physics.ucsd.edu

Michael Kaufman
Colorado School of Mines
mkaufman@mines.edu

Richard LeSar
Iowa State University
lesar@iastate.edu

Jeffrey Lynn
National Institute of Standards and Technology
Jeff.Lynn@nist.gov

Christine Orme
Lawrence Livermore National Laboratory
orme1@llnl.gov

Thomas Russell
Air Force Office of Scientific Research
Thomas.russell@afosr.af.mil

Adam Schwartz
Lawrence Livermore National Laboratory
Schwartz6@llnl.gov

LANS Science and Technology Committee Representatives
Alexandra Navrotsky
University of California, Davis
anavrotsky@ucdavis.edu

Rochus (Robbie) Vogt
California Institute of Technology
vogt@caltech.edu

University of California Observer
Robert Powell
Robert.Powell@ucop.edu

Agenda

Final

Materials Capability Review
Los Alamos National Laboratory

April 29-May 2, 2012

Hilton @ Buffalo Thunder 5th Floor Executive Lounge

Sunday Evening, April 29, 2012 *(By Invitation Only)*

6:00 Opening Session – Committee Gathering and Reception

6:30 Director's Welcome and Committee Charge ....Alan R. Bishop
PADSTE: Principal Associate Director, Science, Technology & Engineering

7:00 ADEPS Welcome and Expectations ....Susan J. Seestrom
ADEPS: Associate Director, Experimental Physical Sciences

7:15 LANL LDRD (Laboratory Directed Research & Development) Overview
....William Priedhorsky
LDRD-PO: Program Director, Laboratory Directed Research & Development

7:30 Executive Session *(Committee Only)*...Gary S. Was
Committee Chair

Purpose:	**Annual Capability Review**	Classification Level:	Unclassified/Classified
Institutional Host(s):	Susan J. Seestrom, ADEPS, 505-665-4454	Dress:	Business/Business Casual
Technical Host(s)	Toni Taylor, MPA-DO, 5-1131	Revised:	April 24, 2012
Protocol POC:	Peggy S. Vigil, CGA-GAO, 7-8448 or cell 699-2195		
Catering:	ARAMARK		
LANL Update:	505-667-6622 or 1-877-723-4101: Provided information about changes in the Laboratory schedule (i.e., closings or delays) Protocol Office will adhere to all weather delays/closings.		

Monday, April 30, 2012

7:00 Meet Visitors in Lobby of the Hilton @ Buffalo Thunder .... Peggy S. Vigil
CGA-IVE: PADSTE, Protocol

7:05 Travel to LANL Badge Office (bus leaves hotel promptly @ 7:05 a.m.) LANS Taxi Service

7:30 Badge Office Processing .... Peggy S. Vigil
CGA-IVE: PADSTE, Protocol

8:00 Walk to J. Robert Oppenheimer Study Center (breakfast provided for committee)

J. Robert Oppenheimer Study Center
TA-3, Bldg. 207, Jemez/Cochiti Room

8:20 Welcome and Logistics .... Susan J. Seestrom
ADEPS: Associate Director, Experimental Physical Sciences

8:30 Materials@LANL .... Antoinette (Toni) Taylor
MPA-DO: Division Leader, Materials Physics & Applications

9:30 MaRIE Overview .... John L. Sarrao
SPO-SC: Program Director, Office of Science

10:00 Break

10:15 Isolating the Influence of Kinetic and Spatial Effects of Dynamic Damage Evolution .... Ellen K. Cerreta
MST-8: Scientist, Materials Science in Radiation and Dynamic Extremes

11:15 LDRD-DR Discussion Led By .... William Priedhorsky
LDRD-PO: Program Director, Laboratory Directed Research & Development
including Susan Seestrom, John Sarrao, and Toni Taylor

11:45 Working Lunch with Early Career Staff and Postdocs *(By Invitation Only)*
(San Ildefonso Conference Room and Gallery Area)

Purpose:	**Annual Capability Review**	Classification Level:	Unclassified/Classified
Institutional Host(s):	Susan J. Seestrom, ADEPS, 505-665-4454	Dress:	Business/Business Casual
Technical Host(s)	Toni Taylor, MPA-DO, 5-1131	Revised:	April 24, 2012
Protocol POC:	Peggy S. Vigil, CGA-GAO, 7-8448 or cell 699-2195		
Catering:	ARAMARK		
LANL Update:	505-667-6622 or 1-877-723-4101: Provided information about changes in the Laboratory schedule (i.e., closings or delays) Protocol Office will adhere to all weather delays/closings.		

1:00 Co-design At Los Alamos National Laboratory .... Antonio Redondo
T-DO: Division Leader, Theoretical

1:30 Exascale Co-Design Center for Materials in Extreme Environments .... Timothy C. Germann
T-1: Scientist, Physics and Chemistry of Materials

2:00 Discussion and Questions .... Antonio Redondo
T-DO: Division Leader, Theoretical

2:15 Poster Presentation .... Various Staff
Poster Titles and Presenters: See Appendix A, Page 7

3:00 Poster Session
Santa Clara Gallery

4:00 Voice of the Customer *(By Invitation Only)*
San Ildefonso Conference Room

5:00 Executive Session *(Committee Only)* .... Gary S. Was
Committee Chair

6:00 Travel to Gabriel's Restaurant *(Transportation for Committee Only)* .... Taxi Service

6:30 Hosted Working Dinner *(By Invitation Only)*
Strategy Pillar Discussion .... Antoinette (Toni) Taylor
MPA-DO: Division Leader, Materials Physics & Applications
.... Frank J. Alexander
CCS-DO: Deputy Division Leader, Computer, Computational & Statistical Sciences
.... Eugene (Gene) J. Peterson
ADCLES: Senior Advisor, Chemistry, Life & Earth Sciences

8:30 Travel to the Hilton @ Buffalo Thunder .... Taxi Service

---

Purpose: **Annual Capability Review**
Institutional Host(s): Susan J. Seestrom, ADEPS, 505-665-4454
Technical Host(s) Toni Taylor, MPA-DO, 5-1131
Protocol POC: Peggy S. Vigil, CGA-GAO, 7-8448 or cell 699-2195
Catering: ARAMARK
LANL Update: 505-667-6622 or 1-877-723-4101: Provided information about changes in the Laboratory schedule (i.e., closings or delays) Protocol Office will adhere to all weather delays/closings.

Classification Level: Unclassified/Classified
Dress: Business/Business Casual
Revised: April 24, 2012

Tuesday, May 1, 2012

7:00 Meet Visitors in Lobby of the Hilton @ Buffalo Thunder .... Peggy S. Vigil
CGA-IVE: PADSTE, Protocol

7:05 Travel to LANL, (bus leaves hotel promptly @ 7:05 a.m.) .... Taxi Service
(breakfast provided for committee)

TA-35, Bldg. 86, Room 205

7:45 Committee Photo .... Robert W. Kramer
ADEPS Communications Team

8:00 Energetic Materials and High Pressure Science .... David J. Funk
WX-DO: Division Leader, Weapons Experiments

8:30 Recent Impact Experiments Probed with Synchrotron X-rays at the Advanced Photon Source .... Brian J. Jensen
WX-9: Scientist, Shock and Detonation Physics

9:00 Discussion and Questions .... David J. Funk
WX-DO: Division Leader, Weapons Experiments

9:15 Posters Presentations... Various Staff
Poster Titles and Presenters: See Appendix B, Page 8

9:30 Poster Session (Uncleared)
NHMFL (TA-35-127) Lobby

10:15 Q Cleared Members Travel to Target Fabrication Facility, TA-35-213-E102

10:30 Overview: Materials Science Research and Development for the Nuclear Weapons Program – On the Path to Prediction and Control (U) .... David F. Teter
MST-DO: Division Leader, Materials Science & Technology

11:00 Applications for Fundamental High Explosives Research for Stockpile Transformation (U) .... Daniel E. Hooks
WX-9: Scientist, Shock and Detonation Physics

Purpose:	**Annual Capability Review**	Classification Level:	Unclassified/Classified
Institutional Host(s):	Susan J. Seestrom, ADEPS, 505-665-4454	Dress:	Business/Business Casual
Technical Host(s)	Toni Taylor, MPA-DO, 5-1131	Revised:	April 24, 2012
Protocol POC:	Peggy S. Vigil, CGA-GAO, 7-8448 or cell 699-2195		
Catering:	ARAMARK		
LANL Update:	505-667-6622 or 1-877-723-4101: Provided information about changes in the Laboratory schedule (i.e., closings or delays) Protocol Office will adhere to all weather delays/closings.		

11:30 A Co-Design Approach to Plutonium Casting Development (U) .... Deniece Korzekwa
MST-16: Group Leader, Nuclear Materials Science

12:00 Classified Poster Session .... Various Staff

12:45 Return Q Cleared Members to Building 86

UNCLEARED COMMITTEE MEMBERS:

10:15 Uncleared Members travel to DARHT Facility, TA-15, Access Center Building 446

10:45 Tour of DARHT .... Juan Barraza
.... *WX-2: Group Leader, DARHT Engineering*

12:15 Uncleared members return to TA-35, Building 86, Room 205

1:00 Working Lunch – Committee Time *(Committee Only)*

2:00 National High Magnetic Field Laboratory .... Charles H. Mielke
MPA-CMMS: Director, NHMFL-PFF; Deputy Group Leader, Condensed Matter & Magnet Science

2:30 Science in Extremes of High Magnetic Fields..Neil Harrison
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

3:00 Poster Presentations .... Various Staff
Poster Titles and Presenters: See Appendix C, Page 10

3:15 Tour of Magnet Facilities... Charles H. Mielke
MPA-CMMS: Director, NHMFL-PFF; Deputy Group Leader, Condensed Matter & Magnet Science

4:00 Poster Session
NHMFL (TA-35-127) Lobby

5:00 Travel to the Hilton @ Buffalo Thunder .... Taxi Service
Committee: Executive Session @ Buffalo Thunder

Wednesday, May 2, 2012

7:00 Meet Visitors in Lobby of the Hilton @ Buffalo Thunder .... Peggy S. Vigil
CGA-IVE: PADSTE, Protocol

7:05 Travel to LANL (bus leaves hotel promptly @ 7:05 a.m.)................... LANS Taxi Service

J. Robert Oppenheimer Study Center
TA-3, Bldg. 207, Jemez/Cochiti Room

7:30 Committee Members Arrive (breakfast provided for committee) .... Gary S. Was
Committee Chair

8:00 Overview: Condensed Matter Physics .... Michael F. Hundley
MPA-CMMS: Group Leader, Condensed Matter & Magnet Science

8:30 Creating Magnetoelectric Effects with Non-Coplanar Spins............................. Vivien Zapf
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

9:00 Electronic Hot Spots in the Spectral Function of Actinides ....Matthias J. Graf
T-4: Scientist, Physics of Condensed Matter & Complex Systems

9:30 Discussion and Questions .... Michael F. Hundley
MPA-CMMS: Group Leader, Condensed Matter & Magnet Science

9:45 Poster Presentation... Various Staff
Poster Titles and Presenters: See Appendix D, Page 11

10:00 Poster Session
Santa Clara Gallery

11:00 Working Lunch – Committee Time *(Committee Only)*

12:00 Director's Outbrief *(Closed Session)* .... Charles F. McMillan
Laboratory Director

1:00 Open Outbrief .... Gary S. Was
Committee Chair

2:00 Committee Members Depart

Purpose: **Annual Capability Review**
Institutional Host(s): Susan J. Seestrom, ADEPS, 505-665-4454
Technical Host(s) Toni Taylor, MPA-DO, 5-1131
Protocol POC: Peggy S. Vigil, CGA-GAO, 7-8448 or cell 699-2195
Catering: ARAMARK
LANL Update: 505-667-6622 or 1-877-723-4101: Provided information about changes in the Laboratory schedule (i.e., closings or delays) Protocol Office will adhere to all weather delays/closings.

Classification Level: Unclassified/Classified
Dress: Business/Business Casual
Revised: April 24, 2012

APPENDIX A

CO-DESIGN FOR MATERIALS POSTER SESSION, *Monday, April 30, 2012*

A Multi-mesoscale Predictive Capability for Interface-driven Behavior............Irene C. Beyerlein
T-3: Scientist, Fluid Dynamics and Solid Mechanics

Computational Co-design for Multi-Scale Application in the Natural Sciences........Duan Zhang, *T-3: Scientist, Fluid Dynamics and Solid Mechanics* and Virginie DuPont, *T-1: Scientist, Physics and Chemistry of Materials*

Optimization Principles for Computational Co-design with Applications to Molecular Dynamics...Stephan J. Eidenbenz
CCS-3: Deputy Group Leader, Information Sciences

Co-design for Materials: Confluence of MaRIE and Exascale...............................Turab Lookman
T-4: Scientist, Physics of Condensed Matter and Complex Systems

Increasing the Timescale of Atomistic Simulations through Co-designed Accelerated Molecular Dynamics Methods ....Danny Perez
T-1: Scientist, Physics and Chemistry of Materials

Understanding, Exploiting, and Controlling Competing Interactions in Complex Oxides.. Quanxi Jia
MPA-CINT: Scientist, Center for Integrated Nanotechnologies

Co-design Modeling of Reactions Behind a Shock Front .... Marc J. Cawkwell
T-1: Scientist, Physics and Chemistry of Materials

APPENDIX B

HIGH EXPLOSIVES/HIGH PRESSURE POSTER SESSION, *Tuesday, May 1, 2012*

Homemade Explosives Afghanistan Training at LANL.................................. Virginia W. Manner
WX-6: Scientist, Explosive Applications and Special Projects

Coherent Control Studies for the Initiation and Detection of Explosives .... David S. Moore
WX-9: Scientist, Shock and Detonation Physics

Modeling Microstructure Evolution for High-Pressure / Strain-Rate Phase Transformations .... Francis L. (Frank) Addessio
T-3: Scientist, Fluid Dynamics and Solid Mechanics

High P-T Neutron Diffraction Study of Hydrous Minerals.. Monika Hartl
EES-14: Scientist, Earth System Observations

Computing Raman Spectra On-the-fly in Extended Lagrangian Born-Oppenheimer Molecular Dynamics .... Anders M. Niklasson and Joshua D. Coe
T-1: Scientists, Physics and Chemistry of Materials

Time-resolved Measurements of Phase Transformations Using a “Pressure-jump” Diamond Anvil Cell and X-ray Diffraction... Nenad Velisavljevic
WX-9: Scientist, Shock and Detonation Physics

Thwarting Chemistry in Dynamic Extremes: Multi-shock Compression of High Explosives.. Tariq D. Aslam
WX-9: Scientist, Shock and Detonation Physics

High P-T Neutron Reflectometry of Solid-Fluid Interfaces............................. Donald D. Hickmott
EES-DO: Scientist, Earth & Environmental Sciences

CLASSIFIED SESSION:

Isentropic Compression Experiments on Plutonium (U)..Paulo A. Rigg
WX-9: Team Leader, Shock and Detonation Physics

EOS Development and Compaction Models for Porous Materials (U)..........Darcie Dennis-Koller
WX-9: Scientist, Shock and Detonation Physics

Hydrotest 3648 (U) ....Shirish Chitanvis
XTD-3: Scientist, Primary Physics

Linking Experimental Behavior and Thermodynamic Theory: Development of a Multi-phase EOS (U)..Frank J. Cherne
WX-9: Scientist, Shock and Detonation Physics

Incorporating Deformation Physics into Engineering Simulations (U)..................Rodney McCabe
MST-6: Scientist, Materials Technology--Metallurgy

APPENDIX C

***NATIONAL HIGH MAGNETIC FIELD LABORATORY POSTER SESSION**, Tuesday, May 1, 2012*

Designing High Strength/High Conductivity Wire for Pulsed Electromagnets .... Ryan F. Need
MPA-CMMS: Undergraduate Student, Condensed Matter & Magnet Science

Dirac Materials in High Magnetic Fields..Ross D. McDonald
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

Dimensionality Control in Organic Quantum Magnets ....John Singleton
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

Photo-Induced Magnetization in Copper-Doped Semiconductor Nanocrystals .... Scott A. Crooker
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

Nanometer Resolution Magnetostricion Measurements in Pulsed Magnetic Fields to 100T...Marcelo Jaime
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

High-Field Characterization of High Temperature Superconductors .... Fedor F. Balakirev
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

New Multiferroic States in Frustrated Ising Spin Chain Compound.........................Jae-Wook Kim
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

Binary Alloy Solidification at 35 Tesla .... Jason Cooley
MST-6: Team Leader, Materials Technology-Metallurgy

APPENDIX D

CONDENSED MATTER PHYSICS POSTER SESSION, *Wednesday, May 2, 2012*

Magnetic Non-Uniformity in $(La_{0.4}Pr_{0.6})_{0.67}Ca_{0.33}MnO_3$ Films and Measurement of the Strain-Magnetization Coupling Coefficient ....Michael Fitzsimmons
LANSCE-LC: Scientist, Lujan Neutron Scattering Center

Ultrafast Optical Probes of Coupled Systems .... Rohit Prasankumar, *MPA-CINT: Scientist, Center for Integrated Nanotechnologies*, and Stuart Trugman, *T-4: Scientist, Physics of Condensed Matter & Complex Systems*

Electronic Inhomogeneity in Heavy Fermion Materials.. Eric D. Bauer
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

New Capabilities at MPA: Ultrafast Quasiparticle Dynamics in Actinides ... Tomasz Durakiewicz
MPA-CMMS: Scientist, Condensed Matter & Magnet Science

First Observation of ^{239}Pu Nuclear Magnetic Resonance ....Georgios Koutroulakis
MPA-CMMS: Postdoctoral Researcher, Condensed Matter & Magnet Science

Localized Anharmonic Rattling of Aluminum Atoms in VAl_{10}.................................Doug Safarik
MST-6: Scientist, Materials Technology-Metallurgy

Artificial Spin Ice: Frustration by Design and Magnetic Monopoles......................Cristiano Nisoli
T-4: Scientist, Physics of Condensed Matter & Complex Systems

First-Principles Theory for Correlated Electron Materials .... Jian-Xin Zhu
T-4: Scientist, Physics of Condensed Matter & Complex Systems

CHARTER
For the 2012 Los Alamos National Laboratory Materials Capability Review Committee

Los Alamos National Laboratory (LANL) uses Capability Reviews to **assess** the quality and institutional integration of science, technology and engineering (STE) and to **advise** Laboratory Management on the current and future health of LANL STE. The capabilities are deliberately chosen to be crosscutting over the Laboratory and therefore will include experimental, theoretical and simulation disciplines from multiple line organizations. Capability Reviews are designed to provide a more holistic view of the STE quality, integration to achieve mission requirements, and mission relevance. The scope of these capabilities necessitate that there will be significant overlap in technical areas covered by capability reviews (e.g., materials research and weapons science and engineering). In addition, LANL staff may be reviewed in different capability reviews because of their varied assignments and expertise. The principal product of the Capability Review is the report that includes the review committee's assessments, commendations, and recommendations for STE.

Specifically, the Committees will:

- Assess the quality of science, technology and engineering within the Capability in the areas defined in the agenda. Identify issues to develop or enhance the core competencies within this capability.

- Evaluate the integration of this capability across the Laboratory organizations that are listed in the agenda in terms of joint programs, projects, proposals, and/or publications. Describe the integration of this capability in the wider scientific community using the recognition as a leader within the community, ability to set research agendas, and attraction and retention of staff.

- Assess the relevance of this capability's science, technology and engineering contributions to current and emerging Laboratory programs, including Nuclear Weapons, Global Security, and Energy Security.

- Advise the Laboratory Director/Principal Associate Director for Science, Technology and Engineering on the health of the Capability including the current and future (5 year) science, technology and engineering staff needs, mix of research and development activities, program opportunities, environment for conducting science, technology and engineering.

The specific charges for the Materials Capability Review are:

- Assess the Los Alamos Laboratory Directed Research and Development project titled, "Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage" using the criteria performance, quality, and relevance for the current status of the project. The committee is requested to provide advice on future direction of this work.

Ver. 2012.00
May 16, 2011

Instructions for the Los Alamos National Laboratory Fiscal Year 2012 Capability Reviews

Introduction

Los Alamos National Laboratory (LANL) uses external peer review to measure and continuously improve the quality of its science, technology and engineering (STE). LANL uses capability reviews to assess the STE quality and institutional integration and to advise Laboratory Management on the current and future health of the STE. Capability reviews address the STE integration that LANL uses to meet mission requirements. STE capabilities are define to cut across directorates providing a more holistic view of the STE quality, integration to achieve mission requirements, and mission relevance. The scope of these capabilities necessitate that there will be significant overlap in technical areas covered by capability reviews (e.g., materials research and weapons science and engineering). In addition, LANL staff may be reviewed in different capability reviews because of their varied assignments and expertise. LANL plans to perform a complete review of the Laboratory's STE capabilities (hence staff) in a three-year cycle. The principal product of an external review is a report that includes the review committee's assessments, commendations, and recommendations for STE.

The Capability Review Committees have the primary responsibility of assessing the Laboratory's STE quality through the topics selected for the review. The Committees will also evaluate the integration of STE within the capability. Capability reviews are about the quality of STE, but it is difficult to separate the STE from the Laboratory missions and programs. The Committees are charged with evaluating the relevance of the STE towards the Laboratory's missions and programs, but capability reviews are not program reviews and are not expected to perform an in-depth examination of programs. Finally Capability Review Committees provide advice to Laboratory Management on STE issues identified during the review. The assessments and advice are documented in reports prepared by the Capability Review Committees that are delivered to the Director and to the Principal Associate Director for Science, Technology and Engineering (PADSTE). Laboratory Management will use this report for STE assessment and planning. The report is also provided to the Department of Energy (DOE) as part of LANL's Annual Performance Plan and to the Los Alamos National Security (LANS) LLC's Science and Technology Committee (STC) as part of its responsibilities to the LANS Board of Governors.

LANL has defined thirteen STE capabilities. Table 1 lists the four STE capabilities that LANL Management (Director, PADSTE, technical Associate Directors) have identified for review in Fiscal Year (FY) 2012. The FY 2012 capability reviews must be **completed by June 30, 2012** to allow sufficient time for the reports and results to be incorporated into the 2012 STE evaluations by the Department of Energy National Nuclear Security Agency and the LANS LLC STC for the LANS Board of Governors.

These instructions identify responsibilities and provide guidance to those organizing, participating in and performing capability reviews at LANL in FY 2012. These instructions have been refined based on experiences with capability reviews from 2007 - 2011. Any questions or comments on these instructions should be directed to the Office Leader for the LANL Science and Technology Base Programs Peer Review and Metrics Office at stbprm-admin@lanl.gov or 505-667-7824.

Table 1. FY 2012 LANL science, technology and engineering capability reviews, organizing associate director (AD), and Los Alamos National Security, LLC Science and Technology Committee point-of-contact (STC POC).

Capability	Organizing AD	STC POC/co-POC
Computer and Computational Sciences	ADTSC	Karin/Long
High-Energy Density Plasmas and Fluids	ADEPS	Jeanloz/Falcone
Materials	ADEPS	Bercaw/Vogt/Powell
Weapons Science and Engineering	ADW	Vogt/Karin/Peddicord

Roles and Responsibilities

LANL Director/PADSTE

1. Determines capabilities to be reviewed and review schedule.
2. Appoints an Organizing AD (OAD) for each capability review.
3. Works with the OAD to create a specific charge for each capability review.
4. Participates in Capability Review Committee member selection as needed.
5. In conjunction with the STC Chair approves the Capability Review Chair and members.
6. Invites the Capability Review Chair and members.
7. Hosts the Capability Review Chairs meeting before the review cycle starts.
8. Provides the charge to the Capability Review.
9. Attends executive session at closeout.
10. Ensures report is delivered by requested deadline.
11. Provides the Capability Review report to the STC Chair for distribution to the STC.
12. Addresses the Capability Review recommendations through the PADSTE Management Review Board assigning actions and resources. The PADSTE will determine if the actions are tracked through the LANL performance tracking system.
13. Incorporates review recommendations and issues into LANL STE planning and assigns actions.
14. Provides summary response for all capability reviews to Capability Review Committee Chairs and to the STC Chair.

LANS, LLC STC Chair (STC Chair)

1. Appoints STC members to serve as the point-of-contact (POC) and co-point-of-contact (co-POC) for each Capability Review Committee.
2. In conjunction with the LANL Director/PADSTE, approves the Capability Review Committee Chair and members.
3. The STC Chair or the Vice Chair may attend any Capability Review meeting as observers. Observers may participate in discussions and attend all sessions, but may not participate in drafting the report.

LANS, LLC STC Point of Contact (POC) / co-Point of Contact (co-POC)

1. Working with the Organizing AD (OAD), compiles a list of potential Capability Review Committee members based on input from the Laboratory, University of California (UC), and STC members. (UC Office of the President (UCOP) collects input from UC, including from the Academic Senate). At least one and a maximum of two LLNL staff members and at least one University of California faculty member are to be named to each Capability Review Committee. The POC does not count for either of these requirements.
2. Working with the OAD, prioritizes the list of potential Capability Review Committee Chairs and members. The list is given to the PADSTE and the STC Chair for approval.

3. The POC or OAD, as appropriate, contacts the recommended Capability Review Chair to ask if the person will serve; the PADSTE officially invites the Chair.
4. Reviews the prioritized Capability Review Committee membership candidate list with the selected Capability Review Chair and OAD; the STC Chair and PADSTE are notified of any changes.
5. Works with the Capability Review Committee Chair and OAD to identify potential dates for the Capability Review meeting.
6. With dates in hand, the POC, OAD, or Capability Review Committee Chair, as appropriate, contacts the proposed Capability Review Committee members regarding their willingness to serve until approximately 9 members, including the Chair, are enlisted. At least one and a maximum of two LLNL staff members and at least one University of California faculty member are to be named to each Capability Review Committee. The Capability Review organizing team (i.e., OAD, Capability Review Committee Chair, and POC) maintains contact during this step and consults if issues arise.
7. Participates in developing the Capability Review meeting agenda with the OAD and Capability Review Committee Chair.
8. Attends the Capability Review Chairs meeting hosted by the PADSTE before the review cycle starts.
9. Attends the Capability Review meeting as an ex-officio member, participates as a full member, including attendance at executive sessions, but does not participate in drafting the report.

LANL Organizing Associate Director (OAD)

1. Coordinates with LANL Director/PADSTE and with ADs who contribute to the capability to develop the Capability Review scope.
2. Works with the POC to prioritize the list of potential Capability Review Committee Chairs and members. The list is given to the PADSTE and the STC Chair for approval.
3. The OAD or POC, as appropriate, contacts the recommended Capability Review Committee Chair to ask if the person will serve; the PADSTE officially invites the Chair.
4. Reviews the prioritized Capability Review Committee membership candidate list with the selected Capability Review Committee chair and POC; the STC Chair and PADSTE are notified of any changes.
5. Works with the Capability Review Committee Chair and POC to identify potential dates for the Capability Review meeting.
6. With dates in hand, the OAD, POC, or Capability Review Committee Chair, as appropriate, contacts the proposed Capability Review Committee members regarding their willingness to serve until approximately 9 members, including the Chair, are enlisted. At least one and a maximum of two LLNL staff members and at least one University of California faculty member are to be named to each Capability Review Committee. The Capability Review organizing team (i.e., OAD, Capability Review Committee Chair, and POC) maintains contact during this step and consults if issues arise.

7. Participates in developing the review agenda with the POC and Capability Review Committee Chair.
8. Identifies Los Alamos Laboratory Directed Research and Development (LDRD) project to be reviewed for the current year. The LANL LDRD Office can assist in project identification.
9. Attends the Capability Review Chairs meeting hosted by the PADSTE before the review cycle starts.
10. Compiles and sends background information to the Capability Review Committee before the review.
11. Provides logistics for the Capability Review meeting, including meeting rooms, necessary security for classified sessions, etc.
12. Works with the Capability Review Committee Chair to maintain review agenda and schedule.
13. Provides additional information requested by the Capability Review Committee.
14. Addresses Capability Review recommendations assigned by Director/PADSTE.

Capability Review Committee Chairperson

1. Reviews the prioritized Capability Review Committee membership candidate list with the selected OAD and POC; the STC Chair and PADSTE are notified of any changes.
2. Works with the organizing AD and POC to identify potential dates for the Capability Review meeting.
3. With dates in hand, the OAD, POC, or Capability Review Committee Chair, as appropriate, contacts the proposed Capability Review Committee members regarding their willingness to serve until approximately 9 members, including the Chair, are enlisted. At least one and a maximum of two LLNL staff members and at least one University of California faculty member are to be named to each Capability Review Committee. The Capability Review organizing team (i.e., OAD, Capability Review Committee Chair, and POC) maintains contact during this step and consults if issues arise.
4. Participates in developing the Capability Review meeting agenda with the POC and OAD. The Chair ensures sufficient executive time in the agenda for committee discussions.
5. Attends a meeting of the Capability Review Committee Chairs hosted by the PADSTE before the review cycle starts.
6. Distributes information about the meeting to Capability Review Committee members as necessary.
7. Presides over the review by keeping to the agenda, managing deliberations of the Capability Review Committee, and assigning tasks to Capability Review Committee members as appropriate.
8. Prepares and leads executive out-brief to the Director/PADSTE.
9. Provides Capability Review report to the LANL Director/PADSTE within 30 days of the review.

Capability Review Committee Members

1. Attend review and complete tasks assigned by Capability Review Committee Chair.
2. Provide unbiased and objective evaluation of the topics within the capability being assessed.
3. Provide written material to Capability Review Committee Chair with sufficient time to meet schedule.

Assessment

The evaluation of designated topics must address the following two criteria:

1) Comparison to peers -- State how the work compares to similar or related work conducted by others.
2) Sustainability -- State the extent to which the reviewed activities strengthen or weaken LANL capabilities. How does the activity/contribution build core competencies or other resources that contribute to the vitality of the capability and the long-term vigor of the Laboratory and its ability to meet the needs of the nation?

Laboratory Directed Research and Development Assessments for FY 2012 Capability Reviews

The Director/PADSTE will charge each Capability Review Committee to assess a single Laboratory Directed Research and Development (LDRD) project related to the capability. Many of the three-year LDRD projects will be nearing completion enabling the Capability Review Committee to assess the quality of the work performed and provide guidance on the programmatic development of the project.

The Capability Review Committee is requested to prepare an assessment (one to two pages) of the LDRD project that will be included in the Capability Review report and in the LDRD Annual Report to the DOE. The selected LDRD project will be included in the agenda as a presentation, and the Capability Review Committee will be asked to assess the project using the following criteria:

1. Quality: Are the science and technology results of high quality compared to national and international peers?
2. Performance (project execution): Is the project making good progress against its milestones? Is it well conceived and executed?
3. Relevance: Is the project continuing to support the strategic directions of the Laboratory?
4. Leadership: Are the results of the project defining R&D directions for the broader community?

The LDRD office will provide a guidance sheet to assist the committee in evaluating the project. The use of the guidance sheet will allow a common framework for LDRD project evaluation with other reviews that LANL performs of its LDRD projects. The committee cannot fully implement the guidance because the capability review duration is shorter than allowed for other reviews, but the guidance does indicate some key concepts that we would like to see addressed.

The Capability Review Committee's advice on future directions and opportunities for the project is requested.

Briefing management

At the end of it's meeting, the Capability Review Committee will brief its findings to LANL Management. Attendance at this briefing, other than senior management (Director/PADSTE), remains at the discretion of the Capability Review Committee Chair and the Director/PADSTE. The out-brief should provide executive style highlights of the assessments and advice for the capability. The Capability Review Committee should prioritize its assessment and advice for the out-briefing (and the report). Specifically, the Capability Review Committee should deliberate in its executive session to identify and prepare for presentation:

1) 3 to 7 most notable contributions observed in the review, and
2) 3 to 7 most important "actionable" recommendations.

Each of these components of the out-briefing should be presented in order of decreasing importance or significance (highest, next to highest, etc.). The rationale behind prioritization is to engage the wisdom and experience of the Capability Review Committee to identify the true pinnacles and the most significant challenges. It is the distinctiveness of the greatest achievements and the magnitude of the greatest challenges that characterize the excellence of an organization/program.

By prioritizing a limited number of items, Capability Review Committees are able to focus their feedback and enable meaningful follow up by LANL Management. A template containing recommended content for the out-briefing can be found in the Appendix of this document.

Preparing the Capability Review report

The Capability Review Committee must submit its assessment and advice via written report. The final copy is due to the Program Manager in the Science and Technology Based Programs Peer Review and Metrics Office within 30 working days of the end of the Capability Review meeting. The Capability Review Committee Chair is responsible for delegating writing assignments, coordinating inputs, editing the final document, and submitting it.

A suggested report template can be found in the Appendix of this document. The template includes abstracts of the areas to be assessed and headings delineating the areas in which specific advice has been requested. The assessment of the LDRD project can follow the same format, but the three criteria (performance, quality, and relevance) that were identified in these instructions need to be addressed.

Appendix

Capability Review Out-Brief Template

Acknowledgement and Recognition
  Opening remarks
  Feedback on execution of review
Assessment of Topics in the Agenda
  Comparison to peers, mission/program relevance, integration
  Assessment of LDRD project
Prioritized Conclusions
  Top 3 to 7 Capability Review Committee “actionable” recommendations
  Top 3 to 7 most notable science, technology and engineering contributions
Special topics
  Any needs for additional information or meetings
  Topics of enduring interest beyond the annual review cycle (e.g. from prior reviews)
  Improvements in capability review process

Capability Review Committee Report Template

Title
Table of Contents
Executive Summary
Introduction
Assessment
- Review Elements (*directly from agenda)*
- Review element 1
  - Scope of the review
    - *Can use pre-written element description (single 50-300 word abstract written by LANL contributor summarizing goal of contribution and key results)*
  - Analysis (*in terms of one or more of these 4 facets)*
    - Approach
    - Implementation
    - Results
    - Impact of work
  - Assessment
    - Comparison to peers
    - Sustainability
- Review element 2
- Review element n
- Review of LDRD project
  - Performance
  - Quality
  - Relevance
  - Capability Review Committee's advice on future directions for the project

Prioritized Conclusions
- Top 3 to 7 most notable science, technology and/or engineering contributions (or other high performance indicators)
- Top 3 to 7 Capability Review Committee "actionable" recommendations

Acknowledgements
Appendices
- Capability Review Committee Meeting Agenda
- Roster of Capability Review Committee Members
- Additional inputs or documents used in assessment by Capability Review Committee

Materials@LANL

Antoinette J. Taylor (MPA-DO)

The scientific and technical area of Materials has been a foundational capability at Los Alamos National Laboratory since the Laboratory's inception. The Materials Capability currently encompasses a wide array of technical disciplines, research topics, organizations and sponsors. Central to the Laboratory's Materials Capability is the vision of intentional control of functionality through discovery and application of fundamental materials properties and materials synthesis and fabrication techniques, reaching from the molecular level, through nano- to microscopic scales, to bulk material. Achieving this goal requires a program of synthesis, fabrication, characterization, and theory and modeling across a wide range of materials relevant to current and anticipated missions of the Laboratory. This materials program enables innovative R&D at the boundaries of chemistry, physics, theory and materials science that translates fundamental discovery to materials production in strategic areas such as actinide science.

In this presentation, we will first describe the structure of the current Materials Capability Review (MCR). Next, we will report on progress addressing the recommendations from last year's MCR. We will then describe our benchmarking efforts to critically review the Materials Capability at LANL. We will also provide an update on the Materials Strategy Implementation Plan. Finally, we will present a few technical highlights not covered in other themes of the MCR.

Materials @LANL

Toni Taylor

Division Leader

Materials Physics and Applications

Presentation outline

- LANL update/Trends in metrics
- Progress in Implementation Plan for Materials Strategy
- Technical highlights
- Response to 2011 MCR recommendations
- 2012 Topics

Presentation outline

- **LANL update/Trends in metrics**
- Progress in Implementation Plan for Materials Strategy
- Technical highlights
- Response to 2011 MCR recommendations
- 2012 Topics

The Materials Capability spans the Laboratory: Lab Leadership has changed in the past year

Institutional Leaders

Charlie McMillan
Laboratory Director

Elizabeth Sellers
Deputy Laboratory Director

Alan Bishop (Acting)
Principal Associate Director
Science, Technology & Engineering

Bret Knapp
Principal Associate Director
Weapons Programs

Terry Wallace
Principal Associate Director
Global Security

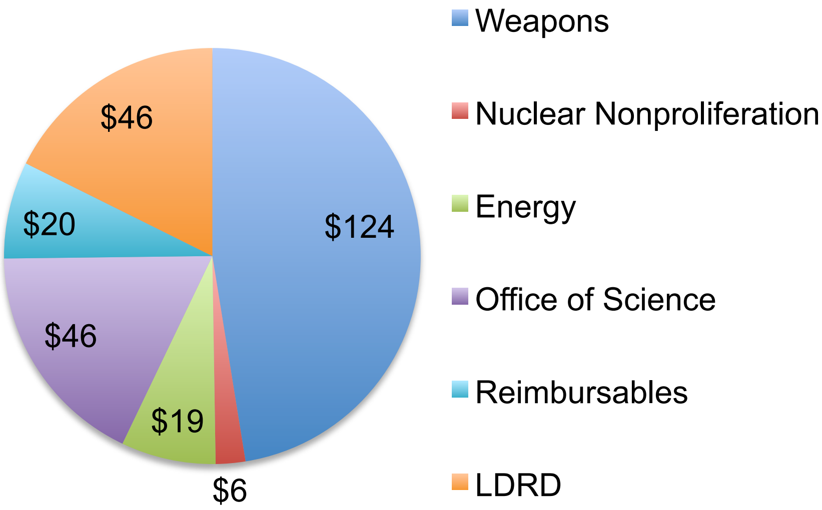
Directorate	Assoc. Director	Code	Divisions
Chemistry, Life, & Earth Sciences	Nan Sauer	ADCLES	Bioscience Chemistry Earth & Environmental Sciences
Engineering & Engineering Sciences	Steve Girrens	ADE	Accelerator Operations & Technology Applied Engineering & Technology Prototype Fabrication
Experimental Physical Sciences	Susan Seestrom	ADEPS	Materials Physics & Applications Materials Science & Technology Los Alamos Neutron Science Center Physics
Information Technology	Carolyn Zerkle	ADIT	Departmental Computing Services Network & Infrastructure Engineering Software & Applications Engineering
Theory, Simulation, & Computation	Paul Dotson (Acting)	ADTSC	Computer, Computational, & Statistical Sciences High Performance Computing Theoretical
Plutonium Science & Manufacturing	Jeff Yarbrough	ADPSM	Integrated Program Management Nuclear Component Operations Manufacturing Engineering & Technology Nuclear Process Infrastructure
Weapons Engineering & Experiments	John Benner (Acting)	ADW	Weapons Experiments Weapons Systems Engineering
Weapons Physics	Robert Webster (Acting)	ADX	Computational Physics Theoretical Design
Threat Identification & Response	Scott Gibbs	ADTIR	Decision Applications International & Applied Technology Intelligence & Space Research Nuclear Nonproliferation

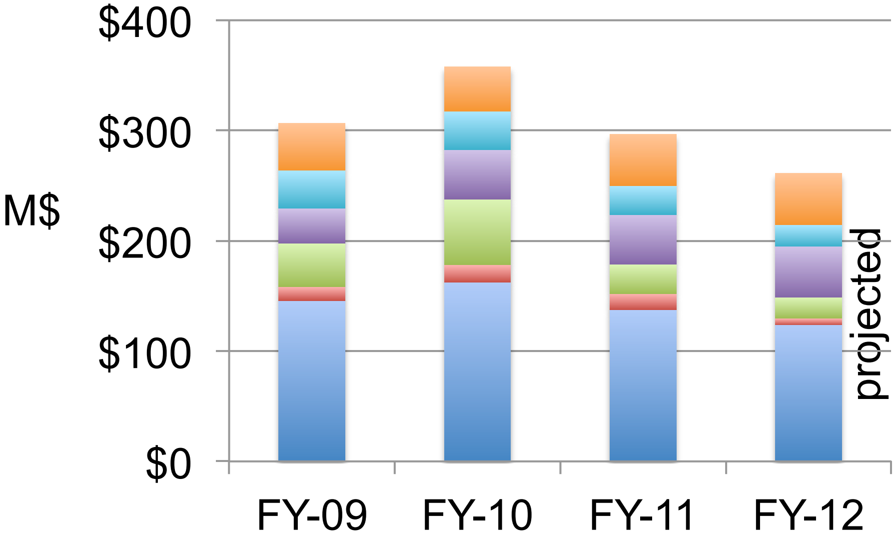
Significant reductions in funding for major program areas are adversely affecting materials R&D

The projected budget for FY-12 is $261M, down from a peak of $357M in FY-10 and average of $320M for FY-09 to FY-11:

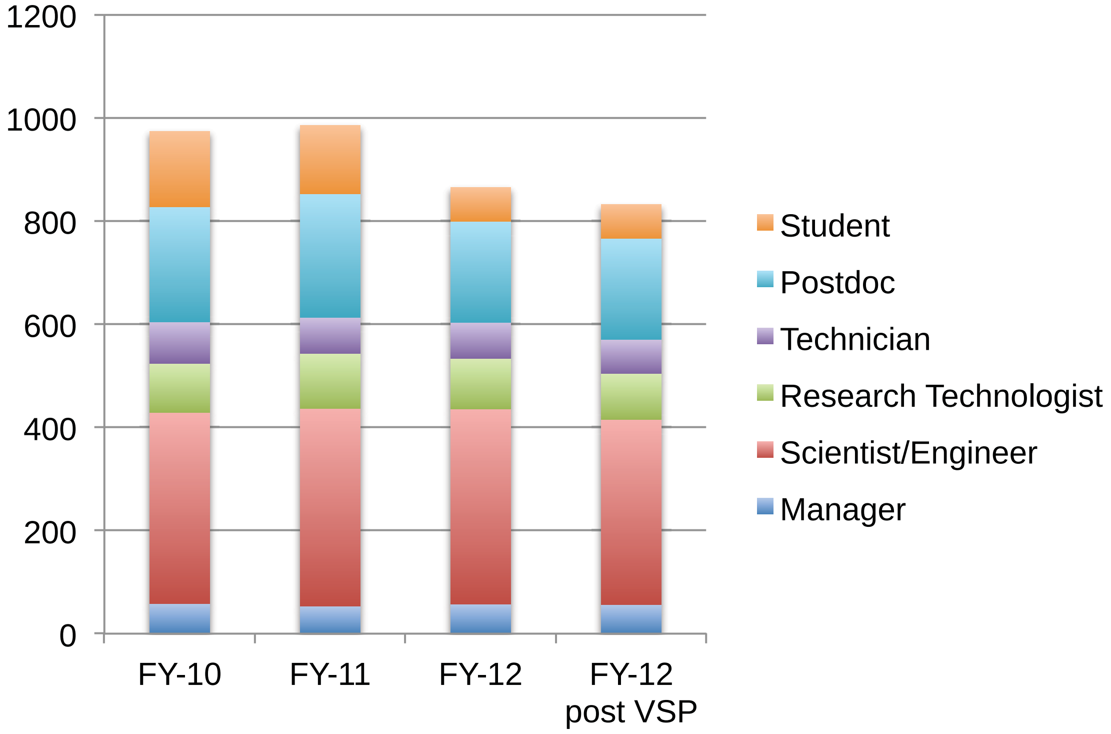
- Weapons down 17% from average
- Energy down 54%
- Reimbursables down 38%
- Office of Science up 14%

FY12: $261M



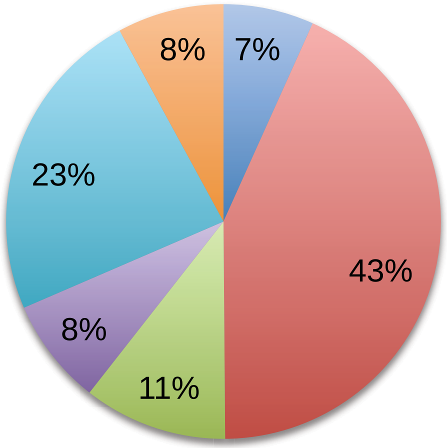


Materials R&D engages over ~800 personnel at LANL



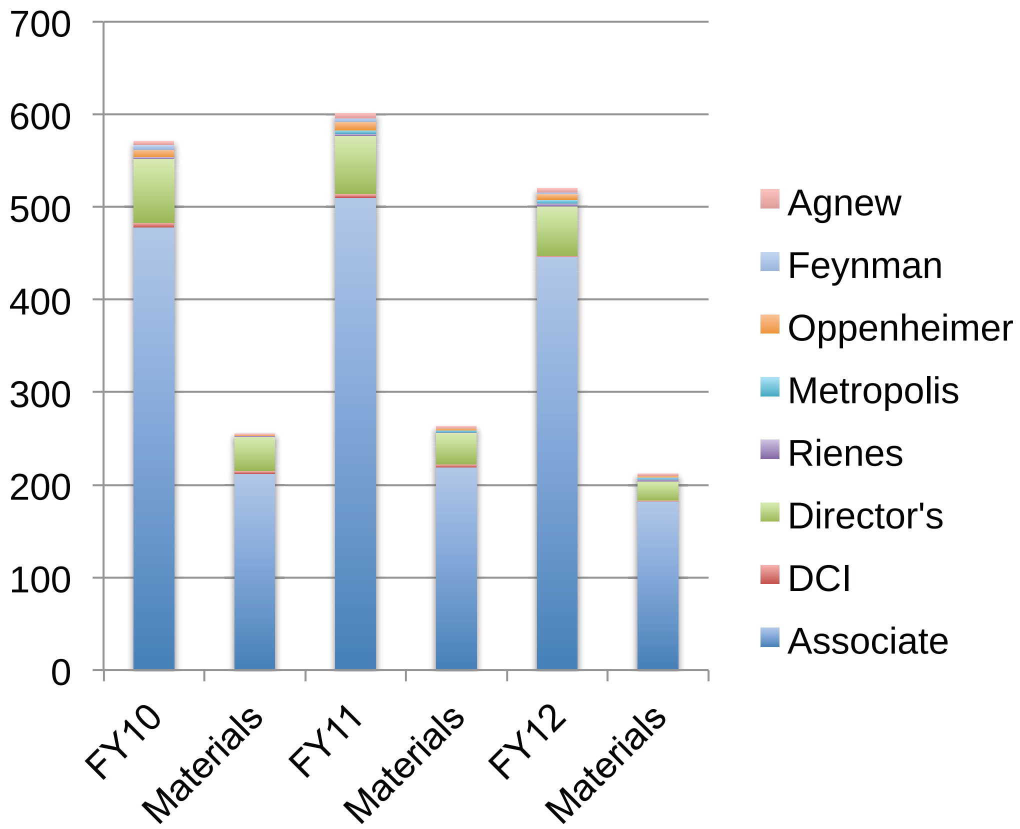
About 5.5% of the core materials R&D personnel participated in the voluntary separation program

FY-12 post VSP



Post docs and students account for one third of the materials R&D personnel mix (total 832)

Materials Science attracts a large number of well-qualified post docs to LANL



Over 40% of the post docs at LANL are engaged in materials research, including post docs in the heavily-competed post doctoral fellows categories.

LANL materials researchers continue to garner external recognition

Robert Field, Amit Misra, and Deniece Korzekwa: **ASM Fellows**

Timothy Germann, Charles Reichhardt, Cynthia Reichhardt, Bogdan Mihaila, and Marcelo Jaime: **APS Fellows**

Paul Burgardt: **American Welding Society Fellow**

Jeanne Robinson, Sasha Balatsky, Jacqueline Kiplinger, and Quanxi Jia: **AAAS Fellows**

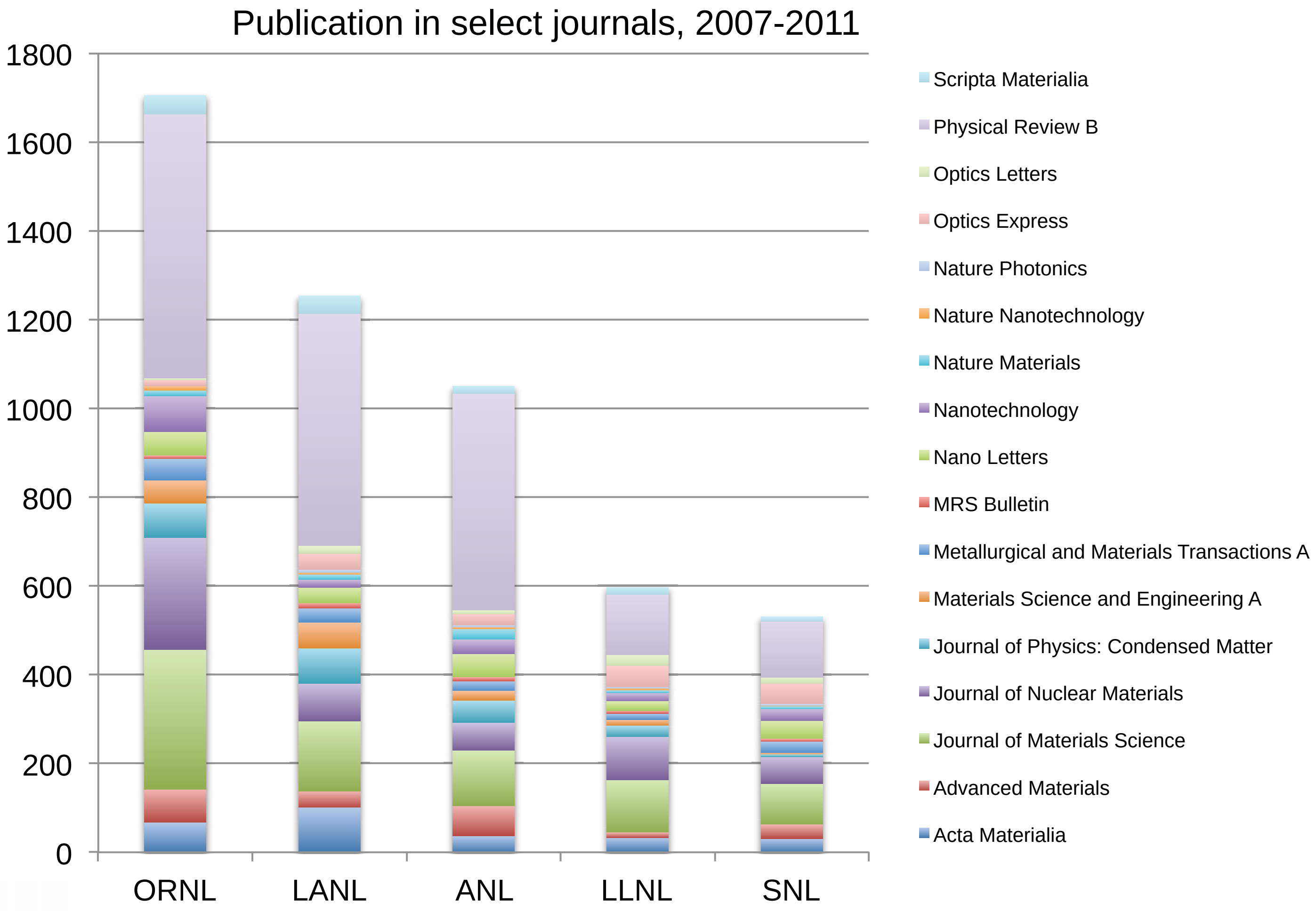
John Carpenter and Nathan Mara: **TMS Young Leaders Professional Development Award**

Michael Nastasi: **MRS Fellow**

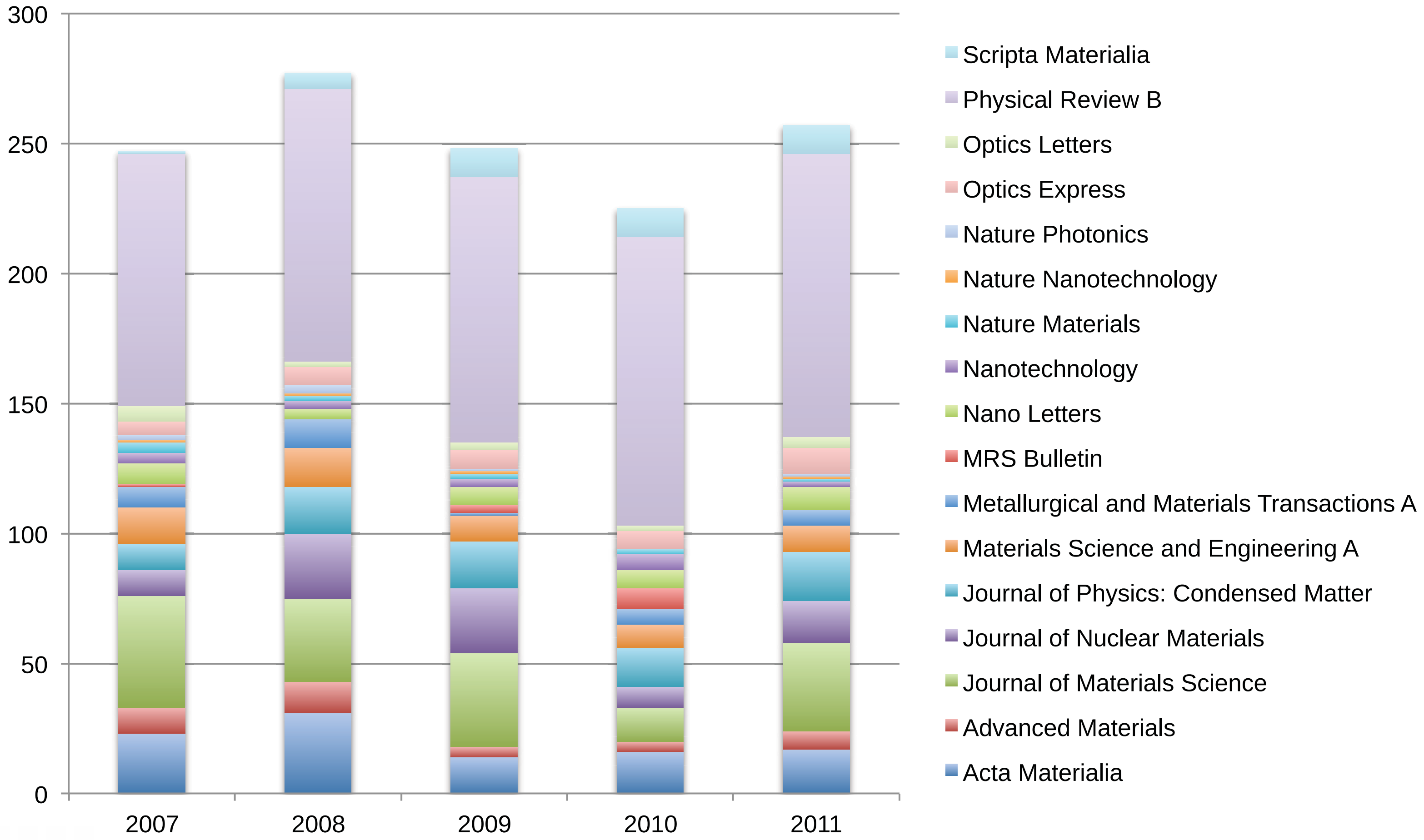
Dane Spearing: **American Ceramic Society Fellow**

David Chavez: **E.O. Lawrence Award**

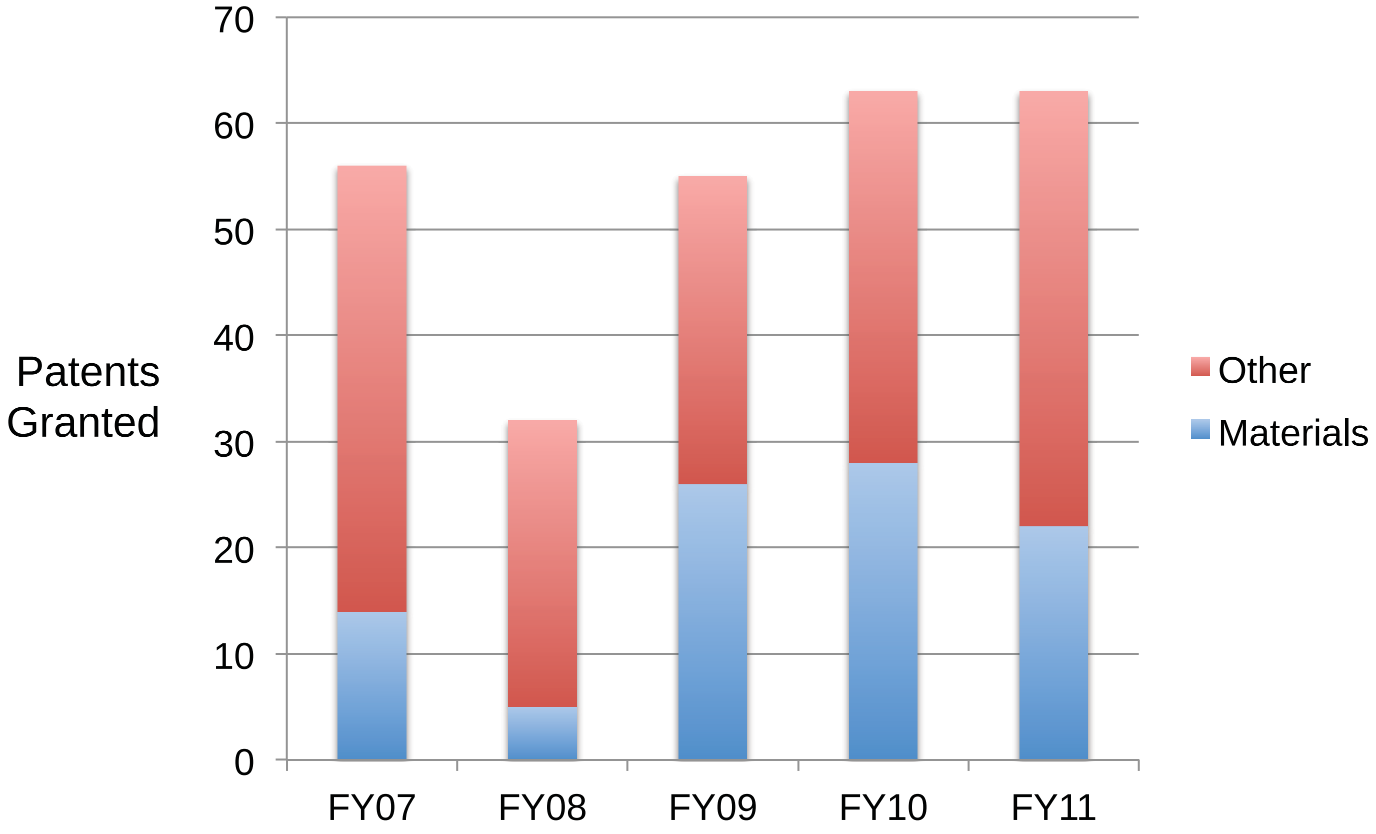
LANL is competitive with other national laboratories in materials publications



LANL'S materials publication output has been relatively constant over the past five years



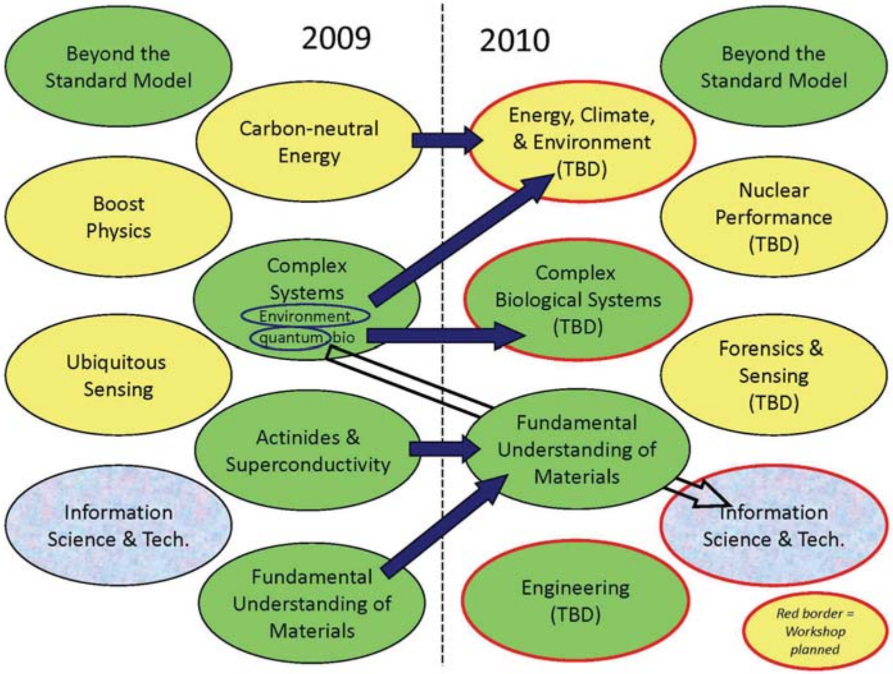
35% of patents granted to LANL over the past five years derive from materials research



Concern:

Changes in the structure of the Grand Challenges in the FY10 competition weaken LDRD DR support for the Materials Pillar

- Materials is one of 3 LANL Pillars
- LANL is designated as the Pu Center of Excellence


2009

2010

Beyond the Standard Model

Carbon-neutral Energy

Boost Physics

Complex Systems

Environment, quantum, bio

Ubiquitous Sensing

Actinides & Superconductivity

Information Science & Tech.

Fundamental Understanding of Materials

Beyond the Standard Model

Energy, Climate, & Environment (TBD)

Nuclear Performance (TBD)

Complex Biological Systems (TBD)

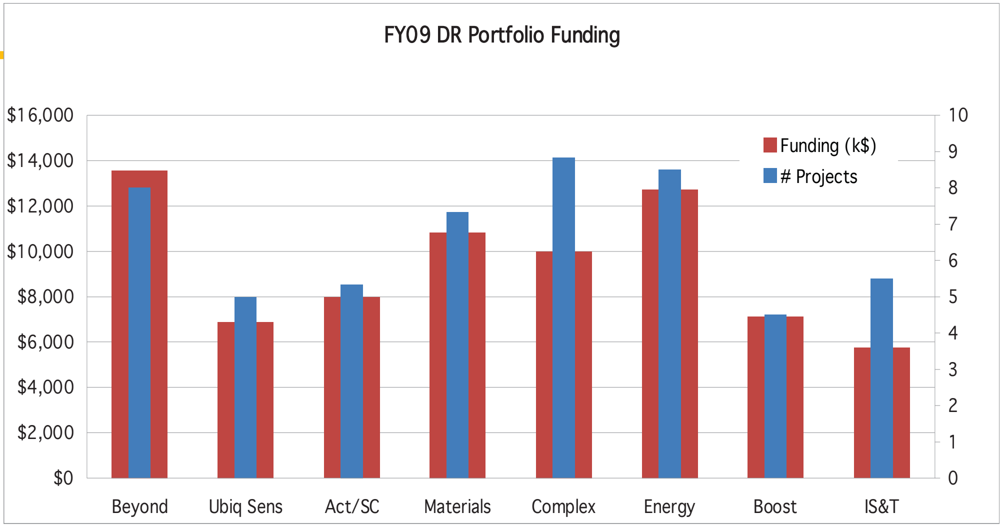
Forensics & Sensing (TBD)

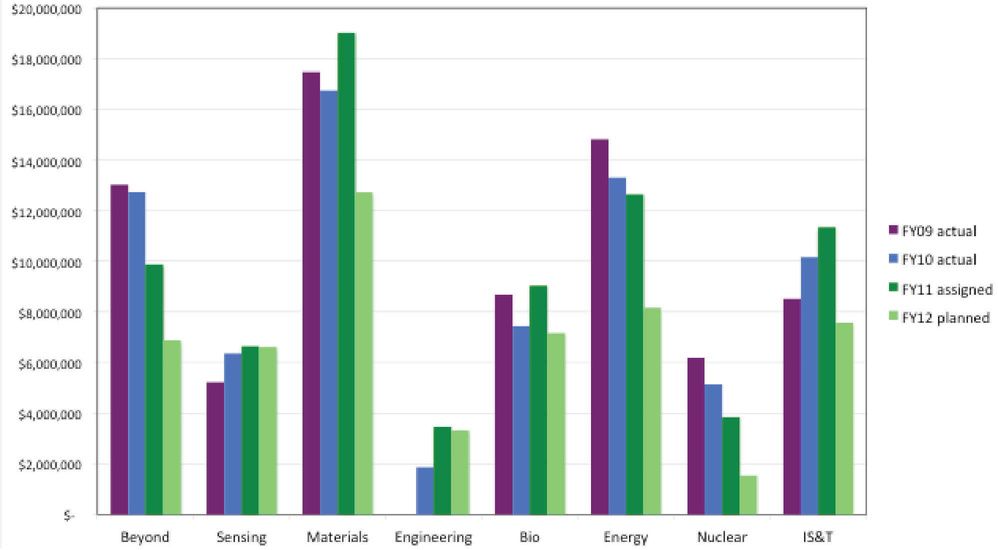
Fundamental Understanding of Materials

Information Science & Tech.

Engineering (TBD)

Red border = Workshop planned

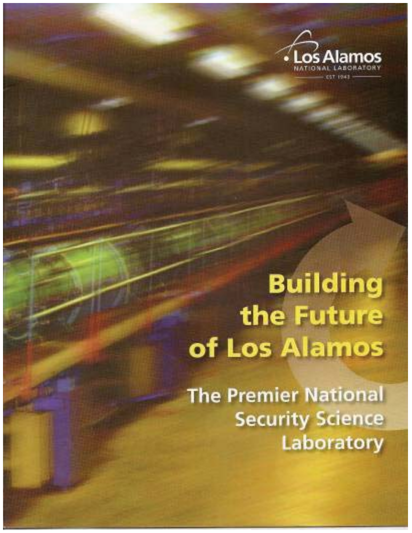

FY09 DR Portfolio Funding



Presentation outline

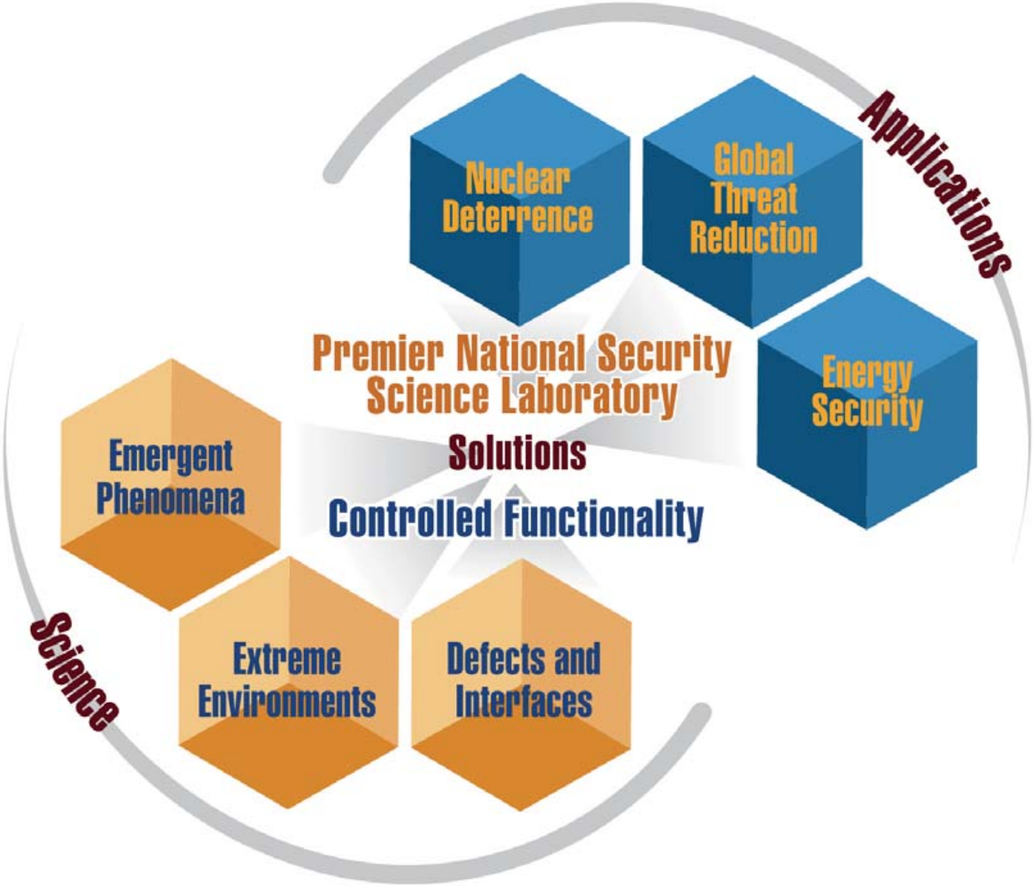
- LANL update/Trends in metrics
- **Progress in Implementation Plan for Materials Strategy**
- Technical highlights
- Response to 2011 recommendations
- 2012 Topics

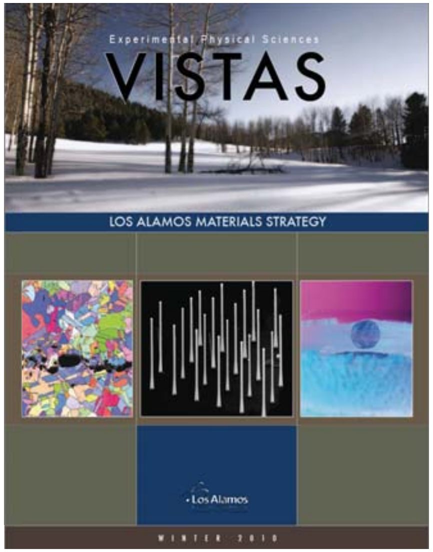
The Materials Strategy advances our vision to develop materials with ‘controlled functionality’ to provide solutions enabling LANL’s missions


Los Alamos NATIONAL LABORATORY EST 1943

Building the Future of Los Alamos

The Premier National Security Science Laboratory




Experimental Physical Sciences

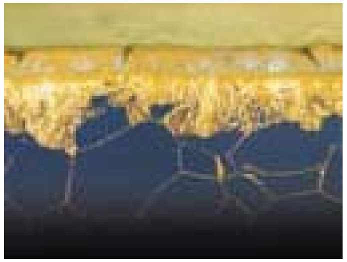
VISTAS

LOS ALAMOS MATERIALS STRATEGY

Los Alamos

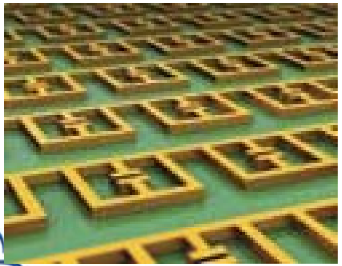
WINTER 2010

LANL Materials will be differentiated through forefront science that cross-cuts three themes



Defects and Interfaces – the mechanistic understanding and control of inhomogeneities, across all appropriate length and time scales, that govern materials functionality

Extreme Environments – the underlying principles enabling the understanding of the interactions of materials with extreme conditions in order to create 1) environmentally tolerant properties and 2) the ability to exploit extreme environments to tune materials functionality



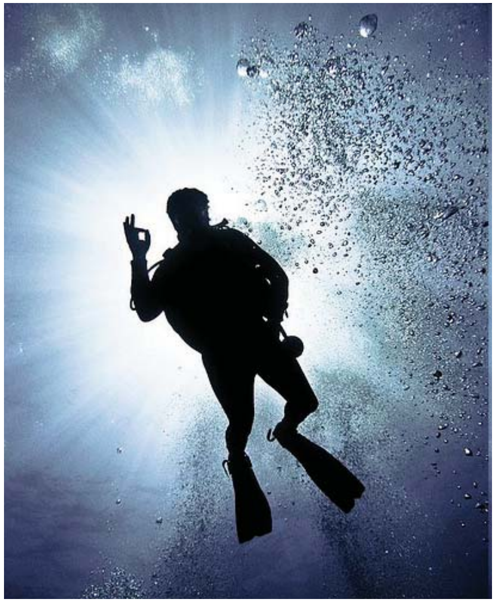
Emergent Phenomena – the science required to discover and understand complex and collective forms of matter that exhibit novel properties and respond in new ways to environmental conditions, enabling the creation of materials with innate functionality

Developing an Implementation Plan: What actions are essential to our vision for Materials S&T?

- **What capabilities are central to our areas of leadership, and how must these evolve over the next decade?**
- **Who are our competitors, and/or our collaborators?**
- **How can we leverage current programmatic efforts and develop new programs that enable our vision to succeed?**
- **What infrastructure is critical to our success, and how must this evolve?**

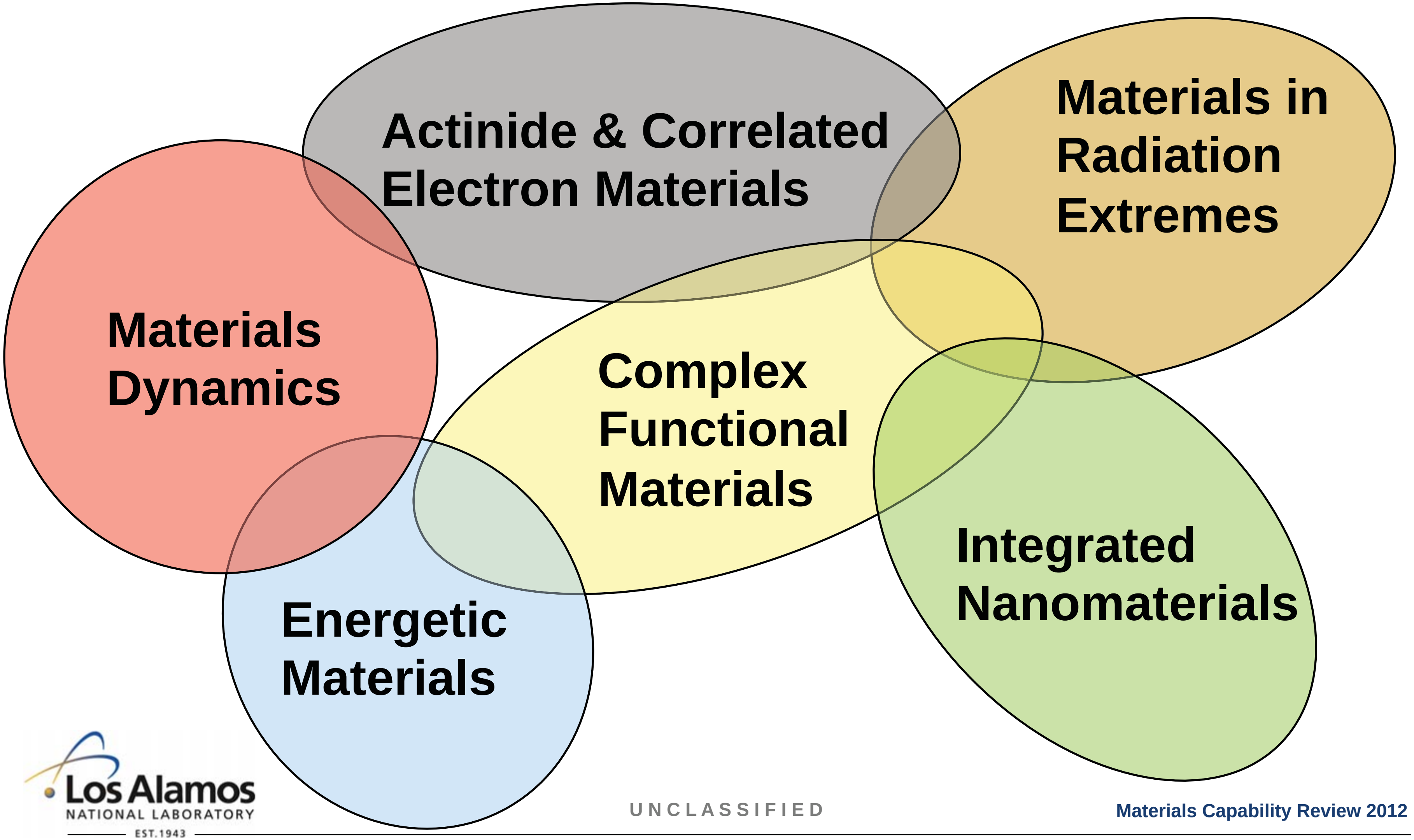
Deep Dives:

Engage LANL Materials community in developing vision in areas of leadership



Engaged >100 scientists across four Laboratory Directorates

Six ‘Areas of Leadership’ span the Materials Pillar



Actinide & Correlated Electron Materials

Materials in Radiation Extremes

Materials Dynamics

Complex Functional Materials

Integrated Nanomaterials

Energetic Materials

FY11 implementation planning was guided by the output from the Deep Dives

- Further refine planning in the Areas of Leadership, identifying Division Leader champions for each area.
- Champion investments in cross-cutting capabilities in ‘making, measuring and modeling.’
- Identify and pursue high impact program development activities
  - Enable underpinning Pu R&D in pursuit of the Nevada scaling initiative
  - Champion and seize OSTP “Functionality by Design” Opportunity
    - Critical Materials Innovation Hub (EERE)
- Pursue institutional strategies underpinning the Materials Strategy
  - Continue the strong connection with the LDRD Investment Strategy
  - Establish the ‘Institute for Controlled Functionality’
- Propose facility/safety basis improvements
  - Implement He recovery for condensed matter physics experiments.
  - Identify an essential activity where risk aversion limits progress (e.g. the inability to perform Pu experiments at pRad) and find a solution.

FY11 implementation planning was guided by the output from the Deep Dives

- Further refine planning in the Areas of Leadership, identifying Division Leader champions for each area.
- Champion investments in cross-cutting capabilities in 'making, measuring and modeling.'
- Identify and pursue high impact program development activities
  - Enable underpinning Pu R&D in pursuit of the Nevada scaling initiative
  - Champion and seize OSTP "Functionality by Design" Opportunity
    - Critical Materials Innovation Hub (EERE)
- Pursue institutional strategies underpinning the Materials Strategy
  - Continue the strong connection with the LDRD Investment Strategy
  - Establish the 'Institute for Controlled Functionality'
- Propose facility/safety basis improvements
  - Implement He recovery for condensed matter physics experiments.
  - Identify an essential activity where risk aversion limits progress (e.g. the inability to perform Pu experiments at pRad) and find a solution.

Champion investments in crosscutting materials capabilities

Leverage MaRIE-relevant investments called out in the Deep Dives

- **Making**
- New facilities for materials chemistry, located in MSC complex
- Processing capability for Pu-242 for small scale experiments
- Plan for a flexible fabrication capability

- **Measuring**
- Advance frontier microscopy capabilities
- Enhance ultrafast x-ray science at LANL and external user facilities
- Develop in-situ synthesis and processing diagnostics

- **Modeling**
- Pilot projects in co-design intimately connected to experiments
  - Structural materials—underway in FY11
  - Functional materials—at a more preliminary stage

Area of Leadership implementation planning for the Materials Strategy

- Definition and strategic vision for each area
  - Key science questions
  - Key thrusts
- Road map
  - Describe actions required on a two-year horizon to realize the vision
  - Additional actions beyond the two year horizon
  - Span the following strategic elements
    - Refinement of capability definition
    - Program Growth
    - Capital and Facility Investments
    - Strategic Staffing
    - Partnerships
- Engage the materials community in developing the implementation plan, communicating it to the materials community and in taking actions aligned with and supporting the plan.

Division level champions led the planning for the ‘Areas of Leadership’

- **Integrated Nanomaterials**
  - Toni Taylor, DL-MPA
  - Jeanne Robinson, DDL-LDRD
- **Complex Functional Materials**
  - David Watkins, DDL-MPA
  - Tony Redondo, DL-T
- **Materials in Radiation Extremes**
  - Jack Shlachter, DDL-T
  - Dave Teter, DL-MST
- **Actinides and Correlated Electron Materials**
  - John Sarrao, DL-SPO-SC
  - Alex Lacerda, DDL-LANSCE
- **Materials Dynamics**
  - Mike Stevens, DDL-WX
  - Cris Barnes, DDL-P
- **Energetic Materials**
  - Dave Funk, DL-WX
  - Carol Burns, DL-C

Actinides and Correlated Electron Materials

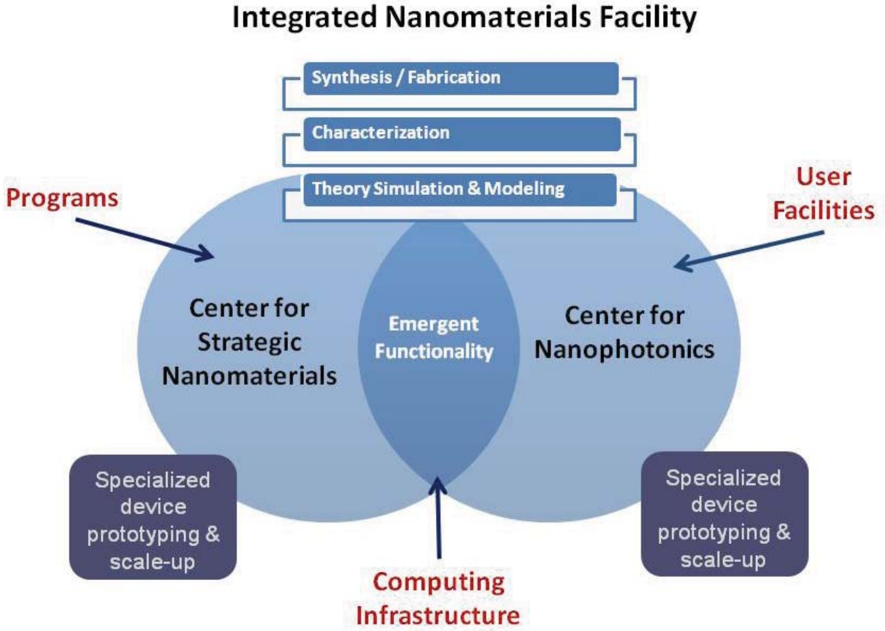
Thrusts

- “Understanding and controlling emergent electronic states”
- “Actinide materials science center of excellence”
- “Predicting and Controlling Plutonium aging and lifetime”

Cross Cutting Grand Challenges

- The grand challenge of achieving controlled functionality is particularly acute in actinide and correlated electron systems due to the unique role of strong electron correlations, acute reactivity, and self-irradiation phenomena in these materials.
- The ability to integrate/bridge results from various techniques on various temporal and spatial scales in diverse environments is a key differentiator and stretch goal (unified theory of actinides).

Integrated Nanomaterials



Integrated Nanomaterials Facility

Synthesis / Fabrication

Characterization

Theory Simulation & Modeling

Programs

User Facilities

Center for Strategic Nanomaterials

Emergent Functionality

Center for Nanophotonics

Specialized device prototyping & scale-up

Specialized device prototyping & scale-up

Computing Infrastructure

‘**Center for Strategic Nanomaterials**’ which will focus on the development of the capability to design and synthesize integrated nanostructures with specified functionality and will include the development of a full range of nanocharacterization techniques, novel synthesis and fabrication capabilities, and theory, modeling and simulation tools to address complexity and interface issues.

‘**Center for Nanophotonics**’ which will focus on establishing the capability to design and synthesize nanostructured materials with functionality optimized for the manipulation of photons on different time and length scales for applications such as radiation detection, low-cost, high efficiency PV and solid-state lighting and photosynthesis, optoelectronics.

Materials under Radiation Extremes

1. **Advanced Nuclear Fuels Nuclear Waste Materials**
2. **Advanced Radiation Temperature Tolerant Structural Materials.**
   - Fundamental understanding and co-design of radiation-tolerant structural and functional materials, non-oxide fuels and novel fuel designs
   - Rapid Certification of Materials for use in reactor applications
   - Designing functionality into materials for radiation environments
   - Developing irradiation environments (Neutrons, ions, gamma, electrons) and in situ measurements within these environments.
   - Modeling and theory capability to examine long-term effects of radiation damage in complex (engineering) materials
   - Understanding and prediction of fission gas release
   - Development of actinide and highly radioactive material handling and characterization and “one-off” production routes

Complex Functional Materials

Key Thrust Areas:

- The synthesis, fabrication and simulation of materials and material systems for energy conversion, storage, and transmission, where optimal performance depends on developing materials to satisfy multiple criteria essential to the overall application.
  - How do we translate molecular and nanoscale properties to macroscale energy functionality?
- Utilization of biological principles and emergent phenomena as inspiration for the creation of materials with enhanced functionality, including the ability to controllably adapt material responses to external conditions.
  - How do we design, synthesize, model and simulate materials that adapt and control functionality across multiple length and time scales?

Energetic Materials

- **Prediction and Control of Explosives Safety, Initiation, and Performance**
  - First principles understanding of performance (safety and intended use) as a function of molecular tailoring and formulation; prediction and control of engineering performance
  - Focused exploration of interplay between thermal, high pressure, shear, shock and light-driven chemical reaction, leading to control
  - Design and synthesis of new explosive molecules enabling formulations tailored to application
- **Invent and Utilize Revolutionary Diagnostics**
  - Develop a suite of diagnostic that transcend orders of magnitude in both length scale and spatial resolution to provide exquisite data for direct comparison with high fidelity simulations
  - Ability to probe both chemical and material properties while accessing a range of temperature, pressure, and density conditions
  - Lifecycle probes that provide relevant physical and chemical data without compromising the performance of the article within which they reside

Materials Dynamics

Key Thrust Areas:

- Linking material microstructure to macroscopic behavior under dynamic deformation conditions – i.e. the Multi-scale Problem;
- Enabling the transition from observation and validation to prediction and control of dynamic processes, and;
- Developing the next generation of diagnostics, dynamic drivers, and predictive models to enable the necessary, transformative research

Near-term goals of the Materials Strategy: Investments in Making, Measuring, and Modeling

- Making
  - Synthesis of Pu samples for small scale experiments (incl. Pu 242)
  - Flexible Fabrication Facility (Space, Personnel, Capital & Operating Model)
- Measuring
  - Enhance nano-micro scale characterization capabilities including, electron microscopy, 3D characterization and nanoscale electronic spectroscopies
  - Develop ultrafast x-ray science at LANL and external user facilities, including the capability to study actinides
  - Demonstrate high-accuracy thermal conductivity measurements
- Modeling
  - Enable midscale, distributed cluster computing for materials modeling
  - Pursue co-design, combining modeling + theory + algorithms + hardware + experiment, particularly with large scale data management via targeted pilot projects

Near-term goals of the Materials Strategy: Partnerships and Strategic Staffing

- Partnerships
  - Promote strategic industrial partnering, in collaboration with TT, with the goal of identifying partners willing to provide matching funds
  - Translate more Lujan/NHMFL/CINT users to institutional collaborators, with the goal of pursuing joint proposals
  - Facilitate (i.e. through DOE NNSA Stockpile Stewardship Academic Alliance) academic research in materials dynamics that increasingly cannot be done at universities
- Staffing
  - Exploit specific opportunities (post VSP) to hire mid-career employees for key leadership positions (e.g. CINT SBCN thrust leader)
  - Encourage quality and diversity in Post Doc hiring and conversion by ensuring competition in post doc hiring
  - Enhance the development of early career scientists into scientific leaders through creative mentoring and career development strategies

Near-term goals of the Materials Strategy: Institutional Strategies and Program Development

- Institutional strategies
  - Evolve the two Materials Institutes into ‘Institute for Controlled Functionality’ supporting the Materials Strategy
  - Develop an experimental facility support business model
  - Institute a searchable, Labwide database for expertise and capability
  - Continue the strong connection with the LDRD Investment Strategy
    - Achieve a stable suite of ~12 materials-centric LDRD-DRs
- Program Development
  - Seize the nascent opportunities for materials R&D in DOE:
    - Critical Materials Hub, Manufacturing Initiative (EERE)
    - Mesoscale Initiative (BES)
    - Advanced Fuels; Used Fuel Disposition; Small Modular Reactors (NE)
  - Pursue underpinning materials R&D associated with new weapons initiatives
  - Promote strategies leading to MaRIE 1.0 in response to the NNSA Signature Facility call

Next steps for the Materials Strategy Implementation Plan

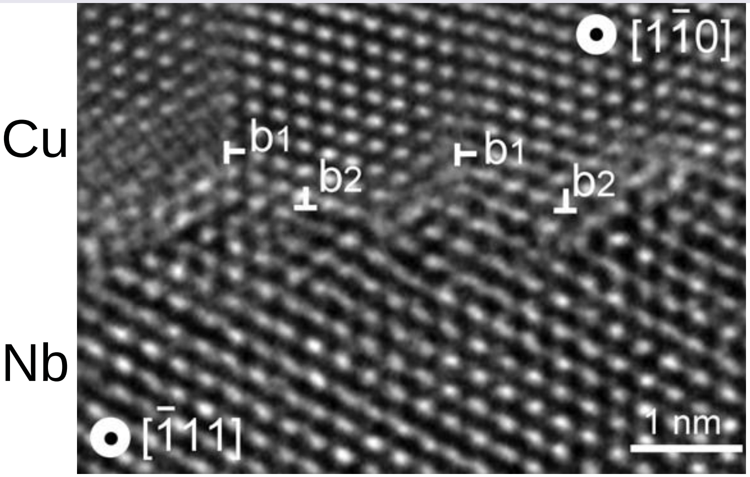
- ✓ Further develop the plan for ‘investment’ in people
  - Address retention and recruitment issues
  - Hold planning session focused on mentoring, career development, succession planning, awards, etc.
- ✓ Continue to present and discuss plan with stakeholders
  - Town halls for materials community
  - Materials Guiding Coalition, Division and Directorate Councils with an emphasis on their role in implementation
  - Targeted discussions with Fellows, Early Career Scientists, Postdocs
  - Discussion with programs: program development opportunities
- ✓ Incorporate feedback from stakeholders and MCR committee
- ✓ Complete implementation document

Presentation outline

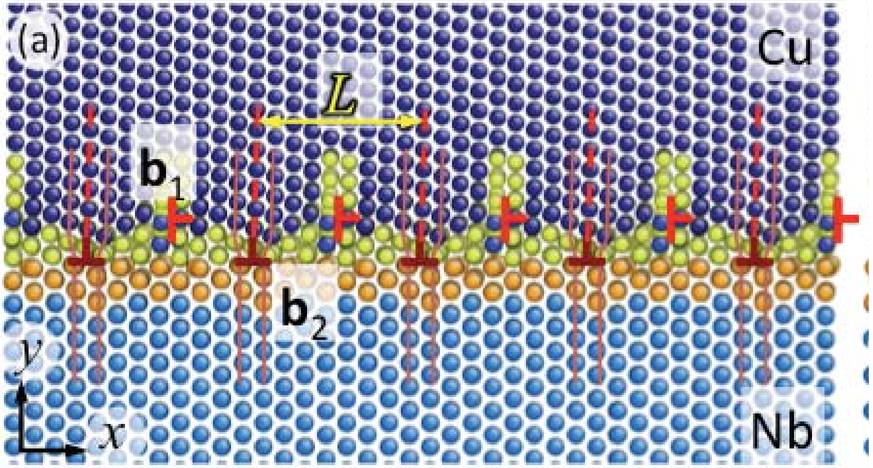
- LANL update/Trends in metrics
- Progress in Implementation Plan for Materials Strategy
- **Technical highlights**
  - **Focusing on S&T not presented in other parts of the review**
- Response to 2011 recommendations
- 2012 Topics

Interface stability in nanocomposites after severe plastic deformation

Discovery of stable, ordered interface after severe straining



Excellent agreement with atomic interface model

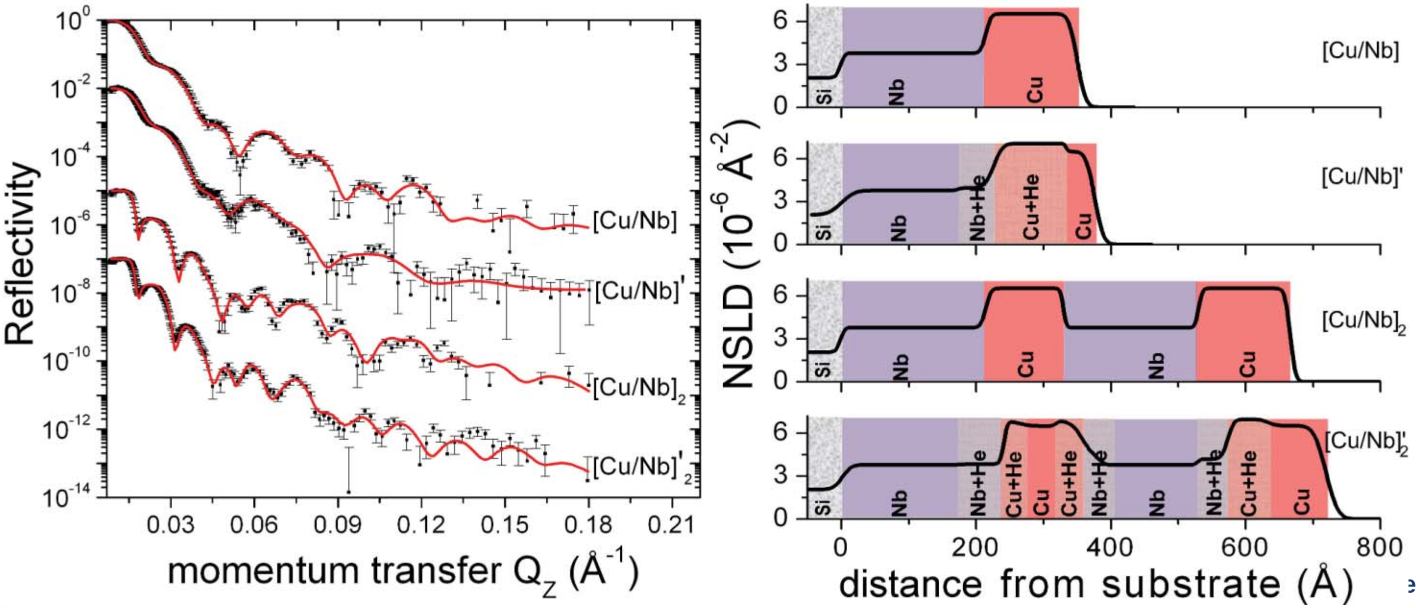


- CMIME researchers showed that certain interfaces (in PVD films) can attract, absorb and annihilate radiation-induced point defects.
- Recent work on accumulative roll bonded Cu-Nb bulk laminate composites shows crystallographic, chemical and morphological stability of interfaces after severe plastic deformation.
- Agreement between the same stable interface found in a heavily deformed material and the atomic model of the un-deformed boundary suggests that the interface is stable because it heals defects introduced during mechanical deformation, analogous to the way it heals radiation-induced defects.

Scripta Mat. **65**, 1022 (2011).; *Appl. Phys. Lett.* **100**, 011911 (2012).; *Acta Materialia*, **60,** 1747 (2012)

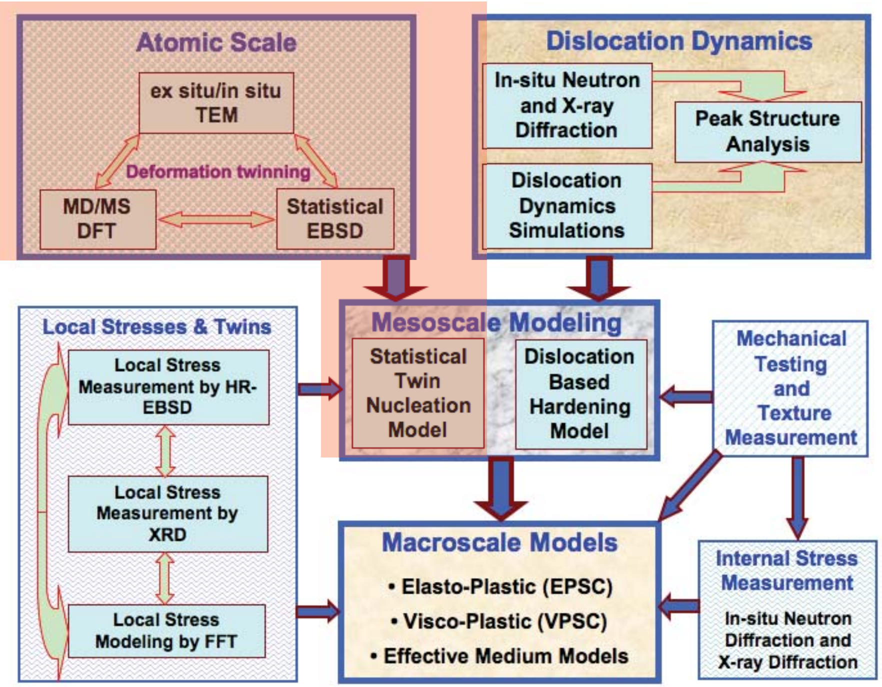
Neutron reflectometry (NR) reveals the performance of radiation-resistant materials

- NR is used to quantitatively determine the changes in the transverse chemical profile of Cu/Nb layered nanocomposites due to He ion migration, absorption, and storage after ion implantation.
- NR enables the high precision measurement of layer parameters such as thickness, density, chemical composition, and interface and surface roughness regardless of the crystallinity of the sample (single crystal, polycrystalline, or amorphous).



APL 98, 241913 (2011), AIP/APS frontier research.

Multiscale Perspective of Understanding Twinning in HCP Metals



Atomic Scale

ex situ/in situ TEM

Deformation twinning

MD/MS DFT

Statistical EBSD

Dislocation Dynamics

In-situ Neutron and X-ray Diffraction

Peak Structure Analysis

Dislocation Dynamics Simulations

Local Stresses & Twins

Local Stress Measurement by HR-EBSD

Local Stress Measurement by XRD

Local Stress Modeling by FFT

Mesoscale Modeling

Statistical Twin Nucleation Model

Dislocation Based Hardening Model

Mechanical Testing and Texture Measurement

Macroscale Models

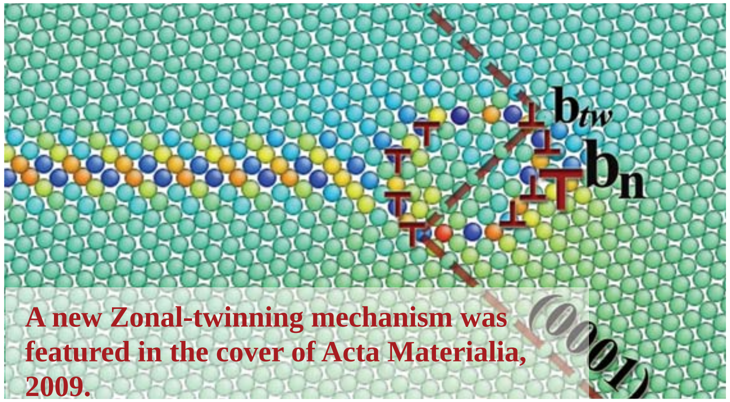
- Elasto-Plastic (EPSC)
- Visco-Plastic (VPSC)
- Effective Medium Models

Internal Stress Measurement

In-situ Neutron Diffraction and X-ray Diffraction

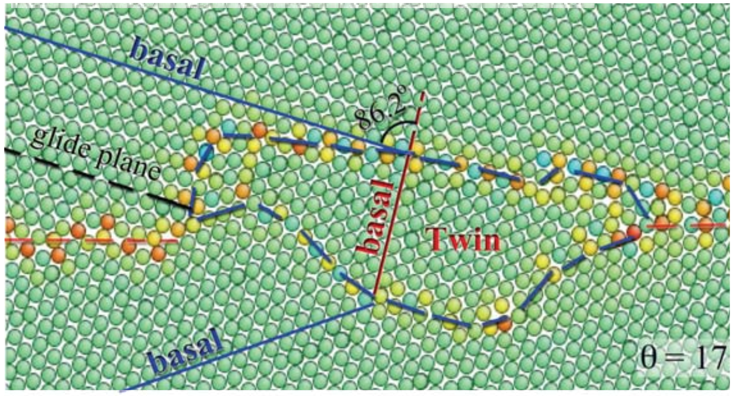
Developing a comprehensive approach for understanding deformation twinning in hcp metals since it is the primary plastic deformation mechanisms, involving molecular dynamics (MD) and TEM at atomic scale, electron backscatter diffraction (EBSD) at micro-scale, and nucleation theory in meso-/macro-scale.

Discoveries of twinning at atomic scale



A new Zonal-twinning mechanism was featured in the cover of Acta Materialia, 2009.

Ref. J. Wang et al. Acta Mater, 57 (2009) 5521



Deformation twinning is preferred at GBs with low misorientation angles, consistent with experiments.

Ref. J. Wang et al. Scripta Mater, 63 (2010) 741

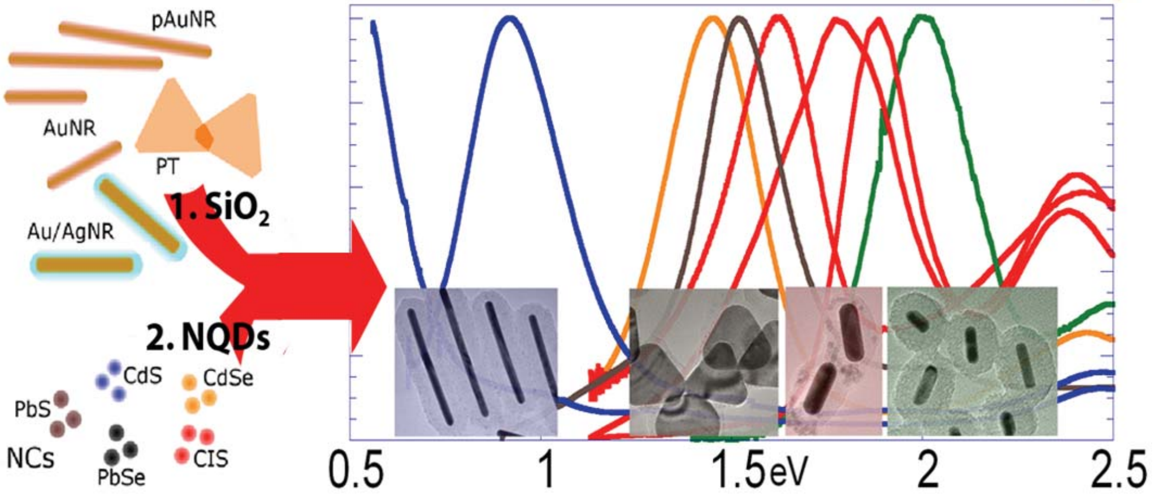
Top 25 Hottest articles: Twinning Mechanisms at atomic-scale

Center for Advanced Solar Photophysics

- **Novel materials**

Spectrally and structure-tunable semiconductor-metal nanohybrids

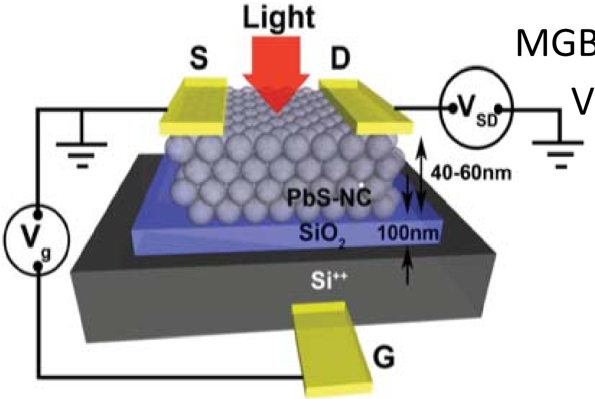
B. Khanal et al. *ACS Nano Lett.* **ASAP** (2012)

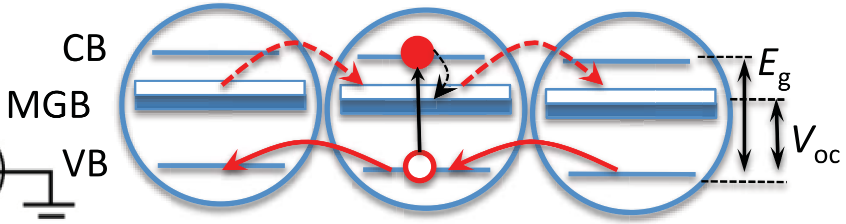


- **Exploratory devices**

NQD-based optical-FETs

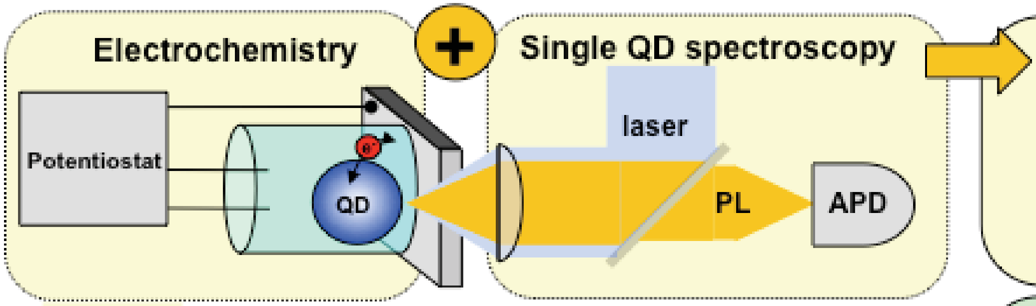
P. Nagpal & V. I. Klimov
Nature Comm. (2011)





Mixed character of photoconduction in PbS NQDs:
Electron transport via MGB states
Hole transport via band-edge states

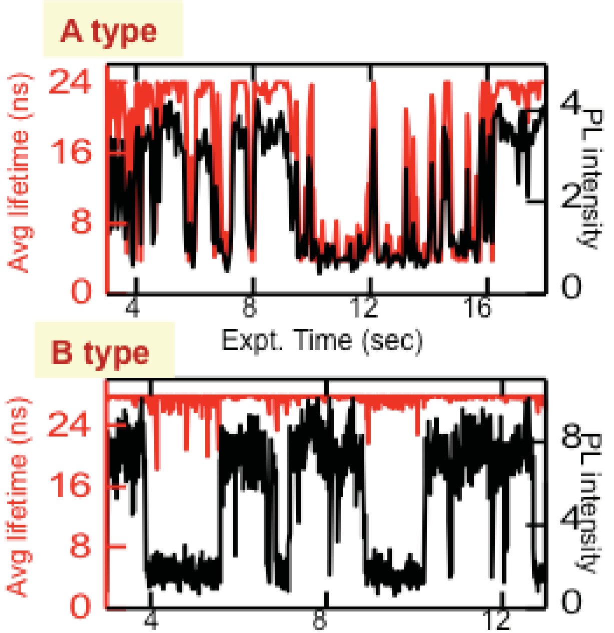
Unraveling the Mystery of Quantum Dot Blinking using Single Dot Spectroelectrochemistry

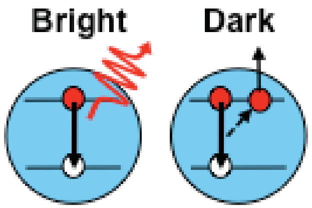


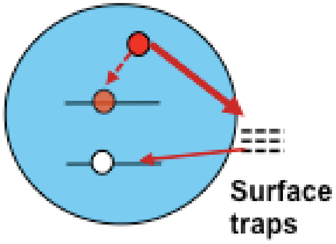
Single QD Spectroelectrochemistry

⇩

Charge injection + *simultaneous* monitoring of optical response







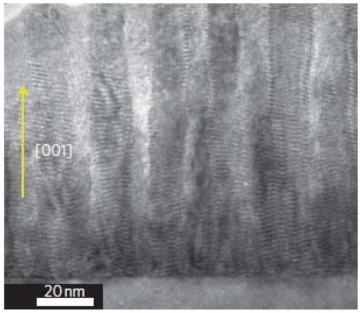
Two types of PL Blinking

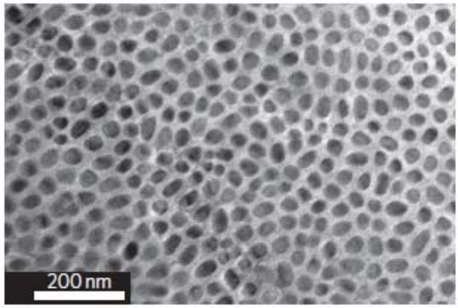
- **A type:** PL intensity and lifetime fluctuate together
- **Auger quenching** of charged exciton is responsible for the "dark" state
- **B type:** Both "bright" and "dark" states have similar PL lifetimes.
- **Trapping of hot electrons** at surface states is responsible for the "dark" state.
- Both blinking types **controlled** by electrochemical potential.
- This novel technique can be applied to a **wide variety of nanomaterials**.

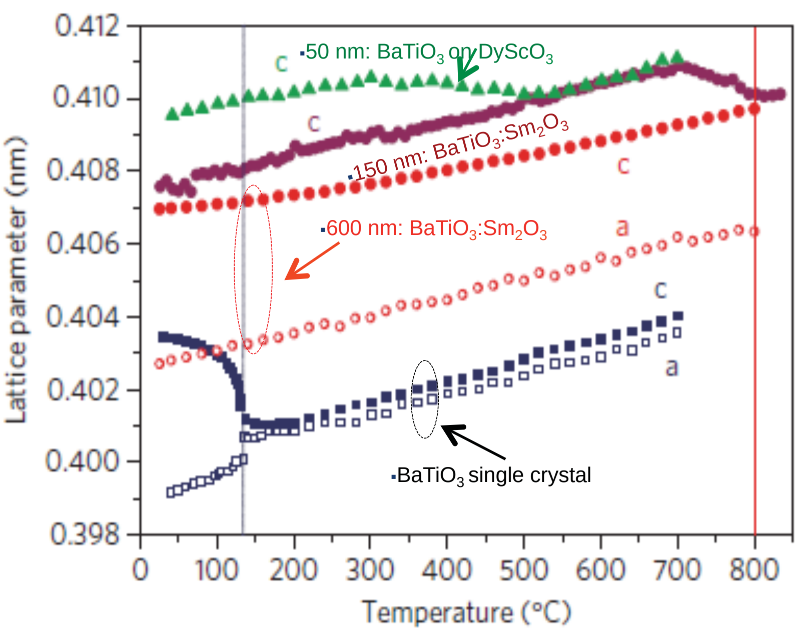
C. Galland, et. al. *Nature* **479**, 203-207, 2011.

Beyond PZT: Thick lead-free ferroelectric films with high Curie temperatures through nanocomposite-induced strain

- Lead-free replacements desired for ferroelectric material, $PbZr_xT_{1-x}O_3$ (PZT).
- The preferred alternative, BTO, contains no lead, and has excellent ferroelectric properties, but its Curie temperature of <130 C is too low to be practical.
- Strain has been used to enhance the Curie temperature of BTO and $SrTiO_3$ films, but only for thicknesses of tens of nms
- Demonstrated self-assembled nanoscale composites of BST and Sm_2O_3 (SmO) up to 1.25 μm thick that exhibit tetragonality up to at least 800°C and strong remnant polarization to at least 330°C (potential for ferroelectricity up to 800°C).
- The nanocomposite improved BTO crystalline quality and reduced the leakage current.







Nature Nanotechnology, 6, 491 (2011).

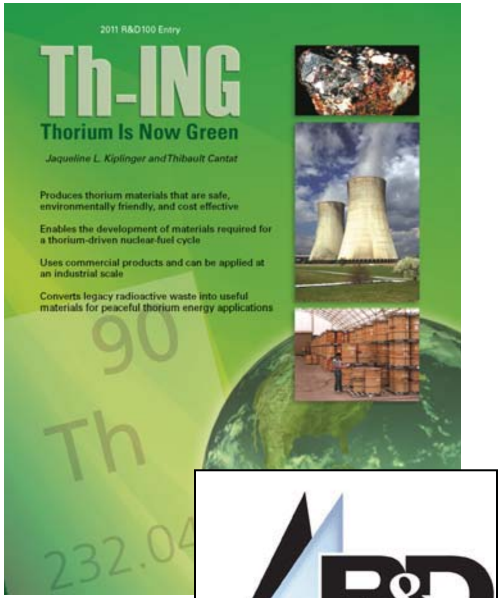
Simplifying Complex Actinide Processes with Th-ING (Thorium is Now Green)

$$Th(NO_3)_4(H_2O)_5 + HCl\ (12\ M) \xrightarrow[-\ NO_x]{H_2O,\ 100°C,\ 6h} ThCl_4(H_2O)_4$$

100% yield

3200 MT Thorium Nitrate Buried at NTS

- **Chemistry is High-Yielding and Safe.**
- **$Th(NO_3)_4(H_2O)_5$ is Commercially Available and Cheap.**
- **Easy to Prepare on a Large Scale.**
- **Safe, Mild Routes to Multigram Quantities of Thorium Chloride Compounds for Chemistry, Materials Science, and Advance Nuclear Fuels Research.**



2011 R&D100 Entry

Th-ING

Thorium Is Now Green

Jaqueline L. Kiplinger and Thibault Cantat

Produces thorium materials that are safe, environmentally friendly, and cost effective

Enables the development of materials required for a thorium-driven nuclear-fuel cycle

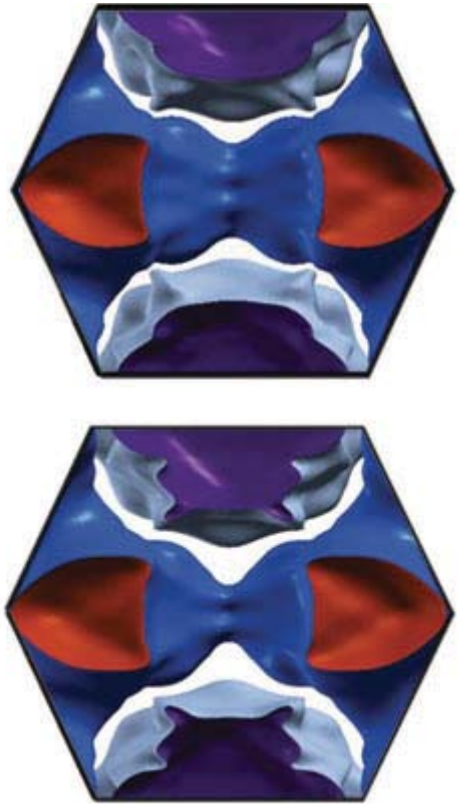
Uses commercial products and can be applied at an industrial scale

Converts legacy radioactive waste into useful materials for peaceful thorium energy applications

- Cantat, T.; Scott, B. L.; Kiplinger, J. L. *Chem. Commun.* **2010**, *46*, 919-921.
- U.S. Patent App. 12/778,891. *Method of Synthesis of Anhydrous Thorium(IV) Complexes*.

Pressure Dependence of Electron-Phonon Coupling in a-uranium

- At ambient pressure, uranium is the only element to exhibit a phase transition to a charge density wave (CDW) state, three modifications below 50 K.
- There is a soft phonon mode at 300 K- a precursor to the CDW.
- Using the European Synchrotron Radiation Facility (ESRF) in France, we measured the dependence of this soft phonon mode under pressure in a diamond anvil cell.
- The new sample preparation at LANL made the measurements possible and measurements were made on three visits. Measurements were made in transmission so crystals of dense uranium had to be in a thin geometry, 15 microns and retain a low mosaic.

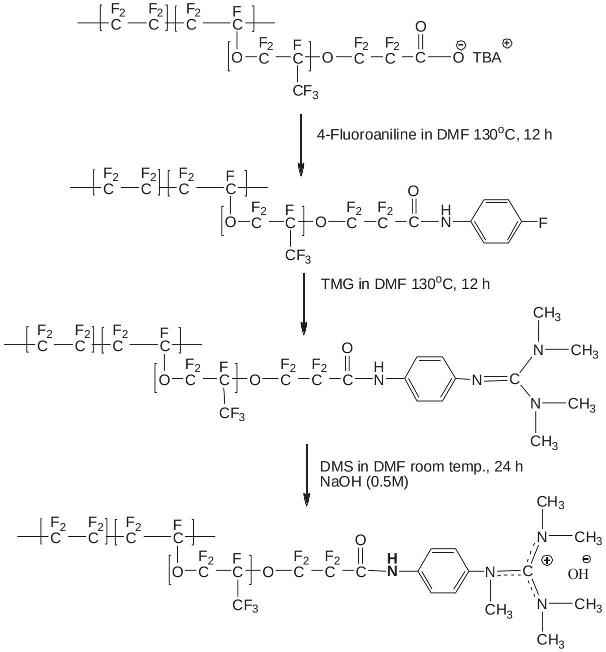


Cross section of the Fermi-surface topology for the α-U structure calculated at ambient pressure (top) and 20 GPa (bottom).

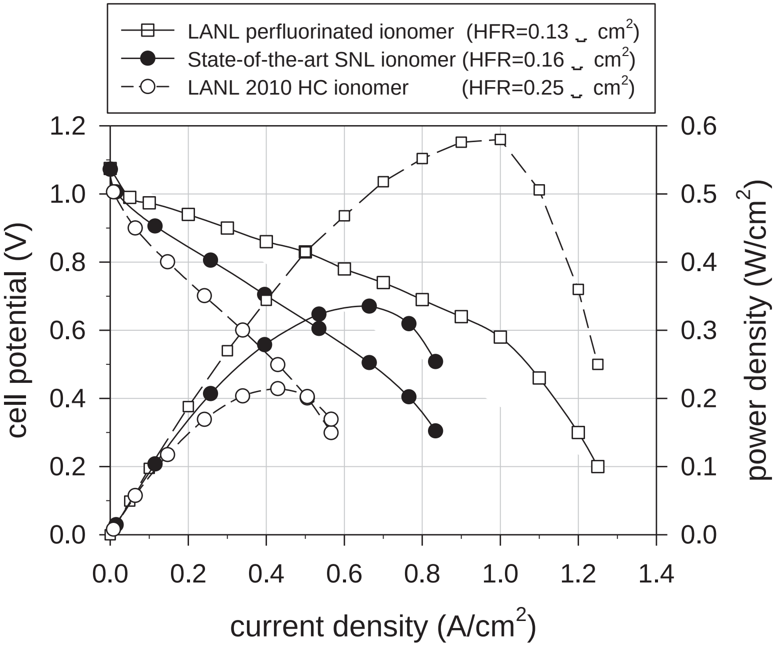
Phys. Rev. Lett. **107**, 136401 (2011)

Novel Polymer Electrolyte for Alkaline Membrane Fuel Cells

Synthesis of perfluorinated ionomer



Alkaline membrane fuel cell (AMFC) performance

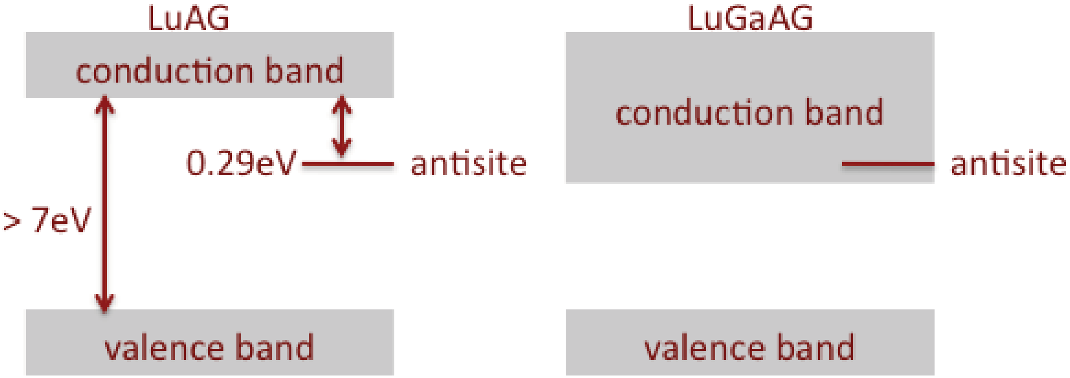


- Stable perfluorinated ionomer for alkaline membrane fuel cells prepared by activated fluorine-amine reaction
- H_2-O_2 alkaline fuel cell with that ionomer generating a power density of 0.58 W/cm² – 75% improvement over the state of the art in the AMFC technology

D.S. Kim *et al. Chem Mater.* **23**, 3759, (2011)

Band Gap and Defect Engineering of High Performance Scintillators for Radiation Detection

- **A new high performance scintillator material was recently discovered with 65,000 photons/MeV (almost 8x BGO) with ~4.9% energy resolution.**
- **Multicomponent garnet was developed with important "band gap engineering" insight from first principles modeling.**



LuAG

conduction band

0.29eV

antisite

> 7eV

valence band

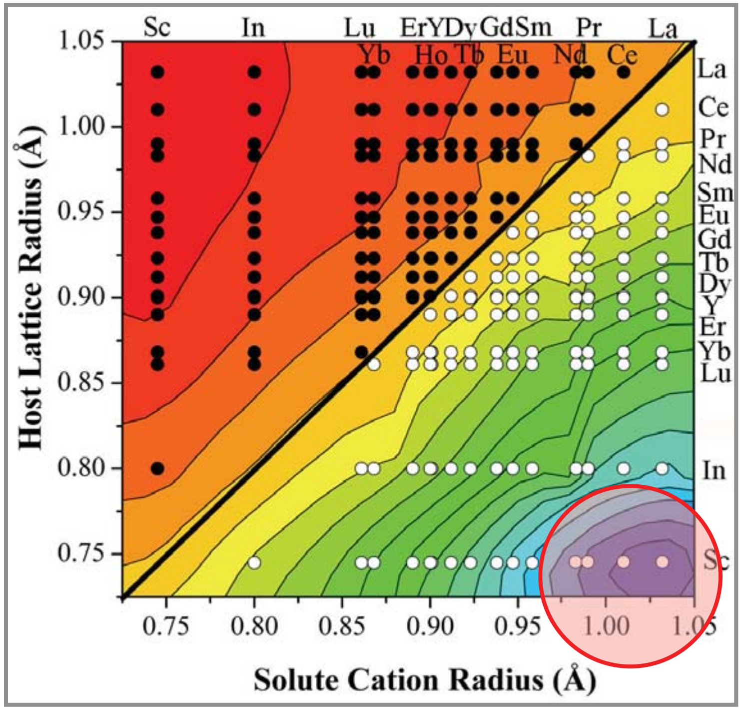
LuGaAG

conduction band

antisite

valence band

Fasoli, et al. *Phys. Rev. B* **84** (2011) 081102(R).



- **Goal is to use similar theoretical techniques to screen wide compositional space for further optimization.**

Presentation outline

- LANL update/Trends in metrics
- Progress in Implementation Plan for Materials Strategy
- Technical highlights
- **Response to 2011 recommendations**
- 2012 Topics

Major concerns/recommendations from 2011 were:

- Bureaucratic burden
- Mid-career hiring and retention
- Facilities renovation
- Importance of LANSCE and MaRIE to the future of the Laboratory
- Integration of modeling and experiment

Laboratory Management recognizes the impact of bureaucracy on the performance of experimental work at the Lab and have taken steps to improve it

- A policy review committee that includes technical representatives has been formed to examine the impact of policies before they are implemented.
- The Deputy Associates Directors (DADs) have successfully implemented the Moderate Hazard Research and Development Integrated Work Management Plan (IWM) that was crucial to continue with laboratory and field experiments from the perspective of Lab's sponsor, NNSA.
- The DADs have also formulated the implementation of the quality program across the Laboratory, again a graded response balancing sponsor (NNSA) requirements with those of the technical organizations.
- Senior management-led effort underway to address NAS report on NNSA management of Labs, specifically focusing on bureaucracy.

Mid-career hiring and retention remains a goal for the Materials Capability, but a viable, comprehensive strategy remains elusive

- **Retention strategy**
  - Understand, as early as possible, reasons for leaving
    - Often, the motivation is a desire to lead but the individual finds the requirements of a Lab management position unacceptable
  - Use of Lab resources for retention packages, in combination with competitive compensation
  - Propose a sabbatical leave program that is funded institutionally through a competitive process
  - Explore partial retention as Lab Associate or formal collaborator
  - Develop a more effective mentoring strategy, perhaps involving retirees

- **Hiring strategy**
  - Successful external mid-career hiring are occurring through user facilities (CINT, Lujan, NHMFL)
  - Provide institutional investments including and G&A for hiring packages, in combination with competitive compensation

UNCLASSIFIED

We have begun to address facility issues, including lack of available space and the renovation of existing space

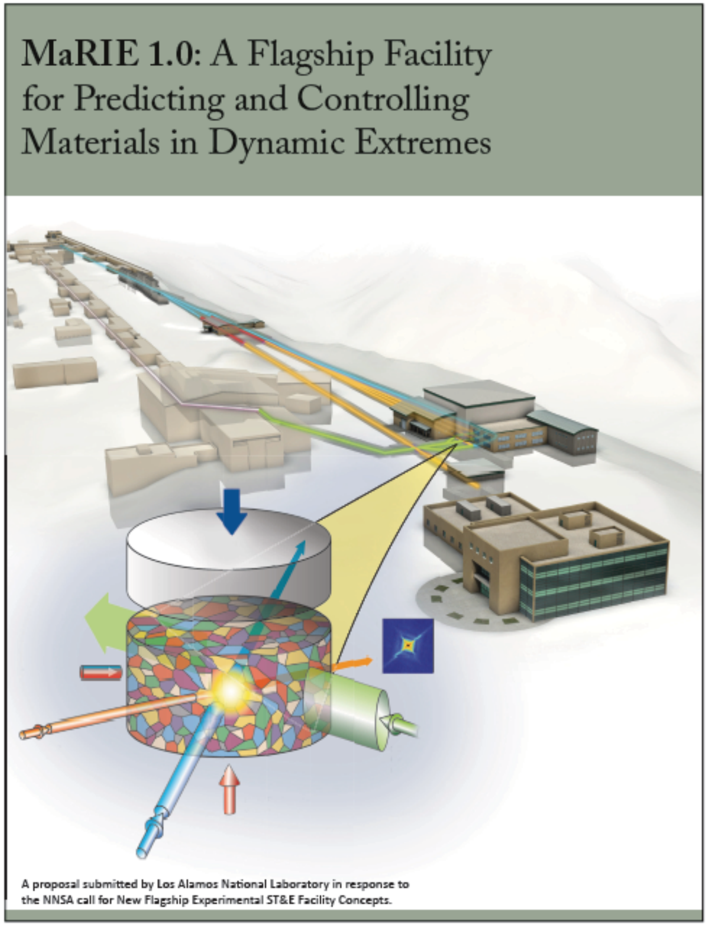
- The Lab is using a modest amount of overhead to refurbish or repair facilities. Planned renovations underway for the Materials Capability:
  - Renovation of the Materials Science Laboratory (MSL) infill to consolidate the Materials Chemistry Group in the Materials Science complex.
  - Renovation of Research Park space for materials for separations R&D.
  - Renovation of space at SM-40 for materials for clean energy R&D.
  - Renovation of uncleared space next to Target Fab for U, NE-driven R&D.
- A long-range planning effort led by the Associate Director for Maintenance and Infrastructure Planning is underway. Our input to this process is guided by the Materials Strategy.
- Alternatives for Pu R&D, resulting from the postponement of the construction of CMRR, are being investigated through an NNSA-commissioned 60-day study, with leadership from the materials community.

The future health of the LANSCE facility has been strongly embraced by the senior Lab management

A three component plan has been implemented that establishes:

1. sustainable operations funding through weapons funding in Readiness in Technical Base and Facilities (RTBF),
2. sustainable facility funding through Institutional Support and RTBF,
3. future operational risks to ensure high-reliability operations through the Linac Risk Mitigation effort.

MaRIE 1.0, LANL's priority response to the NNSA Facilities call, will enable us to observe and ultimately control how mesoscale materials properties affect weapons performance



MaRIE 1.0: A Flagship Facility for Predicting and Controlling Materials in Dynamic Extremes

A proposal submitted by Los Alamos National Laboratory in response to the NNSA call for New Flagship Experimental ST&E Facility Concepts.

- **A mission need exists** for a facility focused on predicting and controlling materials in extreme environments, exploiting *in situ* transient measurements on real materials in relevant dynamic extremes to address key nuclear weapons challenges.

- Achieving controlled functionality at the mesoscale through co-design is the **frontier of materials research**.

- MaRIE 1.0 meets this need with a robust preconceptual reference design that is grounded in **community-defined mission and scientific requirements**.

- **LANL can realize MaRIE 1.0** by FY20 for a total project cost of ~ $1300M ($950M - $1800M).

MaRIE 1.0 is urgently needed to steward the stockpile and contribute to broader national security challenges early in the next decade

We believe full integration of modeling and experimentation are essential to the success of the Materials Pillar

- LANL has a strong history of integrated modeling and experiments which has been formalized in the area of CoDesign.

- 2012 MCR theme on CoDesign will illustrate this connection, as will the other 2012 MCR themes and the LDRD review.

- The Applied Energy Programs, reviewed in 2011, emphasize applied R&D (TRL 2-4), with a limited modeling component.

- We note that most user facilities (LANSCE, NHMFL) are funded to provide experimental support only.
  - CINT (and the NSRCs) are the exception, since they all maintain strong theory thrusts.

Minor concerns/observations from 2011

- The policy on use of the larger computers/supercomputers at LANL should be reviewed, with regard to allocation of cpu's and storage.
  - Recommendations for computer resources optimized for materials modeling are part of the Materials Strategy Implementation Plan.
- The Lab needs to provide mentoring to early-career scientists… We recommend that a Lab-wide mentoring program be instituted to ensure uniform treatment of early-career scientists in all divisions.
  - An early-career mentoring plan is under development.
- Early-career scientists commented on the difficulty in getting access to equipment….LANL should work on developing more instrumentation facilities, either using the CINT model or a pure recharge model....Nanofabrication should be one major priority under this theme.
  - Recommendations for equipment access, including a nano/micro fabrication facility, are part of the Materials Strategy Implementation Plan.

Presentation outline

- LANL update/Trends in metrics
- Progress in Implementation Plan for Materials Strategy
- Technical highlights
- Response to 2011 recommendations
- **2012 Topics**

We are organizing our Materials Capability Reviews based on the Materials Strategy

	2010	2011	2012
Overview	▪ Materials Overview ▪ Materials Strategy ▪ MaRIE update	Materials Overview MaRIE Overview Materials Strategy	Materials Overview with Strategy MaRIE Overview Weapons Overview
Emergent phenomena	CINT/Nanoscience	Materials for Renewable Energy	Condensed Matter Physics
Defects and Interfaces	Electronic/ Photonic Materials	Actinides (Nuclear Energy focus)	Codesign as applied to materials
Extreme Environments	Materials Dynamics	Radiation Environments/ IBML	HE/High Pressure
Programmatic Element	Materials for Global Security	LDRD--Martinez	LDRD--Ceretta
Special Topics	Actinide Overview ▪ Pu strategy ▪ LDRD –Martin	LANSCE	NHMFL

2012 Materials Capability Review topics and presenters

- **Materials Overview and Vision (including LANL Pillar discussion)**
  - Materials for Weapons*: Dave Teter, Division Leader, MST*
  - MaRIE update: *John Sarrao, Program Director, Office of Science & MaRIE*
- **LDRD Review: "Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage,"** *Ellen Cerreta, Scientist, MST-8*
- **Extreme Environments: Energetic Materials/High Pressure**
  - Lead: *Dave Funk, WX (Weapons Experimentation) Division Leader*
- **Defects and Interfaces: CoDesign applied to Materials**
  - Lead: *Tony Redondo, T-Division Leader*
- **Emergent Phenomena: Condensed Matter Physics**
  - Lead: *Mike Hundley, Group Leader, Condensed Matter & Magnet Science*
- **Facility: National High Magnetic Field Lab—Pulsed Field Facility**
  - Lead: *Chuck Mielke, Director, NHMFL-PPF*

Your feedback on the performance of the Materials Capability is requested

- **Scientific Leadership as Evidenced by:**
    - Leadership in an international technical community
    - Publication of highly cited research results
    - Flux of innovative ideas and proposals
    - Hiring and training of next generation's leaders
- **Programmatic Impact**
- **Sustaining a *Cross-Laboratory* Materials Community**
- **Direction for the Future**
    - Progress on implementing the Materials Strategy
    - The path to MaRIE

MaRIE Update

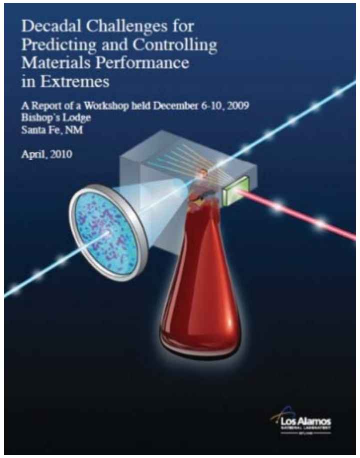
J. L. Sarrao (SPO-SC)

An update on MaRIE with an emphasis on developments since the last Materials Capability Review is presented. In particular, the development and current status of the MaRIE 1.0 proposal, submitted in response to the NNSA New Facilities call, is reviewed. Finally, we discuss ongoing and planned “MaRIE Program” activities that enable MaRIE science today.

MaRIE:

(Matter-Radiation Interactions in Extremes)

An Experimental Facility Concept Revolutionizing Materials in Extremes



Decadal Challenges for
Predicting and Controlling
Materials Performance
in Extremes

A Report of a Workshop held December 6-10, 2009
Bishop's Lodge
Santa Fe, NM

April, 2010

John Sarrao
Los Alamos National Laboratory

Experimental Physical Sciences

VISTAS

MaRIE:
Matter-Radiation Interactions in Extremes

Materials Capability Review 2012

A short history of MaRIE:
Where we've been and where we're going

(2006-2008)

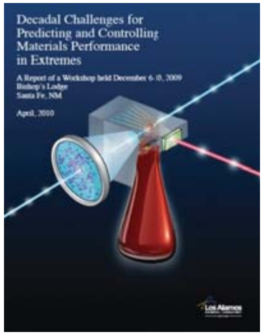
LANS Contract Transition

Concept Definition/Internal Competition

MaRIE selection

Pre-MaRIE

Science Need



Decadal Challenges for
Predicting and Controlling
Materials Performance
in Extremes

A Report of a Workshop held December 6-10, 2009
Bishop's Lodge
Santa Fe, NM

April, 2010

(2009)

Facility Definition

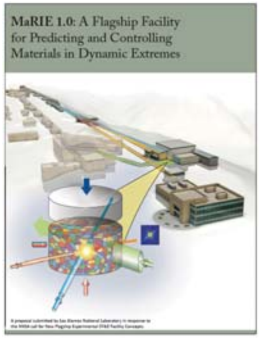
Experimental Physical Sciences
VISTAS

MaRIE:
Matter-Radiation Interactions in Extremes

FALL 2010

(2010)

Pre-conceptual Proposal



MaRIE 1.0: A Flagship Facility
for Predicting and Controlling
Materials in Dynamic Extremes

(2012)

Near Term (FY12) – "MaRIE Proposal":

LANSCE→ Linac Risk Mitigation → MTS

MaRIE 1.0: Response to NA-10 "New Facilities" Call (→ CD-0)

Medium Term (FY12 → FY15) – "MaRIE Project":

Facility-specific risk reduction r&d with partners (e.g., SLAC)

Ongoing –"MaRIE Program":

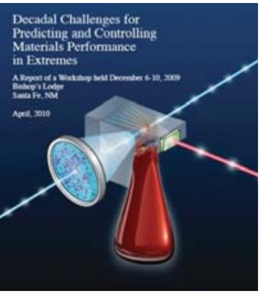
Institutional investments (e.g., LDRD): Materials in Extremes, Co-Design, …

External wins: CMIME EFRC (BES), CASL Hub (NE), ExMatEx (ASCR co-design center)

(In the weapons program,) we have not yet achieved a predictive, process-aware understanding of materials performance

Materials research is on the brink of a new era – from observation of performance to control of properties

- **The confluence of unprecedented experimental capabilities (e.g. 4th generation light sources, controlled synthesis and characterization, …) and simulation advances are providing remarkable insights at length and time scales previously inaccessible**



Decadal Challenges for
Predicting and Controlling
Materials Performance
in Extremes

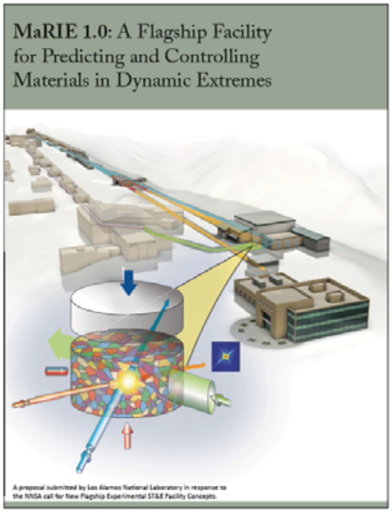
A Report of a Workshop held December 6-10, 2009
Bishop's Lodge
Santa Fe, NM

April, 2010

Experimental Physical Sciences

VISTAS

MaRIE:
Matter-Radiation Interactions in Extremes



MaRIE 1.0: A Flagship Facility
for Predicting and Controlling
Materials in Dynamic Extremes

A proposal submitted by Los Alamos National Laboratory in response to the NNSA call for New Flagship Experimental ST&E Facility Concepts.

New capabilities will be needed to realize this vision:

In situ, dynamic measurements

simultaneous scattering & imaging

of well-controlled and characterized materials

advanced synthesis and characterization

in extreme environments

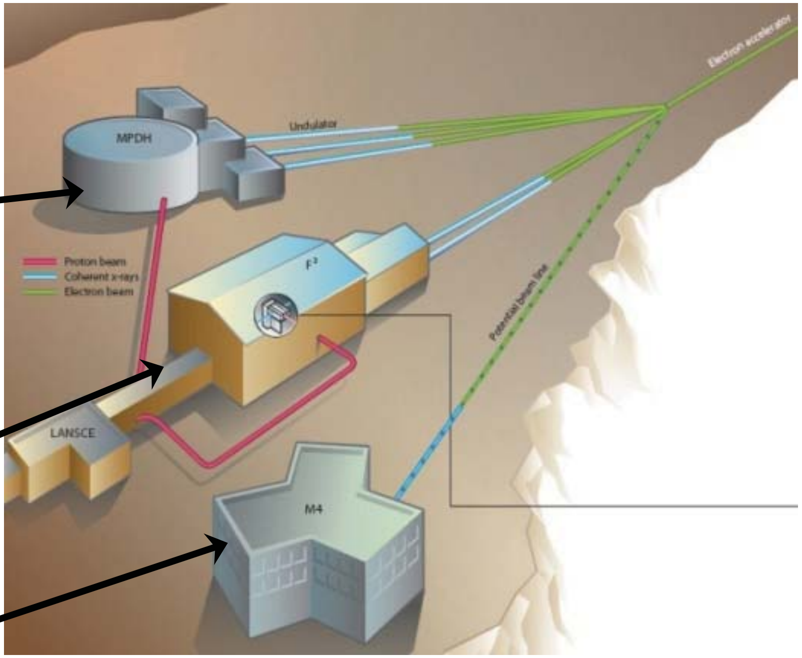
dynamic loading, irradiation

coupled with predictive modeling and simulation

materials design & discovery

MaRIE is a key step towards this vision

MaRIE builds on the LANSCE facility to provide unique experimental tools to meet this need



First x-ray scattering capability at high energy and high repetition frequency with simultaneous charged particle dynamic imaging

(**MPDH**: Multi-Probe Diagnostic Hall)

Unique in-situ diagnostics and irradiation environments beyond best planned facilities

(**F^3**: Fission and Fusion Materials Facility)

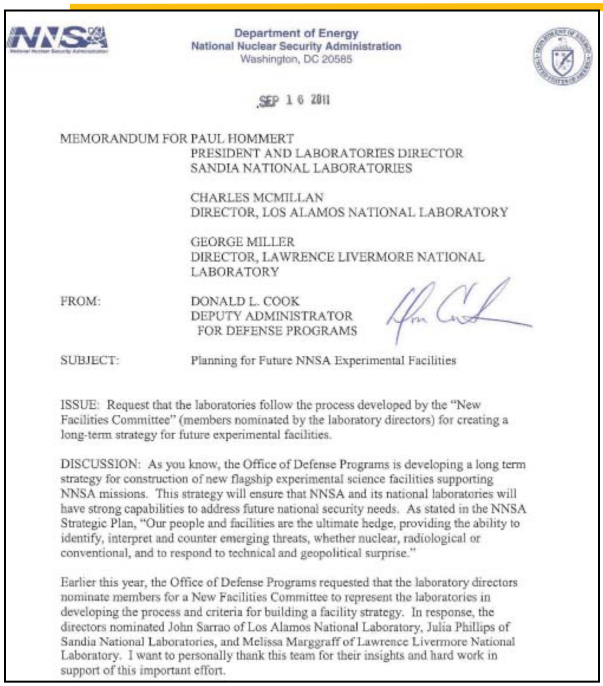
Comprehensive, integrated resource for materials synthesis and control, with national security infrastructure

(**M4**: Making, Measuring & Modeling Materials Facility)

Unique very hard x-ray XFEL
Unique simultaneous photon-proton imaging measurements
Unique spallation neutron-based irradiation capability
Unique in-situ, transient radiation damage measurements
Unique materials design and discovery capability

MaRIE will provide unprecedented international user resources

LANL (and SNL & LLNL) are actively working responses to the NNSA New Facilities Call



Department of Energy
National Nuclear Security Administration
Washington, DC 20585

SEP 16 2011

MEMORANDUM FOR PAUL HOMMERT
PRESIDENT AND LABORATORIES DIRECTOR
SANDIA NATIONAL LABORATORIES

CHARLES MCMILLAN
DIRECTOR, LOS ALAMOS NATIONAL LABORATORY

GEORGE MILLER
DIRECTOR, LAWRENCE LIVERMORE NATIONAL LABORATORY

FROM: DONALD L. COOK
DEPUTY ADMINISTRATOR
FOR DEFENSE PROGRAMS

SUBJECT: Planning for Future NNSA Experimental Facilities

ISSUE: Request that the laboratories follow the process developed by the "New Facilities Committee" (members nominated by the laboratory directors) for creating a long-term strategy for future experimental facilities.

DISCUSSION: As you know, the Office of Defense Programs is developing a long term strategy for construction of new flagship experimental science facilities supporting NNSA missions. This strategy will ensure that NNSA and its national laboratories will have strong capabilities to address future national security needs. As stated in the NNSA Strategic Plan, "Our people and facilities are the ultimate hedge, providing the ability to identify, interpret and counter emerging threats, whether nuclear, radiological or conventional, and to respond to technical and geopolitical surprise."

Earlier this year, the Office of Defense Programs requested that the laboratory directors nominate members for a New Facilities Committee to represent the laboratories in developing the process and criteria for building a facility strategy. In response, the directors nominated John Sarrao of Los Alamos National Laboratory, Julia Phillips of Sandia National Laboratories, and Melissa Marggraff of Lawrence Livermore National Laboratory. I want to personally thank this team for their insights and hard work in support of this important effort.

Deliverables (2/15/12)
Tri-Lab Facility Roadmap
(up to) 4 proposals/Lab

LANL Priorities
MaRIE 1.0
Nuclear Science Complex (WNR+)
HILL (High Intensity Laser Lab)
3 GeV pRad

NNSA is convening an external committee to review proposals and roadmap

-Feedback due 5/1
-Second Round review by 7/1

Desired Outcomes: By 8/1/12,

- NNSA integrates Facility Roadmap into broader planning frameworks
- Best and most urgent proposals move expeditiously to CD-0

The Laboratories have identified a set of facility concepts to fill these gaps

LANL

MaRIE 1.0

Nuclear Science Complex

HILL

3GeV pRad

LLNL

PRIME

Enhanced NIF

Nuclear Security Science Complex

SNL

CHIP²

SPARC

SALSA

The three highest priority proposals address gaps in process aware materials, devices and manufacturing capability

- **urgently needed to support the transition to smaller stockpiles, will enable other NNSA & broader national security missions**
- **progress in process aware materials-manufacturing has the potential to give rise to disruptive technology advances in the 21st century**
- **are qualitatively different than facilities that exist in the tri-lab today**

NNSA Mission Drivers articulate the need for MaRIE 1.0: Dynamic Materials Performance and Process Aware Manufacturing

U.S. Department of ENERGY

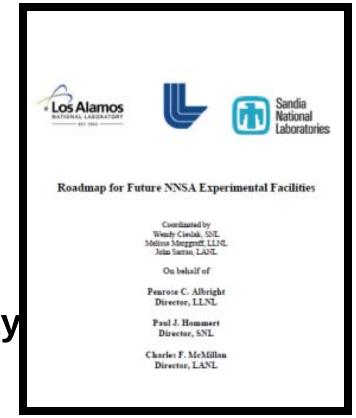
NNSA

FY 2012 Stockpile Stewardship and Management Plan

Report to Congress
April 15, 2011

United States Department of Energy
Washington, DC 20585

"Weapons materials aging and replacement material qualification: … there will be an increasing need for more sophistication in predicting their behavior under weapons conditions. In addition, as unavoidable changes in the stockpile occur, models for materials behavior will need to be more closely related to fundamental thermodynamic and physical properties."



Los Alamos NATIONAL LABORATORY

Sandia National Laboratories

Roadmap for Future NNSA Experimental Facilities

Coordinated by
Wendy Cieslak, SNL
Melissa Marggraff, LLNL
John Sarrao, LANL

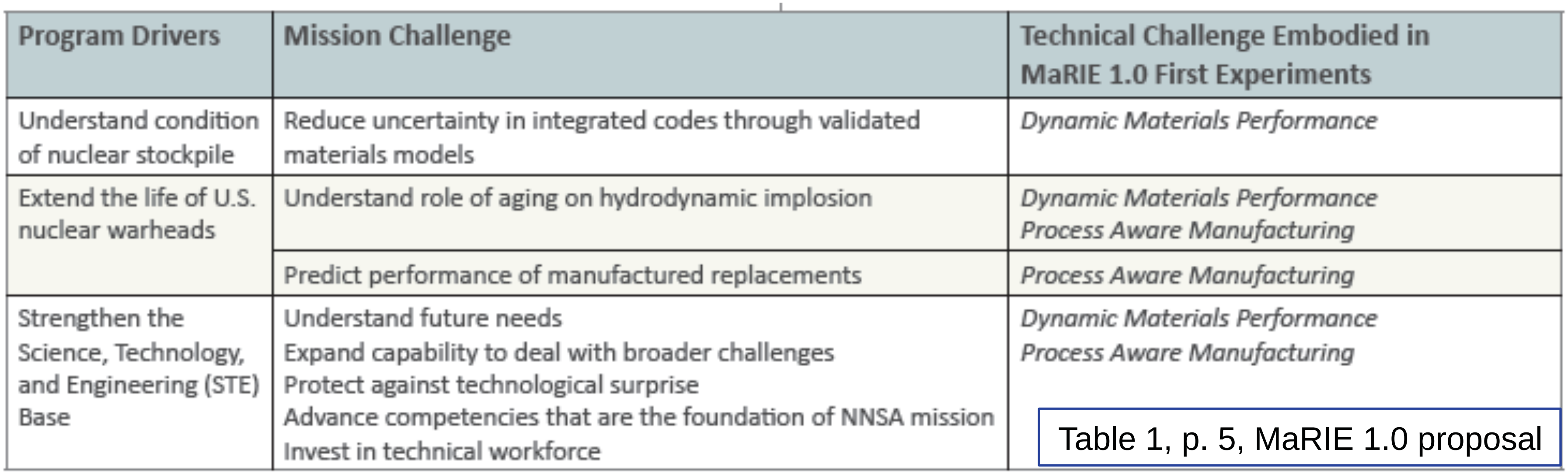
On behalf of

Penrose C. Albright
Director, LLNL

Paul J. Hommert
Director, SNL

Charles F. McMillan
Director, LANL

"In particular, we believe that filling the gap in our ability to 'predict and control from materials and devices to manufacturing processes' is especially urgent."

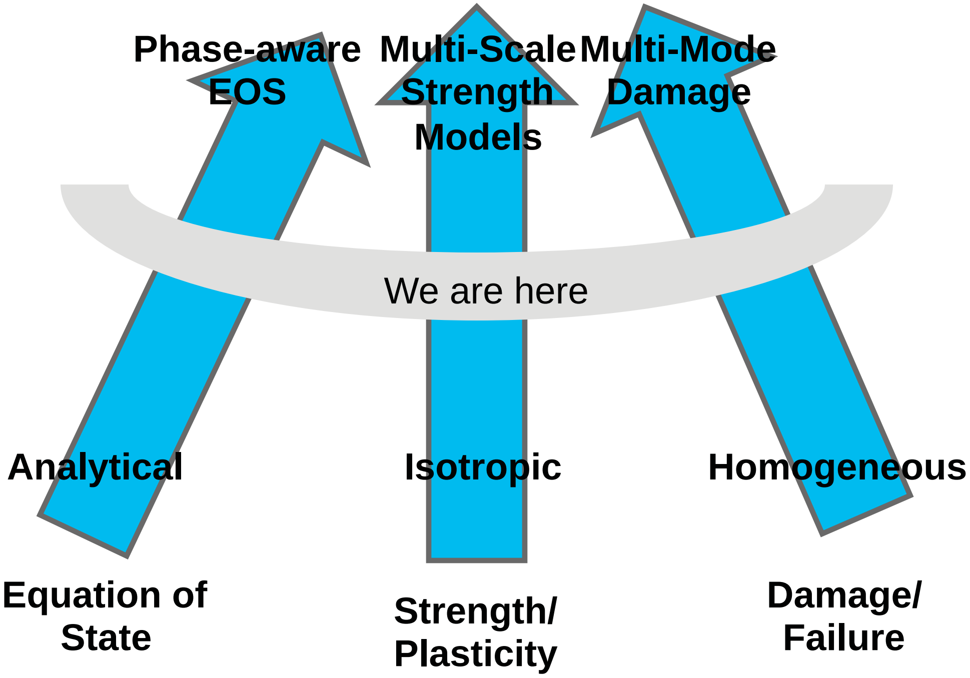


Program Drivers	Mission Challenge	Technical Challenge Embodied in MaRIE 1.0 First Experiments
Understand condition of nuclear stockpile	Reduce uncertainty in integrated codes through validated materials models	*Dynamic Materials Performance*
Extend the life of U.S. nuclear warheads	Understand role of aging on hydrodynamic implosion	*Dynamic Materials Performance* *Process Aware Manufacturing*
	Predict performance of manufactured replacements	*Process Aware Manufacturing*
Strengthen the Science, Technology, and Engineering (STE) Base	Understand future needs Expand capability to deal with broader challenges Protect against technological surprise Advance competencies that are the foundation of NNSA mission Invest in technical workforce	*Dynamic Materials Performance* *Process Aware Manufacturing*

Table 1, p. 5, MaRIE 1.0 proposal

We do not presently possess an adequate predictive, process-aware understanding of materials performance

Dynamic Materials Performance:
Phase-aware integrated models



Phase-aware EOS

Multi-Scale Strength Models

Multi-Mode Damage

We are here

Analytical

Isotropic

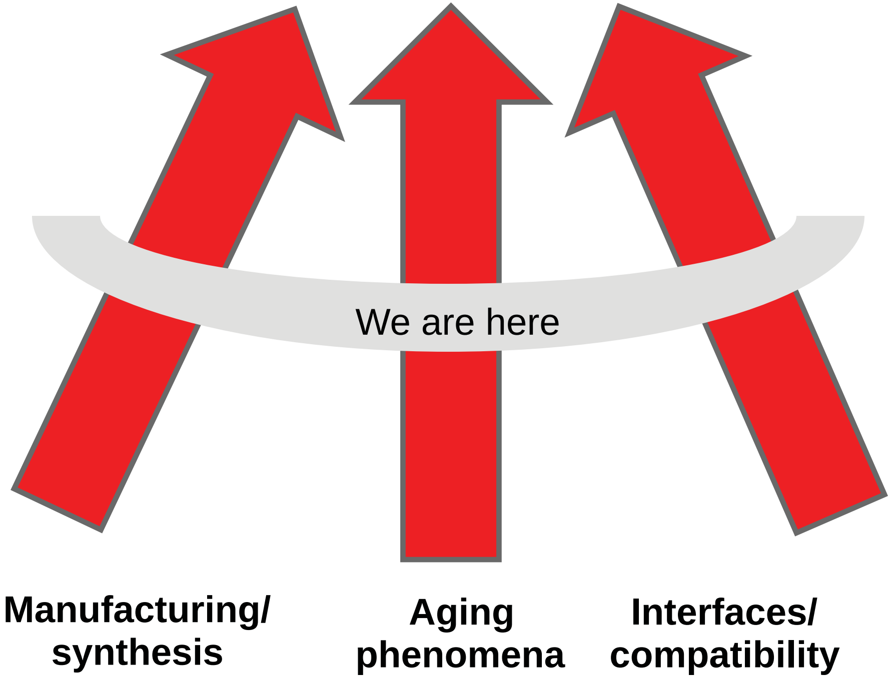
Homogeneous

Equation of State

Strength/ Plasticity

Damage/ Failure

Process Aware Manufacturing:
Process-aware integrated models



We are here

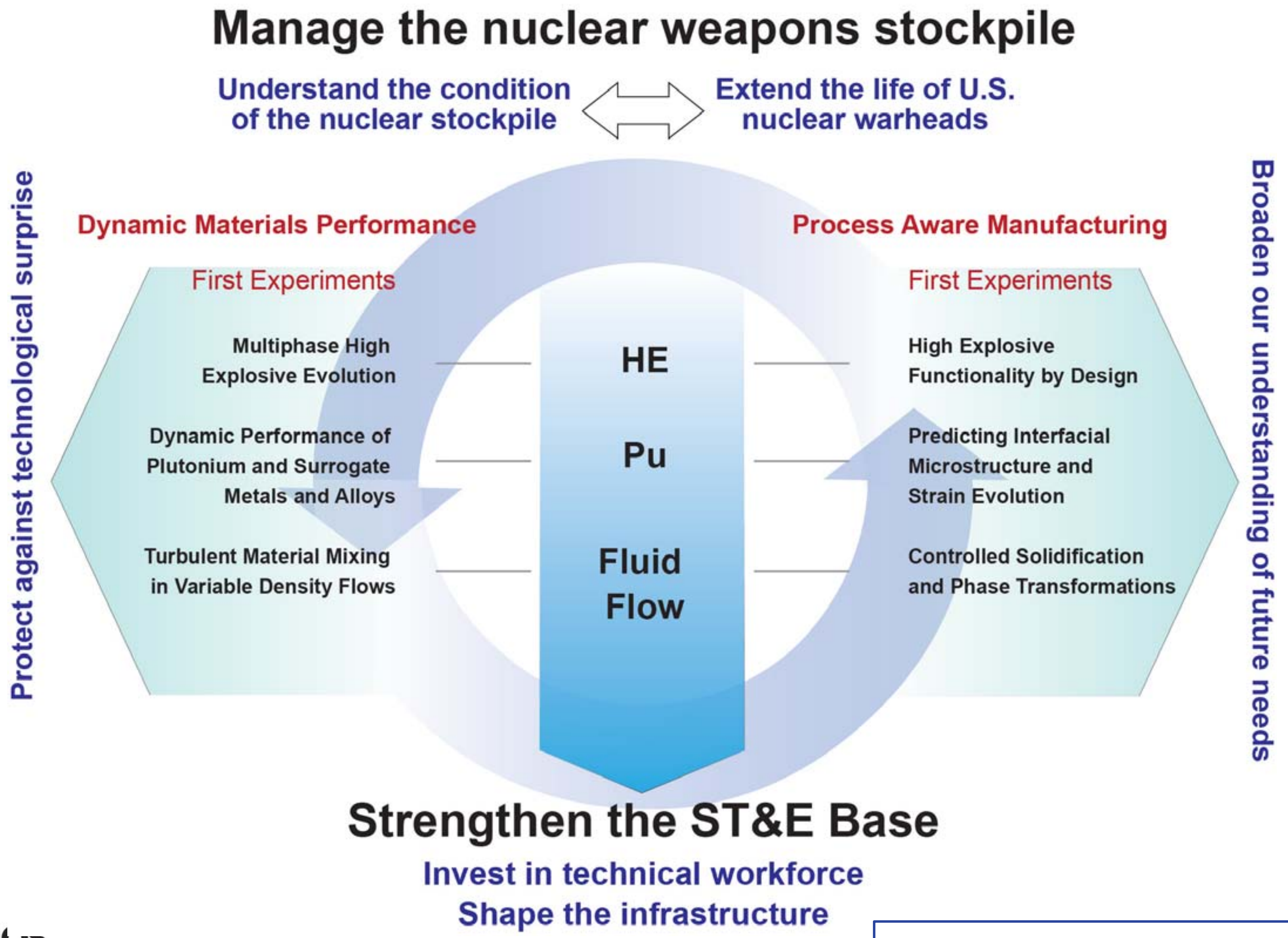
Manufacturing/ synthesis

Aging phenomena

Interfaces/ compatibility

A suite of fundamental, focused, and integrated experiments is required for success

A family of MaRIE 1.0 “First Experiments” span the mission need AND set functional requirements for the facility



Manage the nuclear weapons stockpile

Understand the condition of the nuclear stockpile ⇔ Extend the life of U.S. nuclear warheads

Protect against technological surprise

Dynamic Materials Performance

First Experiments

- Multiphase High Explosive Evolution
- Dynamic Performance of Plutonium and Surrogate Metals and Alloys
- Turbulent Material Mixing in Variable Density Flows

HE

Pu

Fluid Flow

Process Aware Manufacturing

First Experiments

- High Explosive Functionality by Design
- Predicting Interfacial Microstructure and Strain Evolution
- Controlled Solidification and Phase Transformations

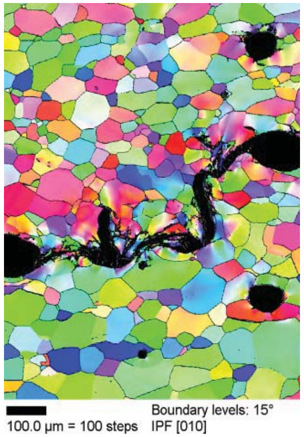
Broaden our understanding of future needs

Strengthen the ST&E Base

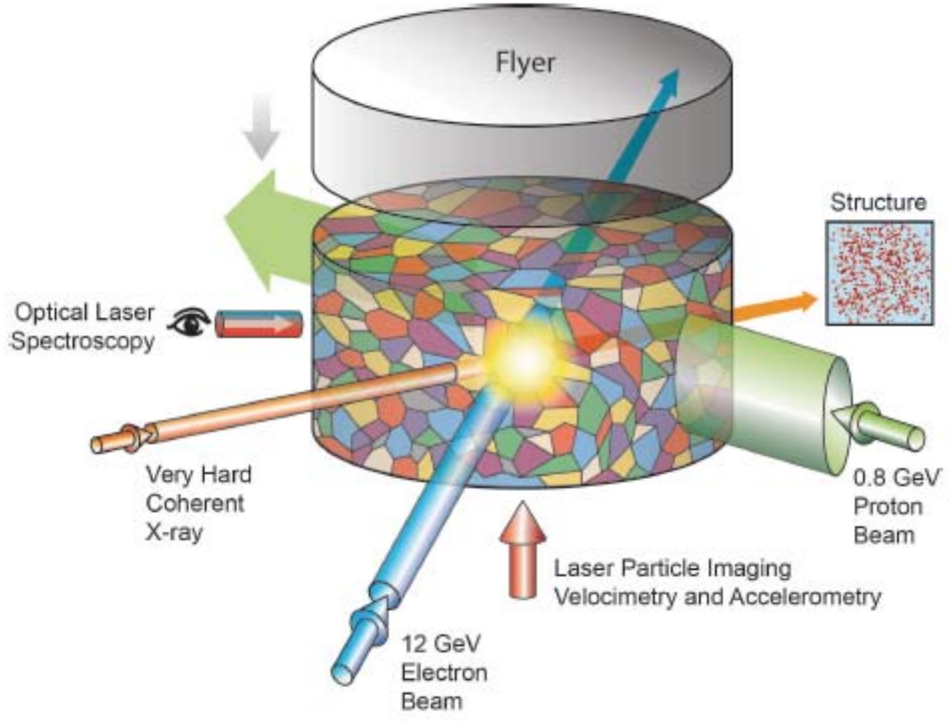
Invest in technical workforce
Shape the infrastructure

Figure 1, p. 7, MaRIE 1.0 proposal

The challenge is to observe the dynamic evolution of polycrystalline materials including Pu at the granular and sub-granular level



The goal
Predict dynamic microstructure and damage evolution



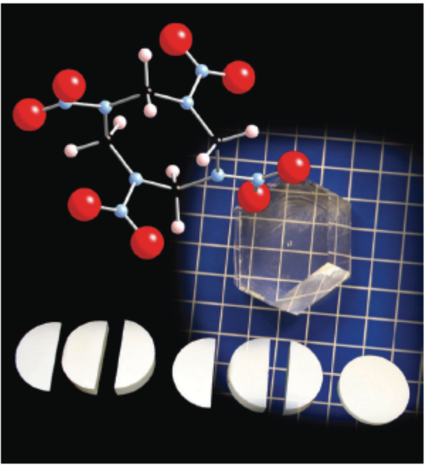
Sub-μm resolution
100’s – 1000’s μm samples
Sub-ns resolution,
~30 frames in
1 μs duration

The first experiment: **Multiple, simultaneous dynamic in situ diagnostics with resolution at the scale of nucleation sites (< 1 μm; ps – ns)**

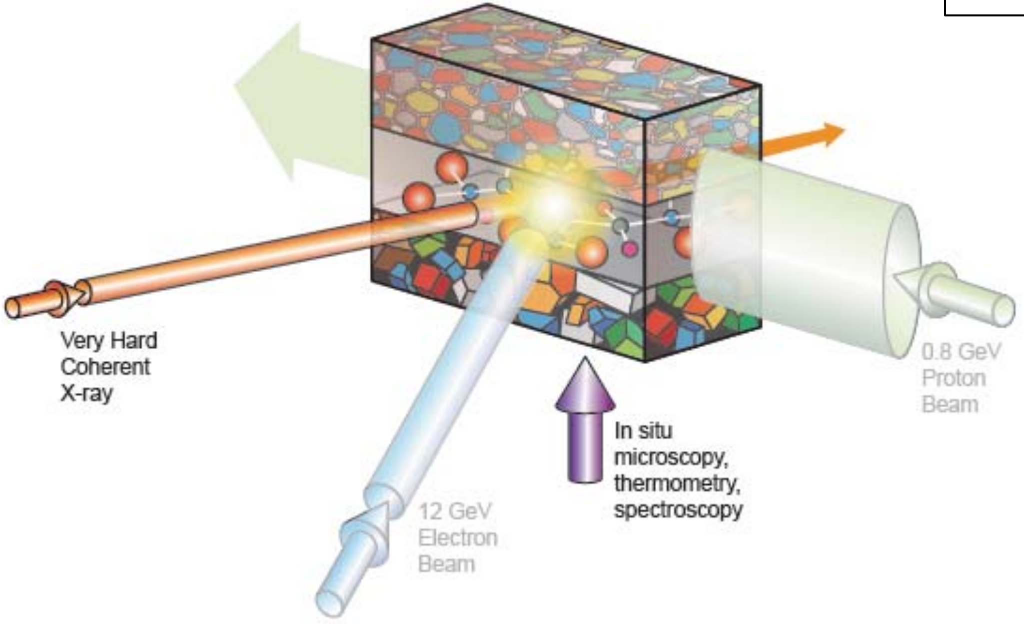
The model: **Accurate sub-grain models of microstructure evolution coupled to molecular dynamics**

Example: High Explosive Functionality by Design

The challenge is to quantify and ultimately control key mesoscale features during the dynamic conditions of materials synthesis from crystallization through component manufacture



Sub-μm resolution
100’s – 1000’s μm samples
Sub-ns resolution,
~100 fs spectroscopy

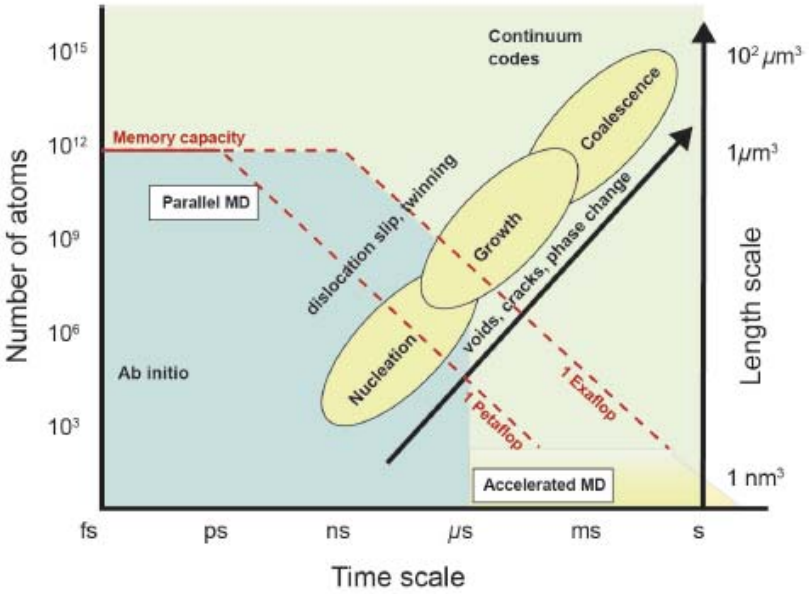


The goal
Design of energetic materials with specific function

The first experiment : **Multi-probe, real-time characterization of HE fabrication “from molecules to microstructure,” including dynamic response**

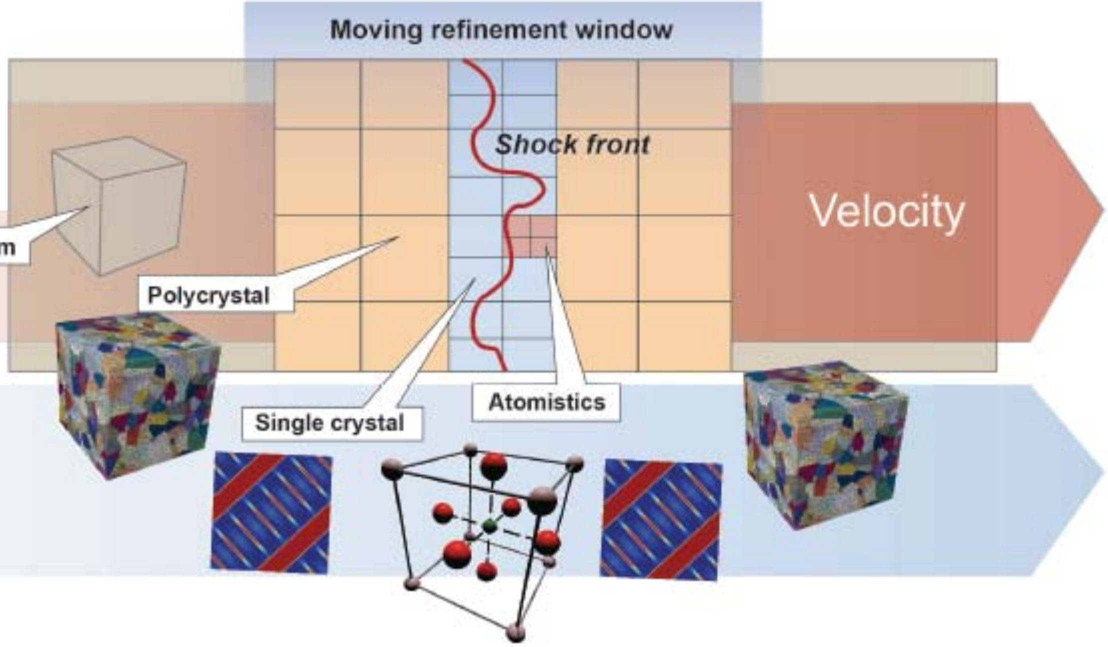
The model : **Prediction of heterogeneity-induced dynamic response of explosives**

MaRIE 1.0 with LANL's integrated co-design approach will couple multi-scale theory and multi-probe experiment on next-generation computing architectures

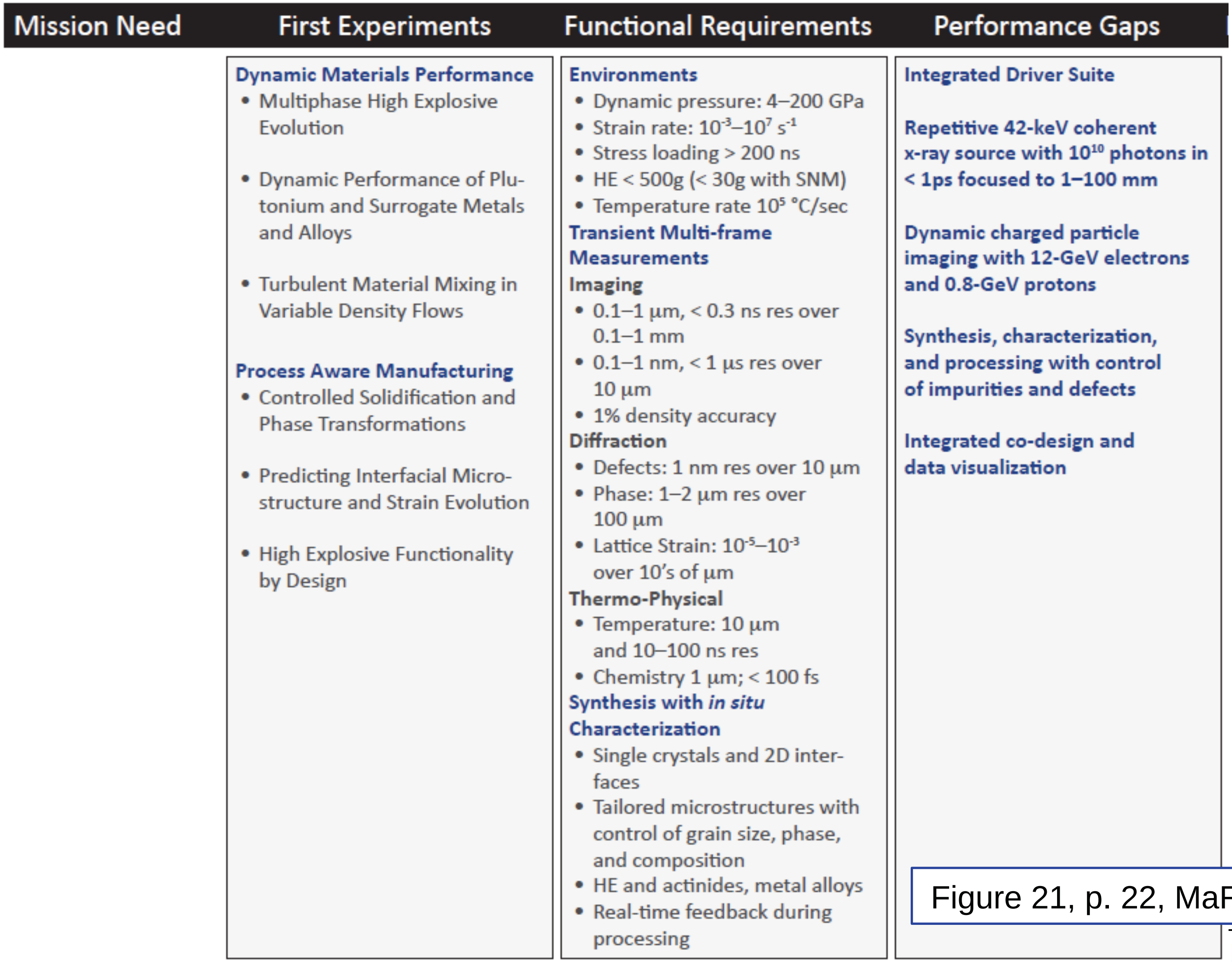


Mesoscale materials phenomena need extreme-scale computing

Variable-resolution models are synergistic with multi-probe, in-situ, transient measurements



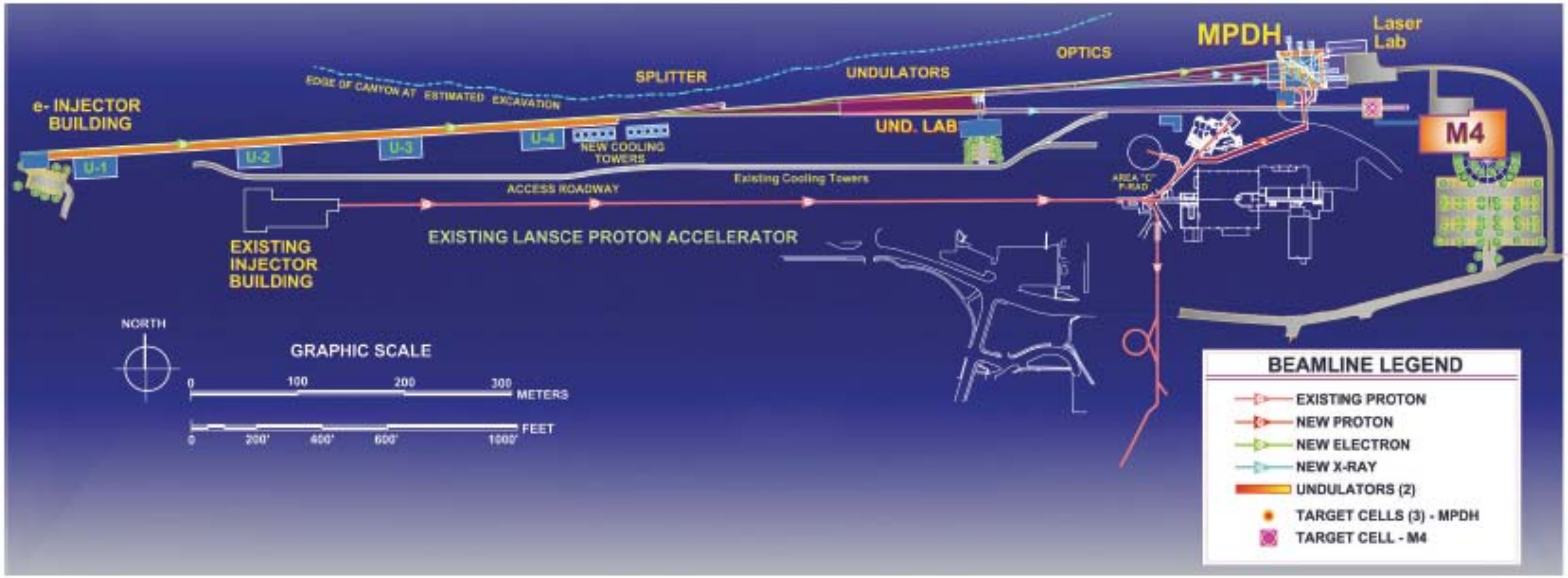
MaRIE 1.0 “First Experiments” define mission-driven functional requirements and reveal performance gaps



Mission Need	First Experiments	Functional Requirements	Performance Gaps
	Dynamic Materials Performance • Multiphase High Explosive Evolution • Dynamic Performance of Plutonium and Surrogate Metals and Alloys • Turbulent Material Mixing in Variable Density Flows **Process Aware Manufacturing** • Controlled Solidification and Phase Transformations • Predicting Interfacial Microstructure and Strain Evolution • High Explosive Functionality by Design	**Environments** • Dynamic pressure: 4–200 GPa • Strain rate: 10^{-3}–10^{7} s^{-1} • Stress loading > 200 ns • HE < 500g (< 30g with SNM) • Temperature rate 10^{5} °C/sec **Transient Multi-frame Measurements** **Imaging** • 0.1–1 µm, < 0.3 ns res over 0.1–1 mm • 0.1–1 nm, < 1 µs res over 10 µm • 1% density accuracy **Diffraction** • Defects: 1 nm res over 10 µm • Phase: 1–2 µm res over 100 µm • Lattice Strain: 10^{-5}–10^{-3} over 10’s of µm **Thermo-Physical** • Temperature: 10 µm and 10–100 ns res • Chemistry 1 µm; < 100 fs **Synthesis with *in situ* Characterization** • Single crystals and 2D interfaces • Tailored microstructures with control of grain size, phase, and composition • HE and actinides, metal alloys • Real-time feedback during processing	**Integrated Driver Suite** **Repetitive 42-keV coherent x-ray source with 10^{10} photons in < 1ps focused to 1–100 mm** **Dynamic charged particle imaging with 12-GeV electrons and 0.8-GeV protons** **Synthesis, characterization, and processing with control of impurities and defects** **Integrated co-design and data visualization**

Figure 21, p. 22, MaRIE 1.0 proposal

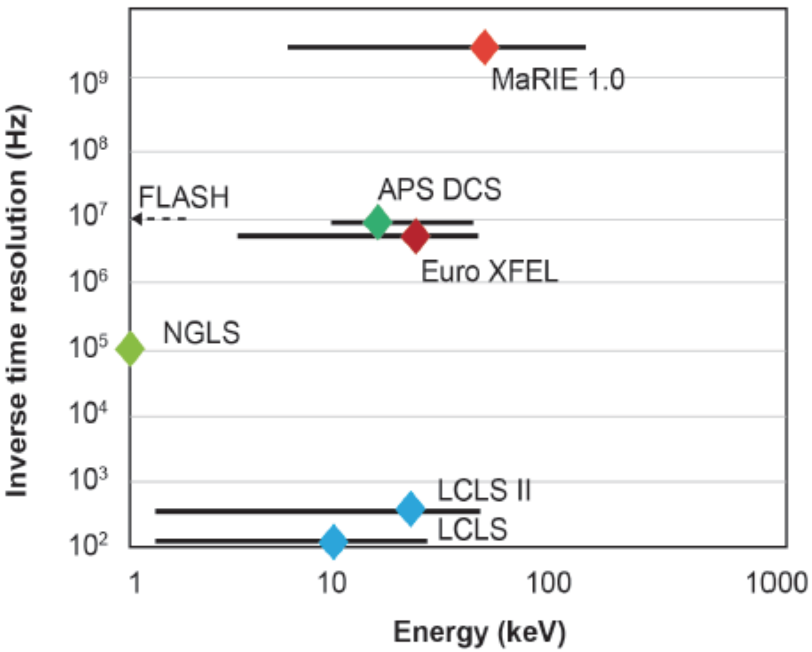
MaRIE 1.0 facility definition derives from “First Experiments” functional requirements and identified performance gaps



Leveraging LANSCE’s existing 1-MW, 0.8-GeV proton accelerator, MaRIE 1.0 will provide

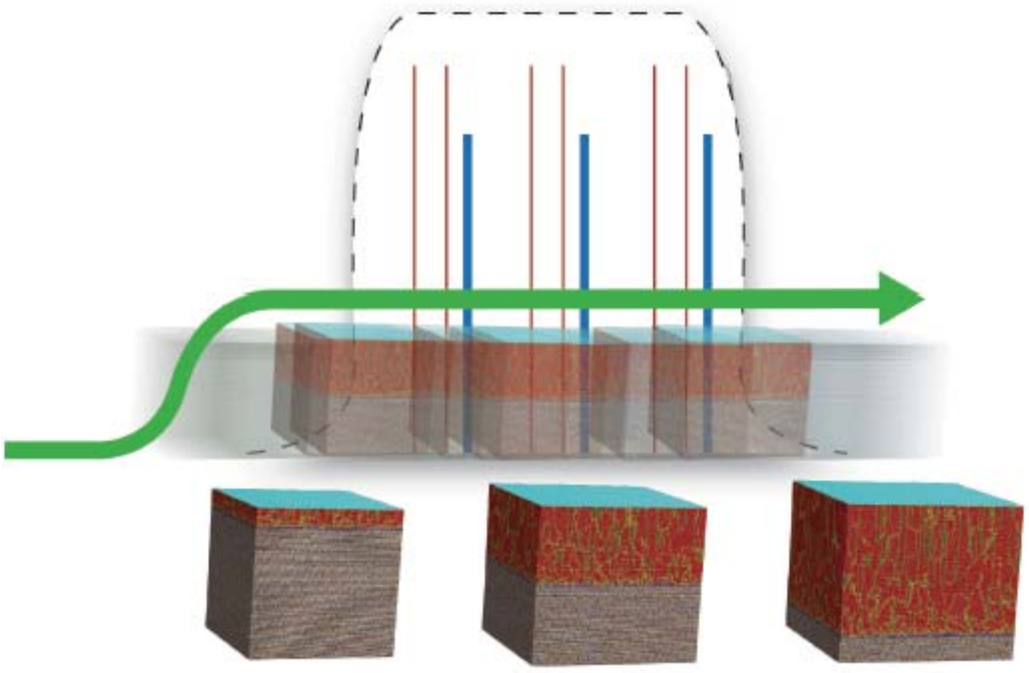
- **the world’s first very hard (42-keV) XFEL**;
- **a new Multi-Probe Diagnostic Hall (MPDH)**, coupling hard, coherent, brilliant x-ray photons with 12-GeV electron and 0.8-GeV proton radiographic tools in dynamic extremes; and
- **a unique Making, Measuring, and Modeling Materials (M4) Facility** for materials synthesis and characterization with high-performance computational co-design focused on the mesoscale.

MaRIE 1.0 photons are unique and the simultaneous use of additional electron and proton probes is unprecedented



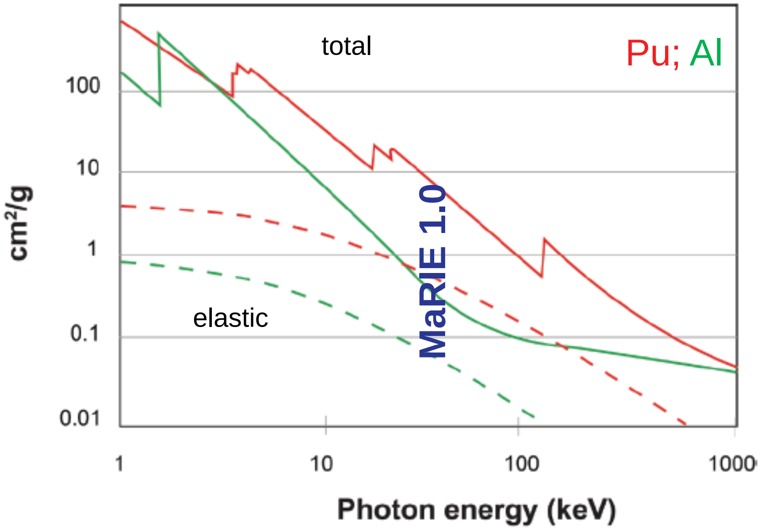
MaRIE 1.0 XFEL is harder and higher repetition rate than peer photon sources

MaRIE 1.0 multiplexes 42 keV x-ray photons (red), 12 GeV electrons (blue), and 0.8 GeV protons (green) during a single dynamic event

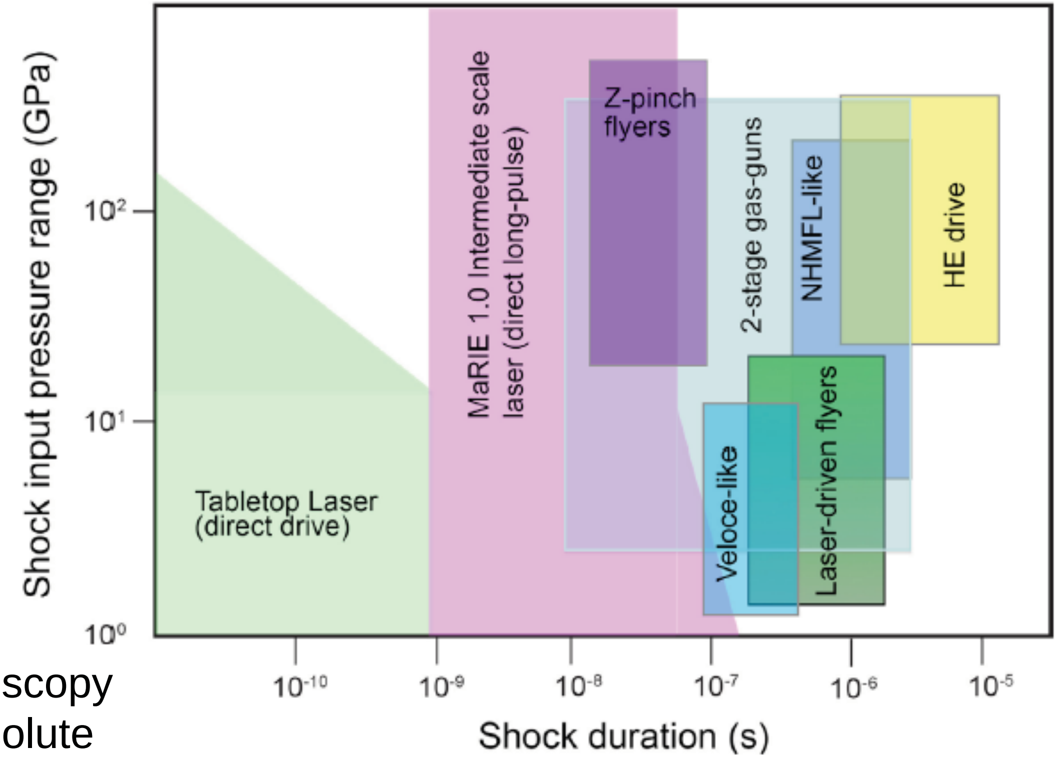


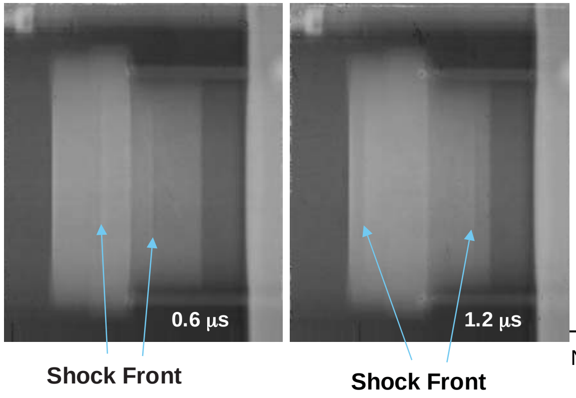
Through the Multi-Probe Diagnostic Hall, MaRIE 1.0 provides a unique capability for simultaneous, multi-probe measurements of in situ transient phenomena in relevant dynamic extremes

42-keV XFEL allows multigranular sample penetration and multipulse dynamics without significant sample perturbation.



MPDH provides a broad suite of loading conditions to the user.

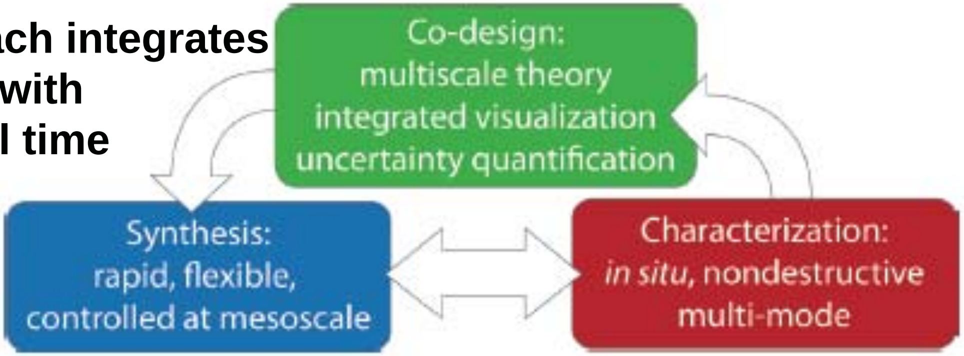


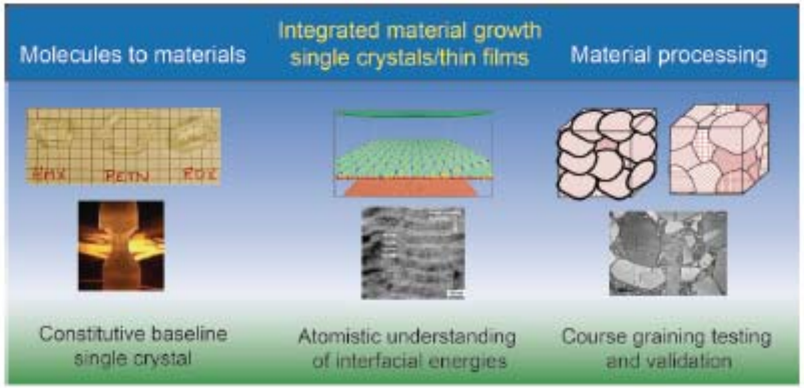


Proton microscopy provides absolute density (~1%) & velocities through sample volume.

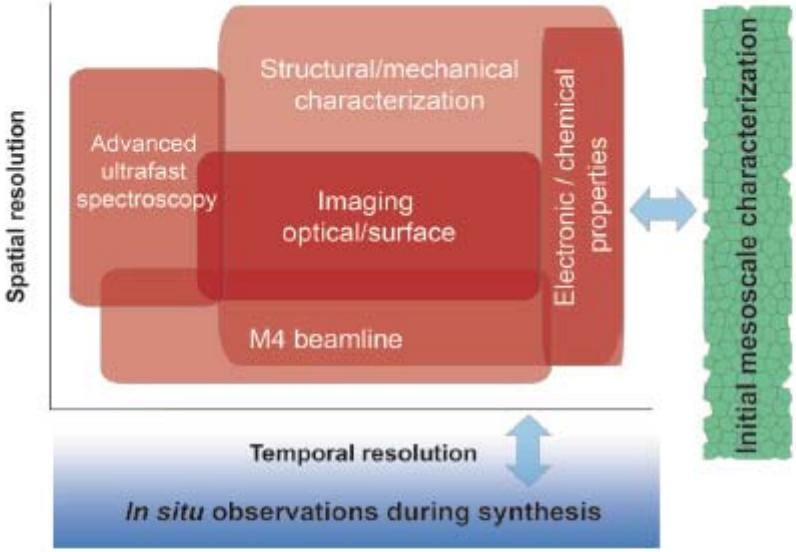
Through the M4 Facility, MaRIE 1.0 provides unique collocated and integrated synthesis, characterization, and co-design capabilities for controlling material properties at the mesoscale

M4's co-design approach integrates theory and simulation with experiment in near real time





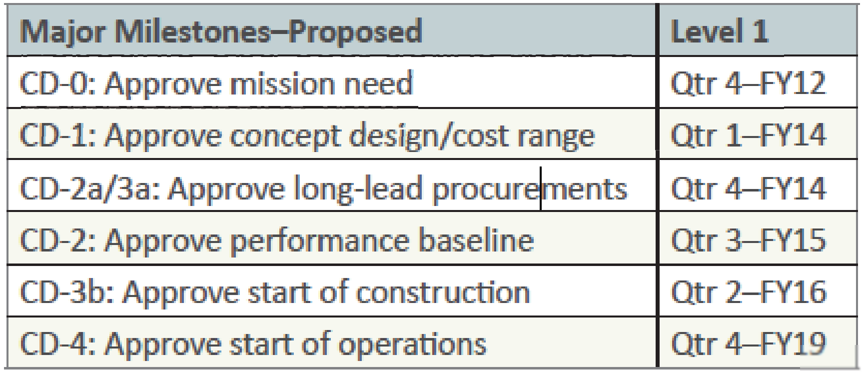
M4 synthesis capabilities span scales from molecular to bulk with emphasis on unique mesoscale/microstructure control



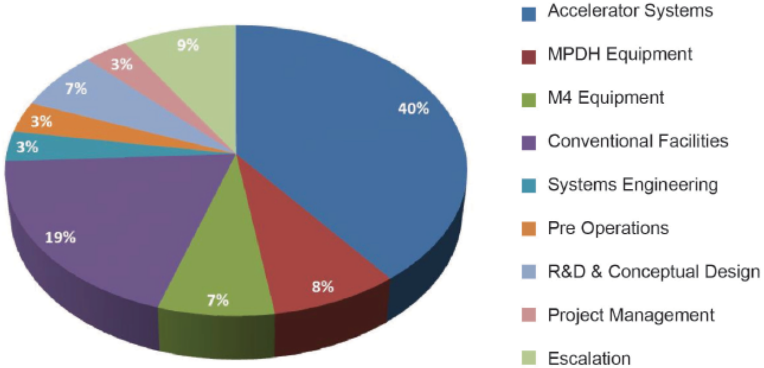
M4 XFEL undulator enables in situ 'science of synthesis' and MPDH pre-characterization

MaRIE 1.0 can be realized by FY20 for a total project cost of $1300M (cost range = $950M–$1800M)

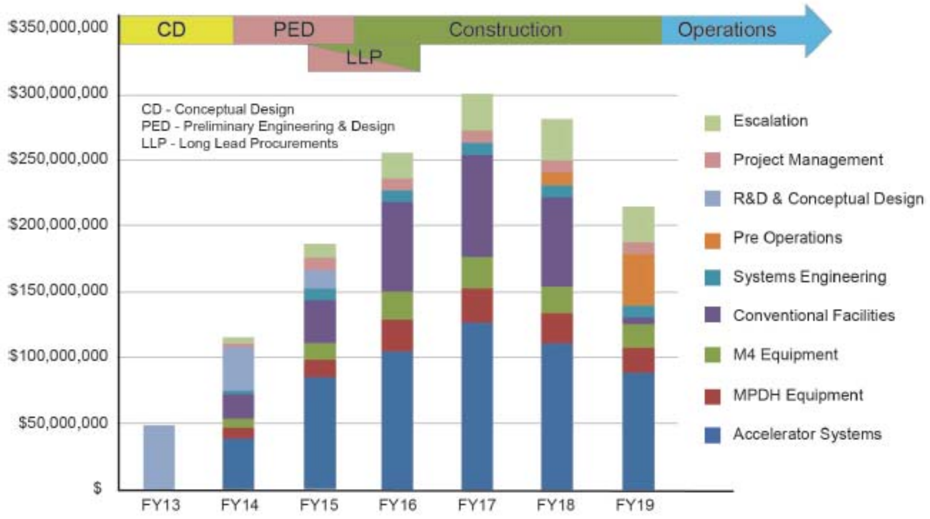
MaRIE 1.0 preconceptual reference design benefits from a robust and frequently peer-reviewed project management infrastructure



Major Milestones–Proposed	Level 1
CD-0: Approve mission need	Qtr 4–FY12
CD-1: Approve concept design/cost range	Qtr 1–FY14
CD-2a/3a: Approve long-lead procurements	Qtr 4–FY14
CD-2: Approve performance baseline	Qtr 3–FY15
CD-3b: Approve start of construction	Qtr 2–FY16
CD-4: Approve start of operations	Qtr 4–FY19



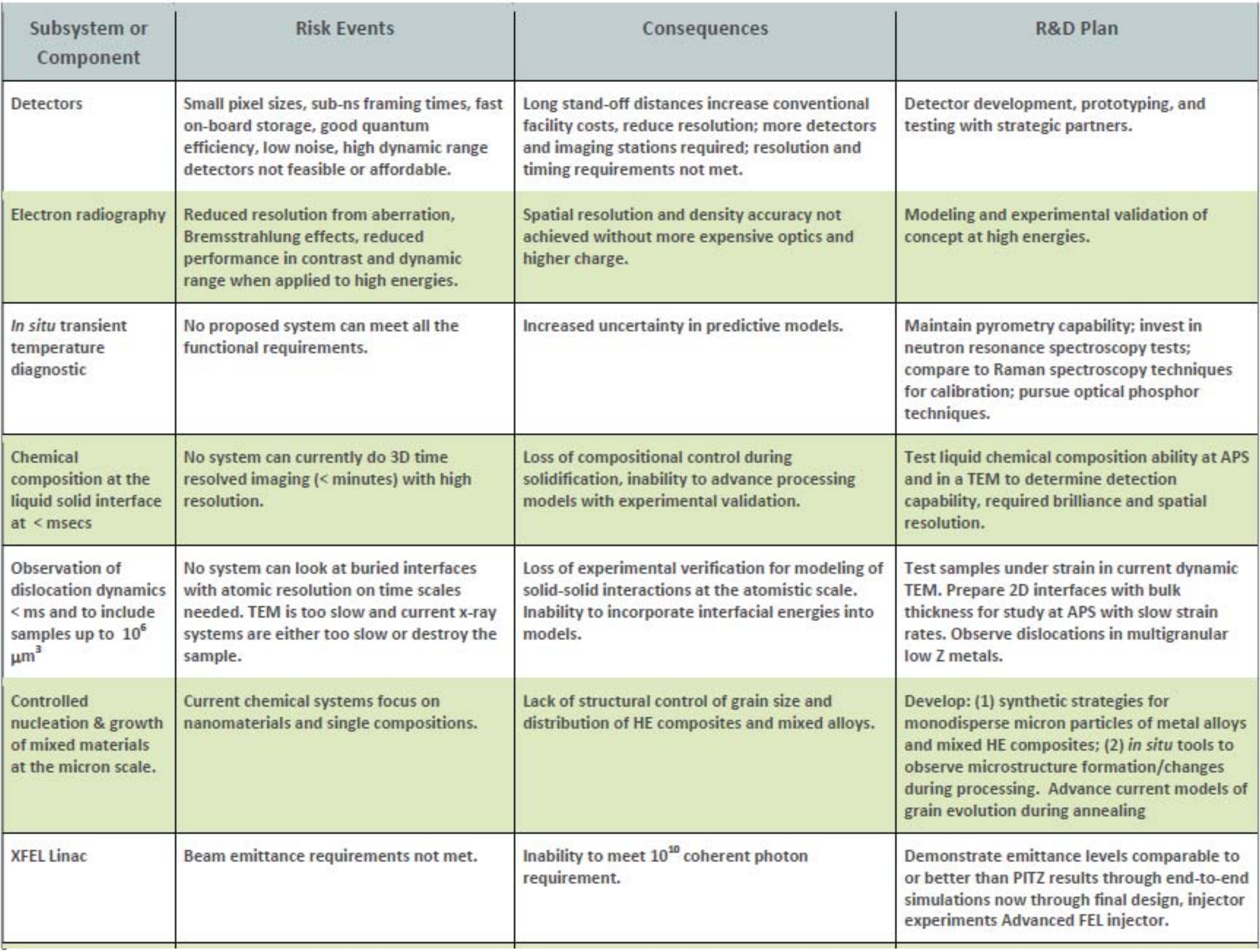
Fully-burdened & escalated cost
TRL-based contingency
Class 4/5 estimate & cost range



Los Alamos
NATIONAL LABORATORY
EST. 1943

Operated by Los Alamos National Security, LLC for NNSA

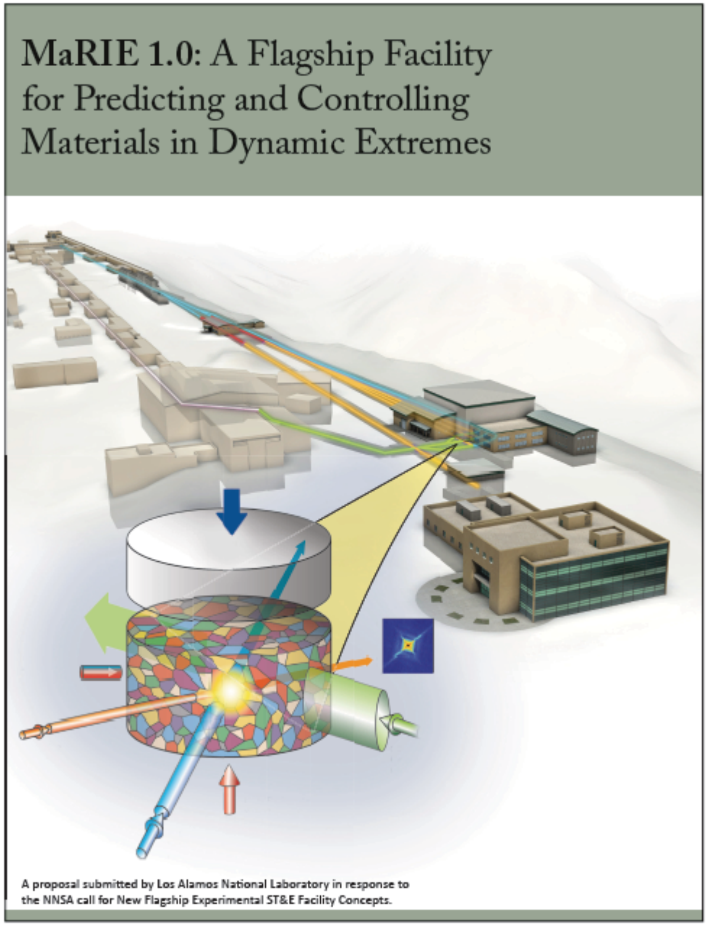
We understand the risks associated with our preconceptual reference design and have an R&D plan to retire those risks



Subsystem or Component	Risk Events	Consequences	R&D Plan
Detectors	Small pixel sizes, sub-ns framing times, fast on-board storage, good quantum efficiency, low noise, high dynamic range detectors not feasible or affordable.	Long stand-off distances increase conventional facility costs, reduce resolution; more detectors and imaging stations required; resolution and timing requirements not met.	Detector development, prototyping, and testing with strategic partners.
Electron radiography	Reduced resolution from aberration, Bremsstrahlung effects, reduced performance in contrast and dynamic range when applied to high energies.	Spatial resolution and density accuracy not achieved without more expensive optics and higher charge.	Modeling and experimental validation of concept at high energies.
In situ transient temperature diagnostic	No proposed system can meet all the functional requirements.	Increased uncertainty in predictive models.	Maintain pyrometry capability; invest in neutron resonance spectroscopy tests; compare to Raman spectroscopy techniques for calibration; pursue optical phosphor techniques.
Chemical composition at the liquid solid interface at < msecs	No system can currently do 3D time resolved imaging (< minutes) with high resolution.	Loss of compositional control during solidification, inability to advance processing models with experimental validation.	Test liquid chemical composition ability at APS and in a TEM to determine detection capability, required brilliance and spatial resolution.
Observation of dislocation dynamics < ms and to include samples up to 10^6 μm^3	No system can look at buried interfaces with atomic resolution on time scales needed. TEM is too slow and current x-ray systems are either too slow or destroy the sample.	Loss of experimental verification for modeling of solid-solid interactions at the atomistic scale. Inability to incorporate interfacial energies into models.	Test samples under strain in current dynamic TEM. Prepare 2D interfaces with bulk thickness for study at APS with slow strain rates. Observe dislocations in multigranular low Z metals.
Controlled nucleation & growth of mixed materials at the micron scale.	Current chemical systems focus on nanomaterials and single compositions.	Lack of structural control of grain size and distribution of HE composites and mixed alloys.	Develop: (1) synthetic strategies for monodisperse micron particles of metal alloys and mixed HE composites; (2) *in situ* tools to observe microstructure formation/changes during processing. Advance current models of grain evolution during annealing
XFEL Linac	Beam emittance requirements not met.	Inability to meet 10^{10} coherent photon requirement.	Demonstrate emittance levels comparable to or better than PITZ results through end-to-end simulations now through final design, injector experiments Advanced FEL injector.

Table 6, p. 44, MaRIE 1.0 proposal

MaRIE 1.0 will enable us to observe and ultimately control how mesoscale materials properties affect weapons performance



MaRIE 1.0: A Flagship Facility for Predicting and Controlling Materials in Dynamic Extremes

A proposal submitted by Los Alamos National Laboratory in response to the NNSA call for New Flagship Experimental ST&E Facility Concepts.

A mission need exists for a facility focused on predicting and controlling materials in extreme environments, exploiting *in situ* transient measurements on real materials in relevant dynamic extremes to address key nuclear weapons challenges.

Achieving controlled functionality at the mesoscale through co-design is the **frontier of materials research**.

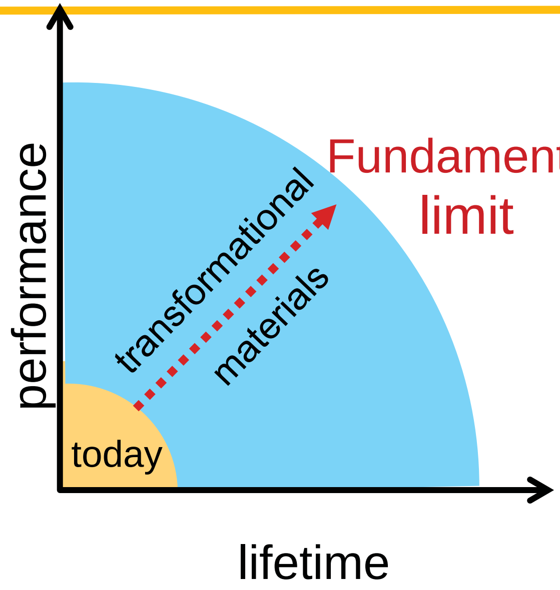
MaRIE 1.0 meets this need with a robust preconceptual reference design that is grounded in **community-defined mission and scientific requirements**.

LANL can realize MaRIE 1.0 by FY20 for a total project cost of ~ $1300M ($950M - $1800M).

MaRIE 1.0 is urgently needed to steward the stockpile and contribute to broader national security challenges early in the next decade

There’s more to MaRIE than MaRIE 1.0…

- **“MaRIE is a compass, not a weathervane”**
  - **MaRIE remains aligned with Laboratory materials strategy**
- **MTS remains a critical Laboratory priority and an essential step towards MaRIE**
- **“MaRIE Program:” We’re investing in “MaRIE science” now, including with partners and collaborators**
  - **BESAC meso initiative**
  - **Growing FESAC awareness of materials challenges**
  - **OSTP: Materials Genome Initiative**
  - **EERE: Critical Materials Hub**



Isolating the Influence of Kinetic and Spatial Effects of Dynamic Damage Evolution

E. Cerreta (MST-8)

While dynamic damage has been studied for many years, our current ability to predict and simulate evolving deformation during dynamic loading remains limited. Reasons for this are related not only to previous limitations in our abilities to characterize damage both during and after deformation, but also our abilities to experimentally mimic well-modeled shock deformation conditions. Specifically, while we believe that both time and length scale of a dynamic loading event are critically important to the development of damage leading to component failure, we have not been able to perform the experiments that allow us to isolate these effects, interrogate their unique contribution to material behavior, and then incorporate this physical understanding into predictive models. Recent advances in bulk characterization techniques and newly developed dynamic loading techniques have made isolation of these effects possible for the first time, therefore have enable model driven dynamic experiments. In this way, this project utilizes a combined experimental and theoretical approach to examining the influence of time and length scales on dynamic damage. Experimental observations are incorporated into materials models to advance the state of the art in dynamic damage modeling. Additionally meso-scale simulations are utilized to help establish correlations between microstructure and damage. This co-design approach to the study of dynamic damage sheds light on materials performance parameters critical to the design of next-generation materials.

Isolating the Influence of Kinetic and Spatial Effects of Dynamic Damage Evolution

LDRD-DR 20100026

LDRD
innovation for our nation

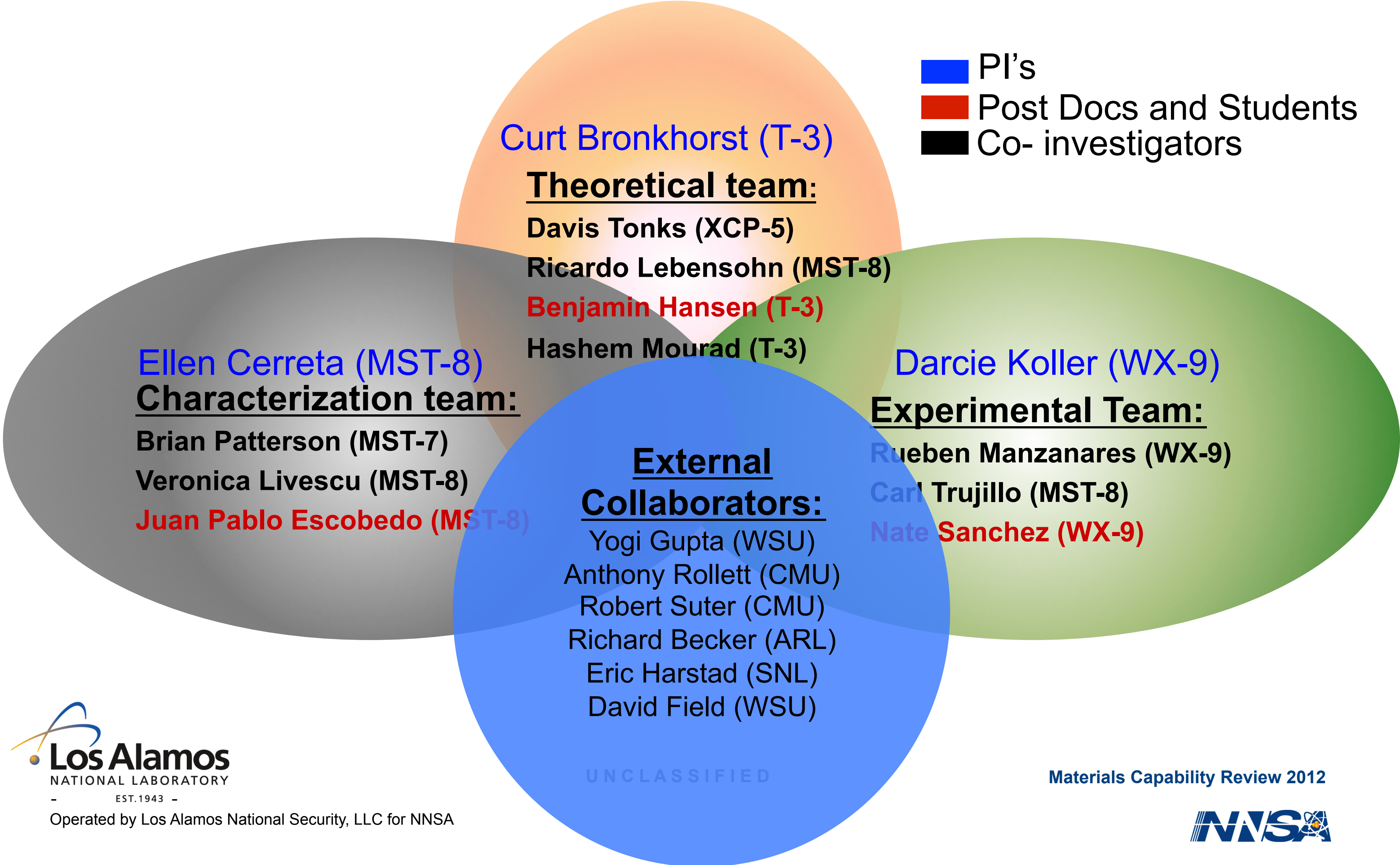
UNCLASSIFIED

Los Alamos
NATIONAL LABORATORY
EST. 1943

Operated by Los Alamos National Security, LLC for NNSA

The People and Teams

🟦 PI's
🟥 Post Docs and Students
⬛ Co- investigators



Curt Bronkhorst (T-3)

Theoretical team:

Davis Tonks (XCP-5)
Ricardo Lebensohn (MST-8)
Benjamin Hansen (T-3)
Hashem Mourad (T-3)

Ellen Cerreta (MST-8)

Characterization team:

Brian Patterson (MST-7)
Veronica Livescu (MST-8)
Juan Pablo Escobedo (MST-8)

Darcie Koller (WX-9)

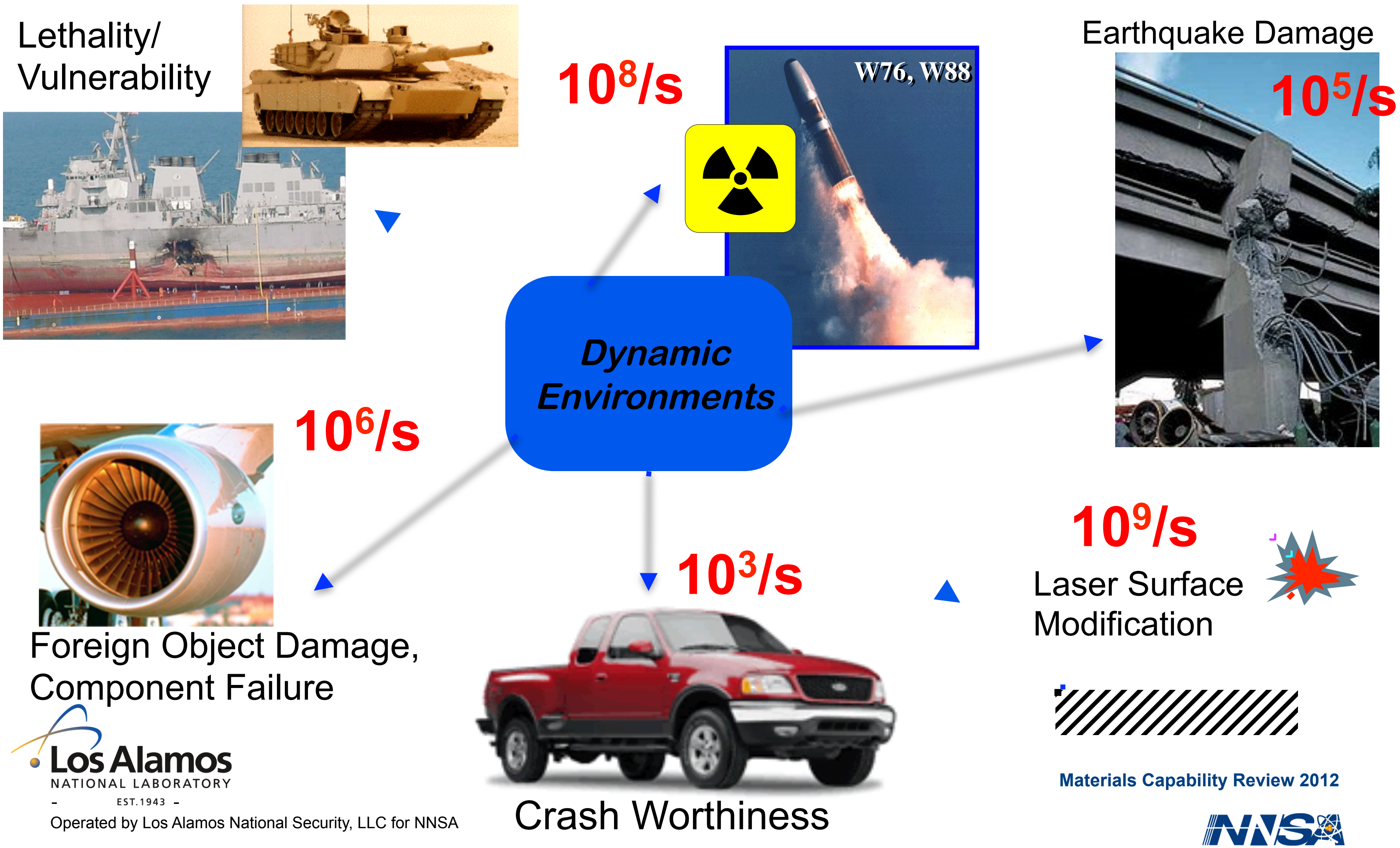
Experimental Team:

Rueben Manzanares (WX-9)
Carl Trujillo (MST-8)
Nate Sanchez (WX-9)

External Collaborators:

Yogi Gupta (WSU)
Anthony Rollett (CMU)
Robert Suter (CMU)
Richard Becker (ARL)
Eric Harstad (SNL)
David Field (WSU)

The Extreme Environment of Dynamic Loading Includes a Spectrum of Rates



Dynamic Environments

Lethality/
Vulnerability

10^8/s

Earthquake Damage

10^5/s

10^6/s

Foreign Object Damage,
Component Failure

10^3/s

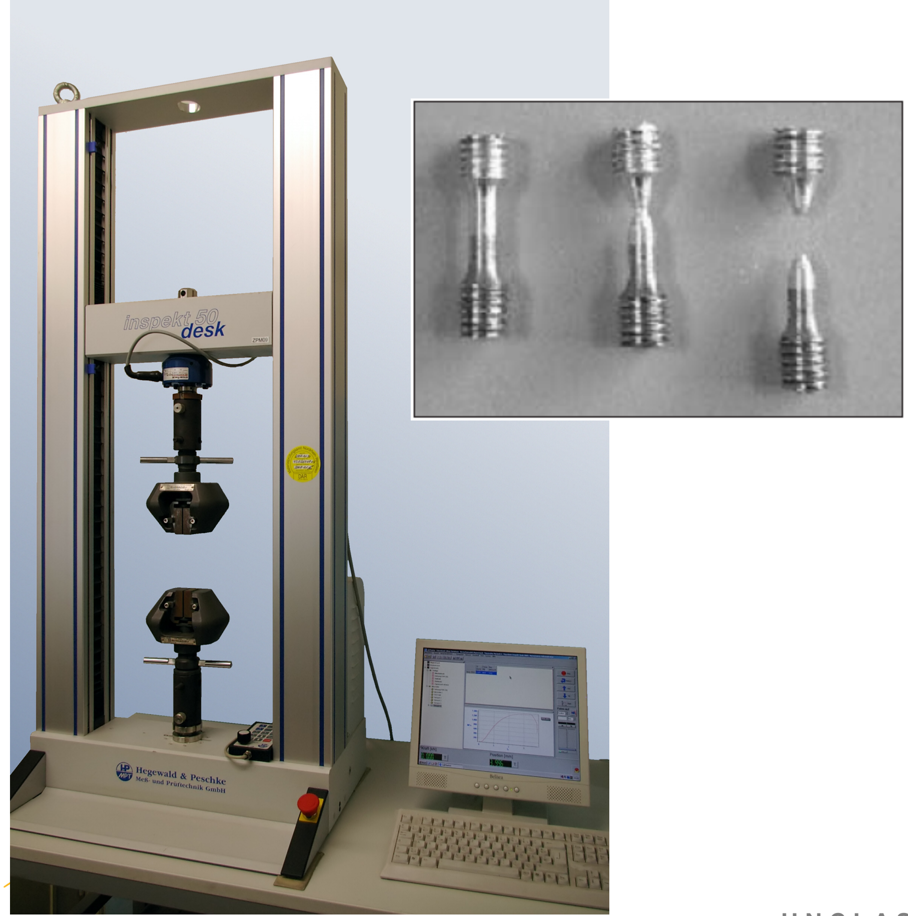
Crash Worthiness

10^9/s

Laser Surface
Modification

Small Scale Experiments are Designed to Isolate Effects of Individual Parameters

Quasi-Static Testing:

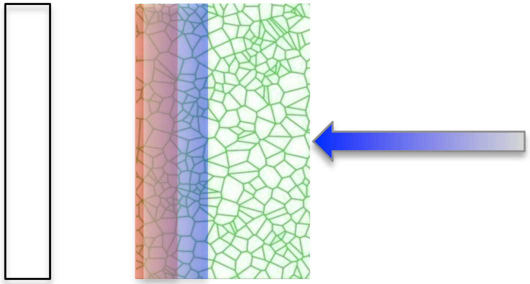


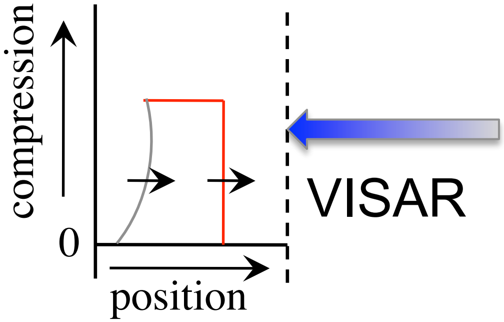
During Shock:

Sample volume under tension is unknown

Rate is not explicitly known because yielding affects wave interactions.

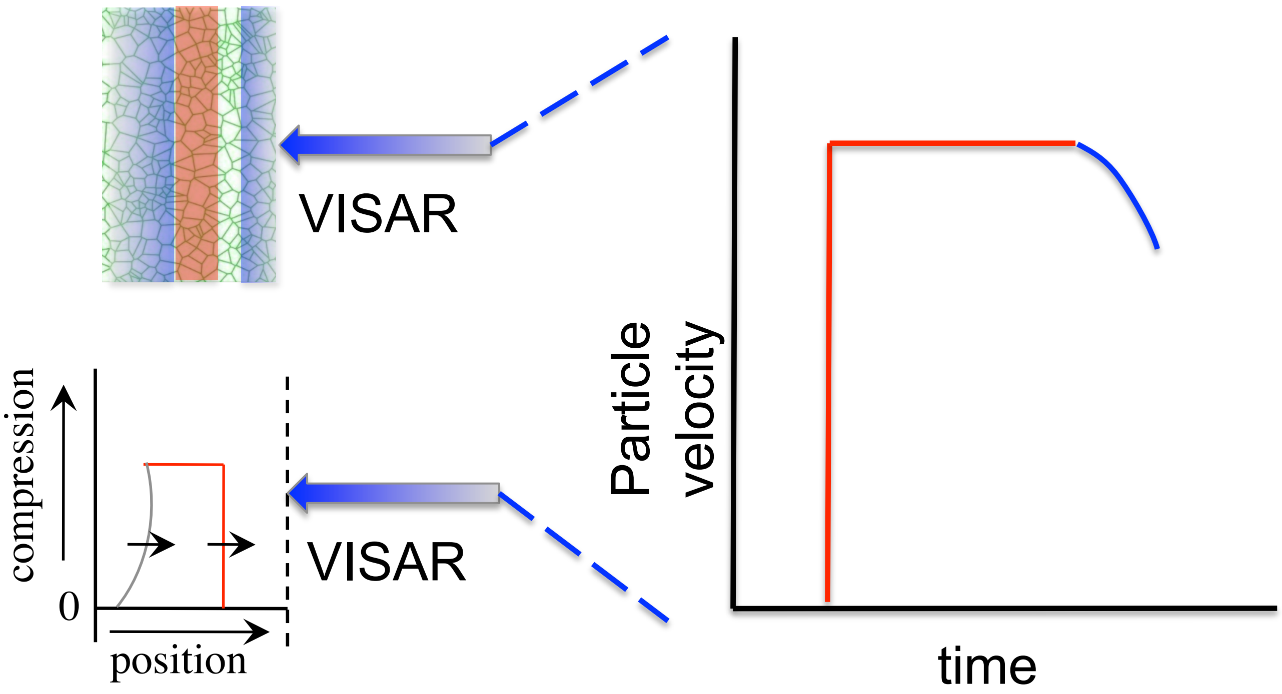
Plate Impact Experiments Enable Characterization of Dynamic Damage



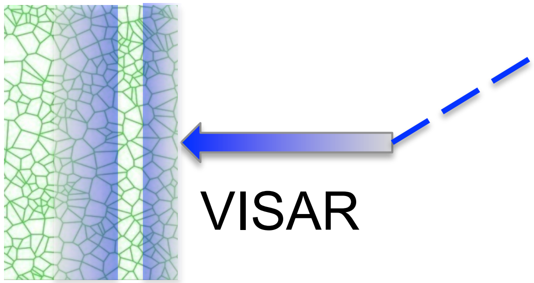


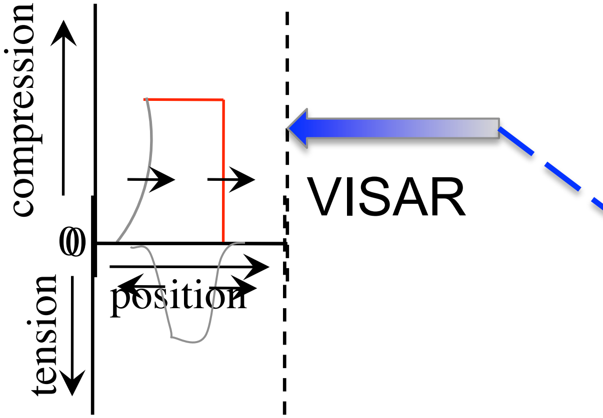
- Plate impact experiments subject materials to both compressive and unloading waves
- Their arrival at the back free surface and interaction within the bulk is examined with in-situ diagnostics

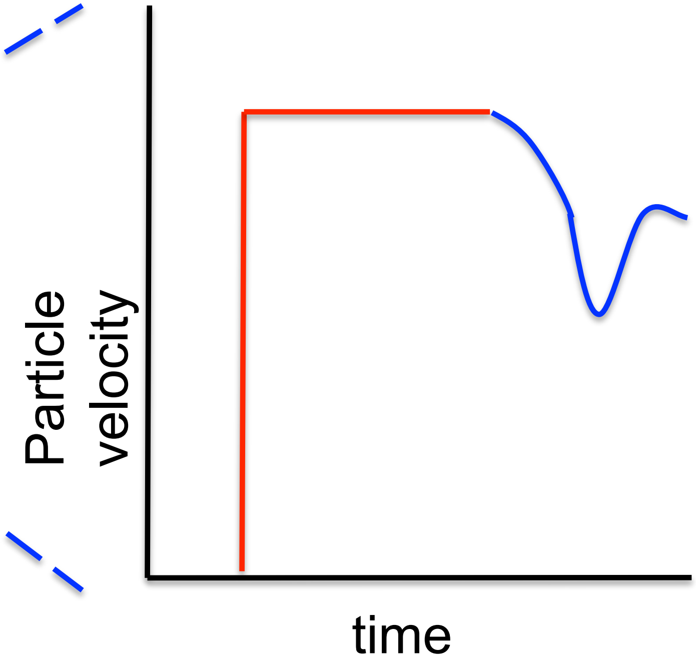
Plate Experiments Have a Complicated Unloading Scenario



Interacting Rarefactions Produce Tension that Leads to Damage

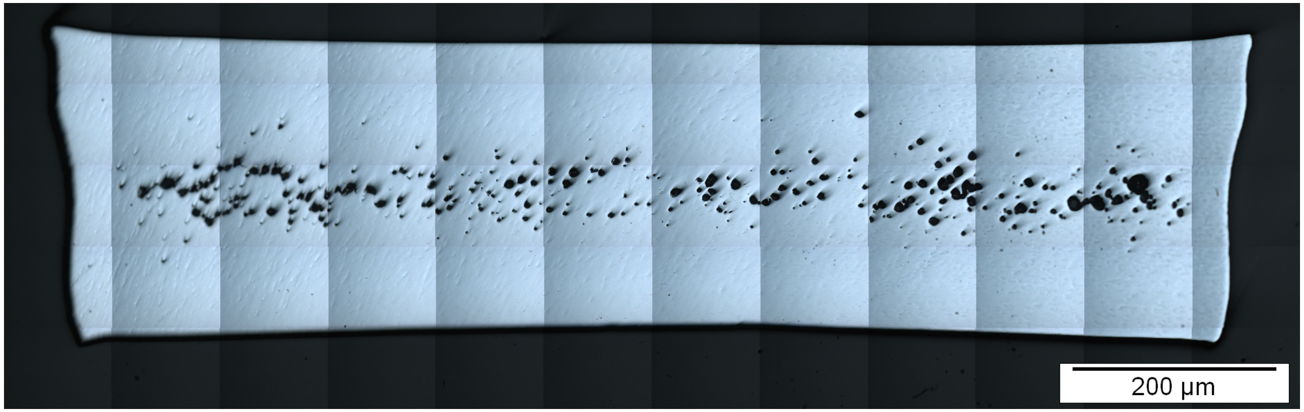




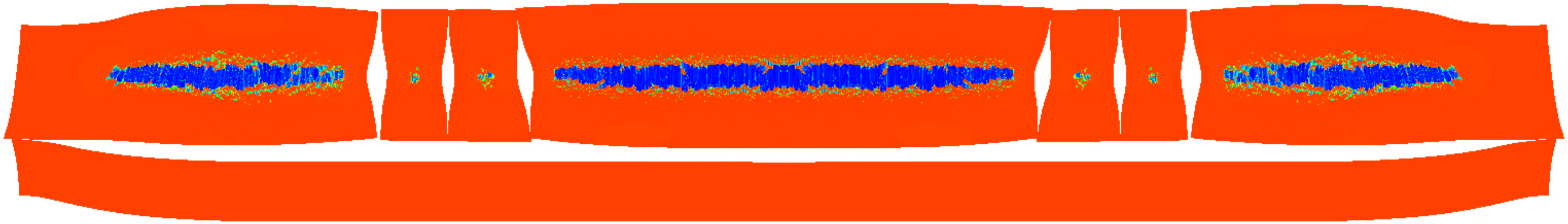


Our Current Understanding of Dynamic Damage Does Not Allow for Accurate Prediction of These Processes

Experiment



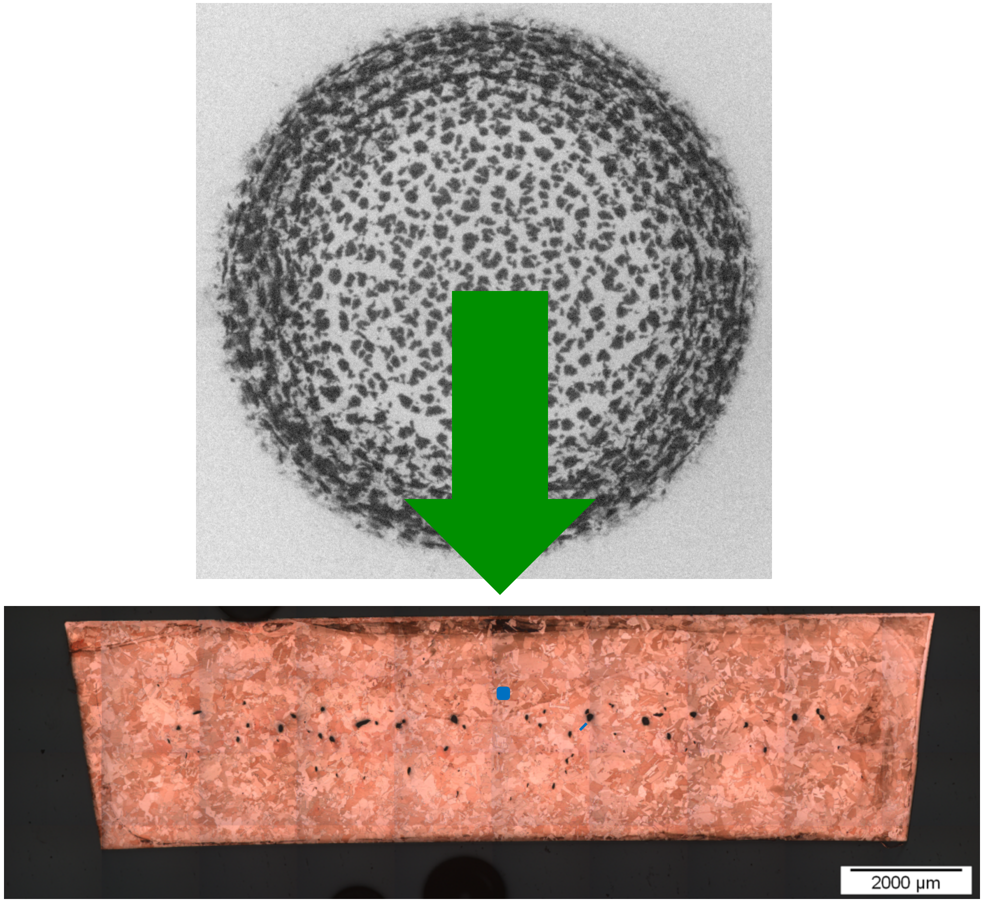
Simulation

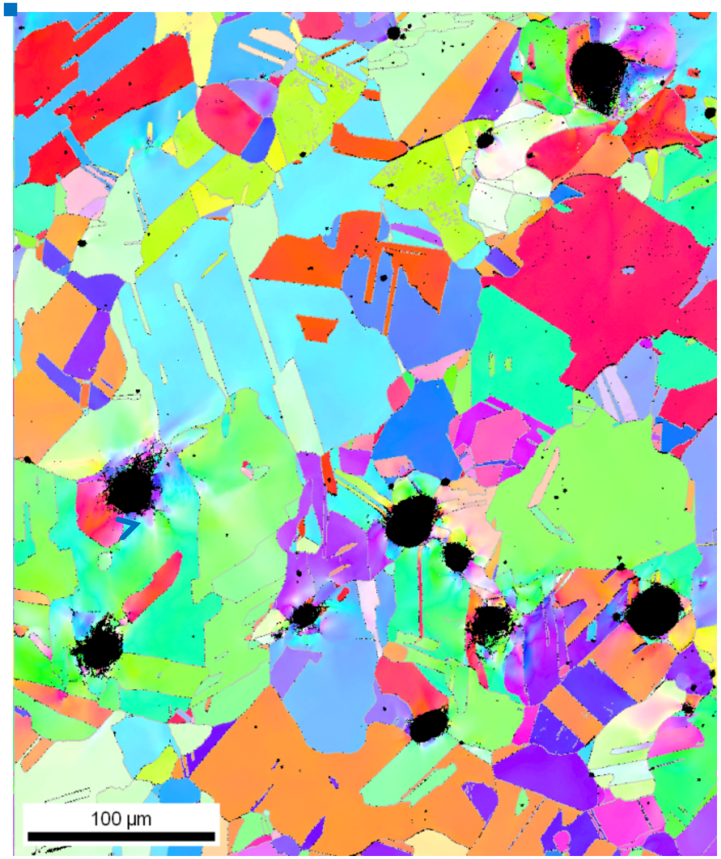


🟥 Fully Dense

🟦 Zero Density

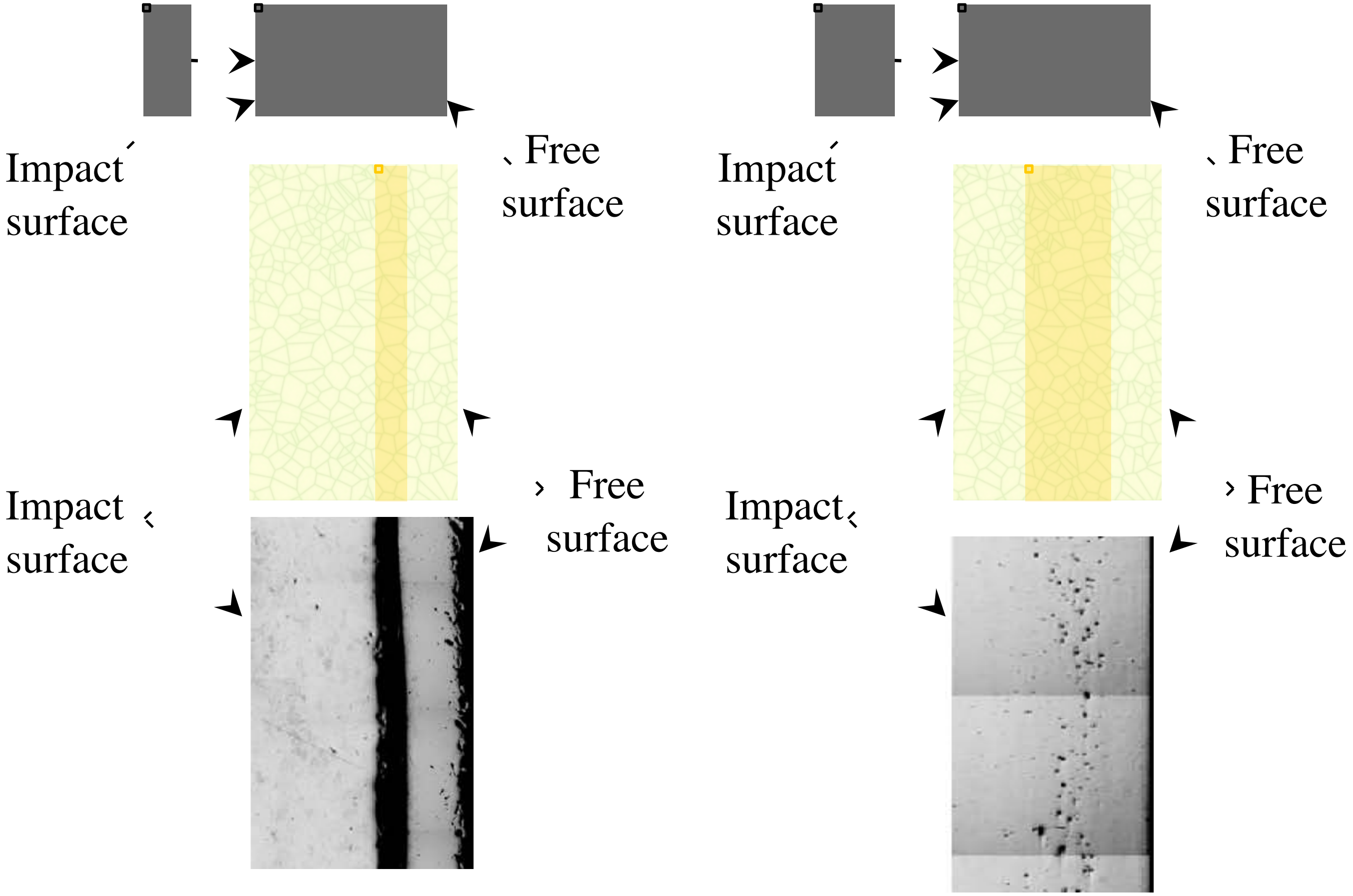
Damage Evolution has been Linked with Features of the Dynamic Loading Profile and Microstructure





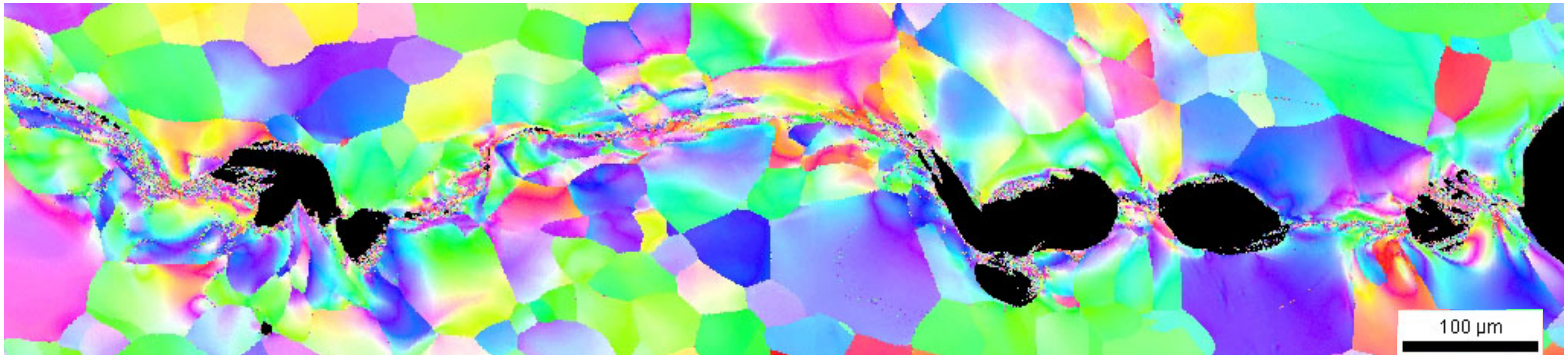
J.P. Escobedo, et al., JAP, 2011

Dynamic Drive Conditions Alter the Tensile Rate and the Volume Sampled



This has made it very difficult to separate the individual effects of microstructural length scales from the effects of kinetics on damage evolution

Key Science Questions Driving our Hypotheses



1. Can we partition deterministic processes vs. stochastic processes?
    - Focus on nucleation and growth of damage
2. Can we develop a multi-scale understanding of these processes?
    - Tie mechanistic understanding of damage phenomena to continuum observations
3. Can we capture the essential physics in our models?
    - Focus on strength and damage models

Hypotheses and Goals that Guide Our Work

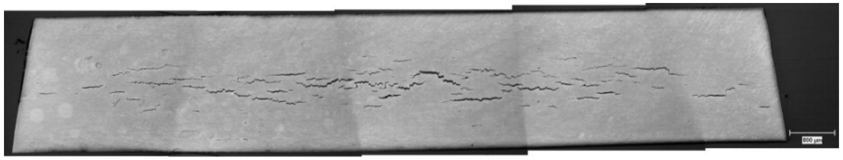
1. **Microstructural length scales are critical to dynamic damage**
   - Length scales can dictate nucleation vs. growth controlled damage
   - Mechanism for damage is influenced by feature types
2. **Kinetics affects the balance of nucleation vs. growth dominated physics**
   - Rate of tensile loading controls availability of damage mechanisms

Goals:

1. Establish kinetic and spatial considerations for dynamic damage
2. Tie meso-scale mechanisms for damage to continuum level observations
3. Guide development of physically based dynamic damage/failure models with a focus on developing meso-scale tools

The Process of Model Development is a Long Term Investment

Discovery Experiments and/or Calculations



New discovery
Requires explanation

Material Model Formulation

$$\tau - \sigma_f(\dot{\varepsilon},\theta)^2[1+q_3\phi^2 - 2q_1\phi\cosh\delta] = 0$$

Material Parameter Evaluation

Tension, compression, gas gun...

Model Validation

Taylor anvil, forced shear, HE loaded ….

Predict well ?

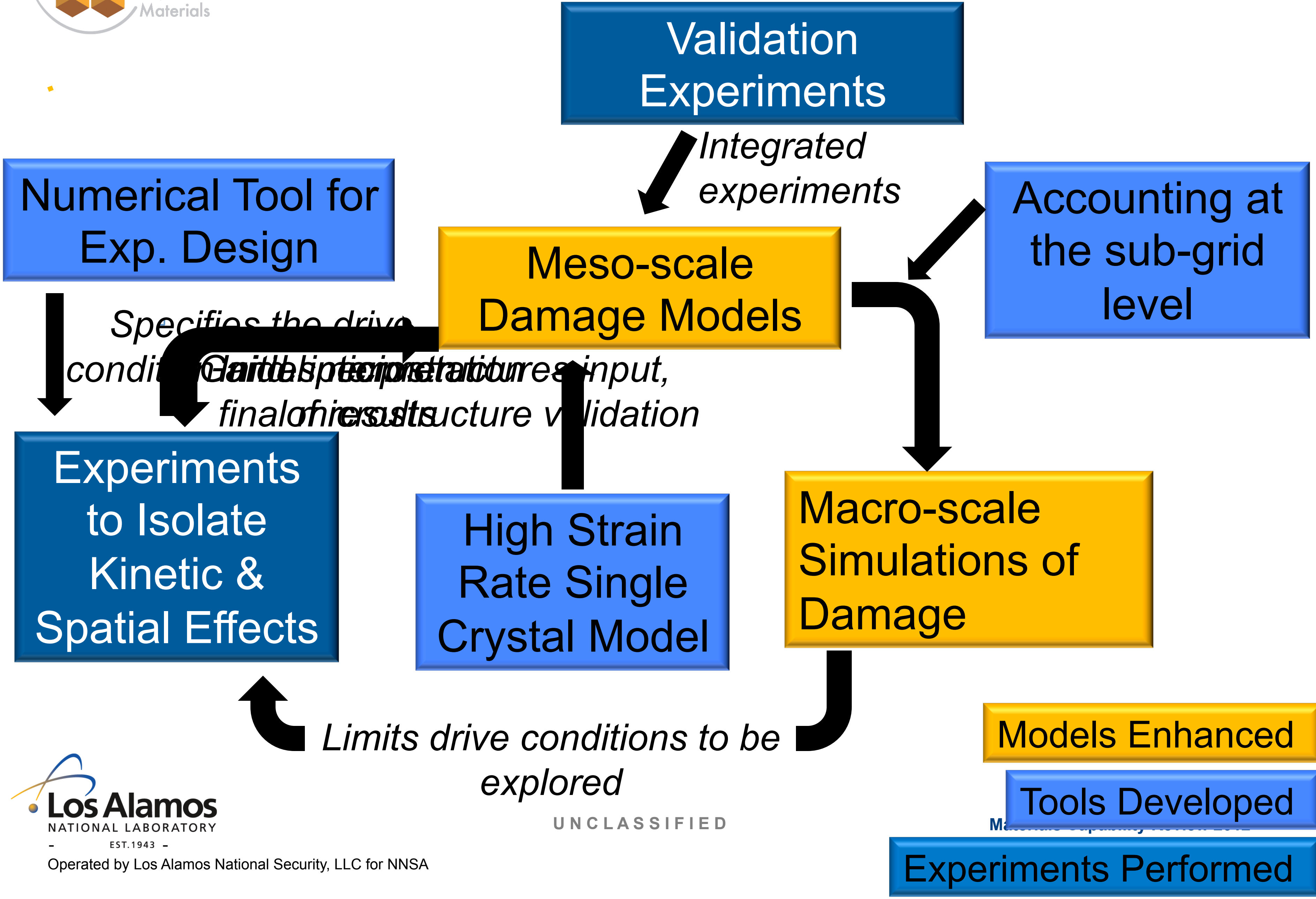
No

explain

Outstanding Dynamic Damage Model and Physics Issues

1. **The physics of ductile damage is approached as a process of nucleation, growth, coalescence, and failure.**
    1. Our models have followed a traditional approach established by Gurson-Tvergaard-Needleman.
    2. Existing macro-scale models are motivated by micro-mechanics of pore/solid interactions – not microstructure
2. **Weak representation of high-rate plastic response**
3. **Results are mesh sensitive and uniqueness of solution is an issue – lack appropriate length scale.**
4. **The role of micro-inertial effects on pore growth rate is believed to be important.**

Model Driven Approach



Validation Experiments

Integrated experiments

Numerical Tool for Exp. Design

Meso-scale Damage Models

Accounting at the sub-grid level

Specifies the drive conditions

Guides interpretation of results

Initial microstructure input, final microstructure validation

Experiments to Isolate Kinetic & Spatial Effects

High Strain Rate Single Crystal Model

Macro-scale Simulations of Damage

Limits drive conditions to be explored

Models Enhanced

Tools Developed

Experiments Performed

Scope of this Project was Designed for the Three Year Time Frame of an LDRD-DR

Theoretical & experimental approach to implement a physical understanding of kinetic & spatial effects in damage models

Task 1: Influence of Microstructural Length Scales on Damage Evolution

Task 2: Influence of Kinetics on Damage Evolution

Task 3: Computational Tool Development

Task 1: Influence of Microstructural Length Scales

What are we doing?

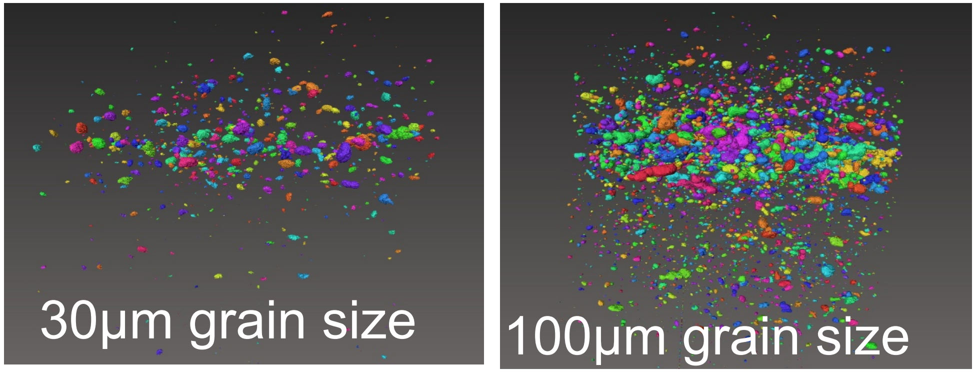
Examine the role of microstructural features suspected to be important to damage nucleation

Why do it? (Goal)

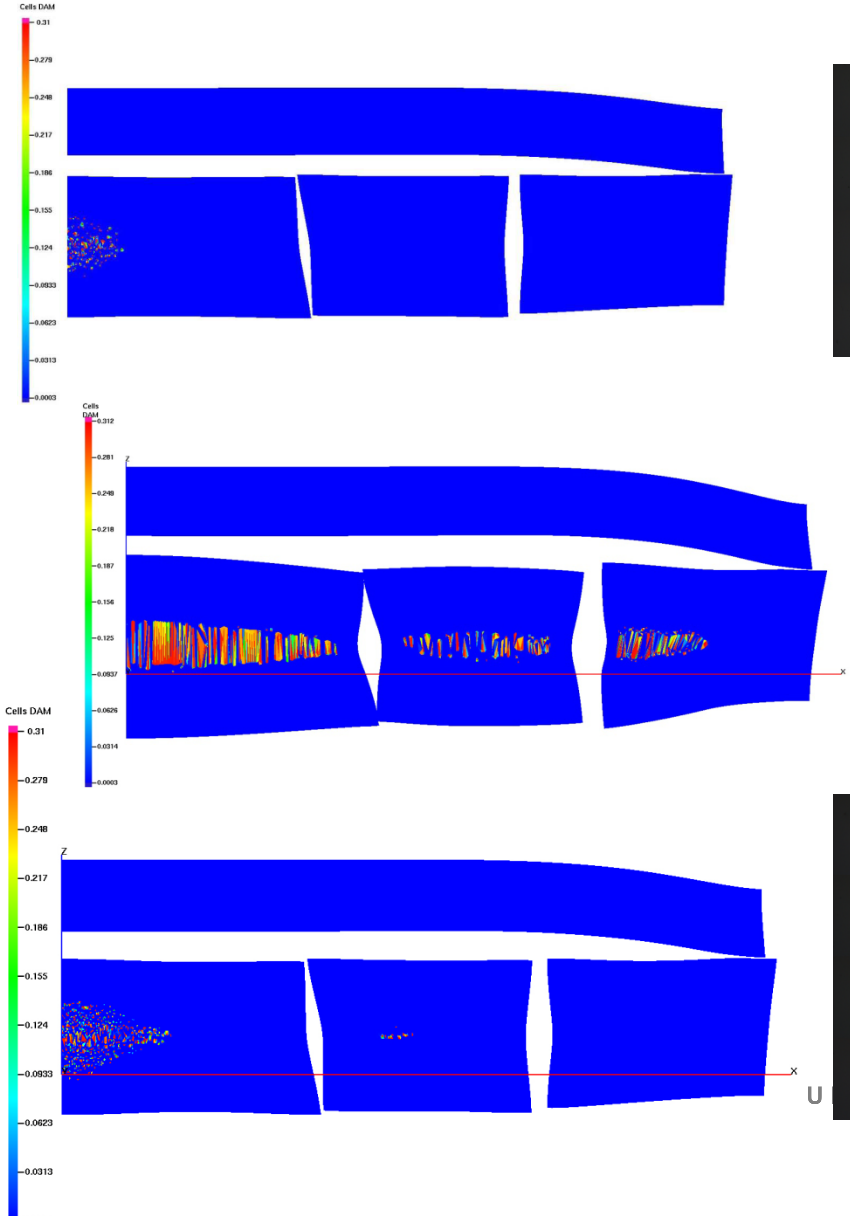
Quantify the role of microstructural length scales on damage to reveal predictable features of damage nucleation and growth

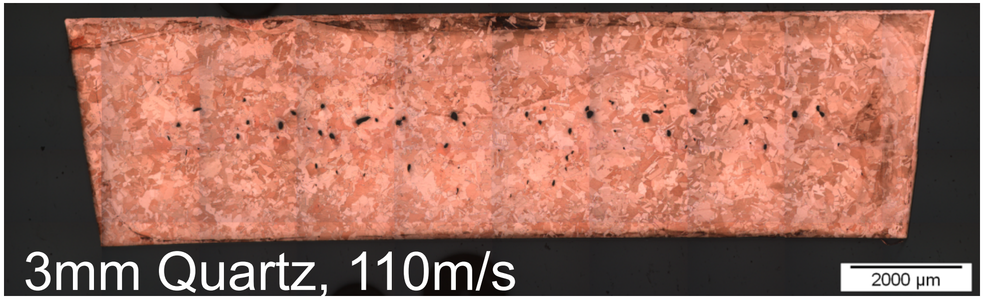
How?

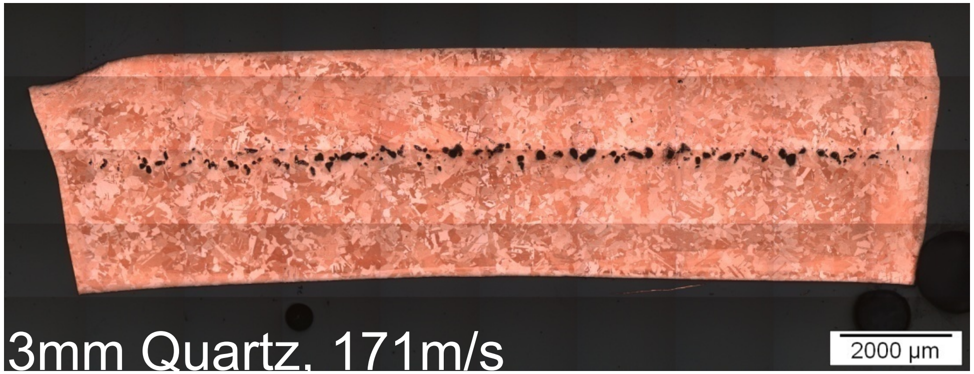
- With one drive condition, shock load 4 different, high-purity Cu microstructures (grain sizes)
- Quantify damage as a function of the changing microstructural length scale

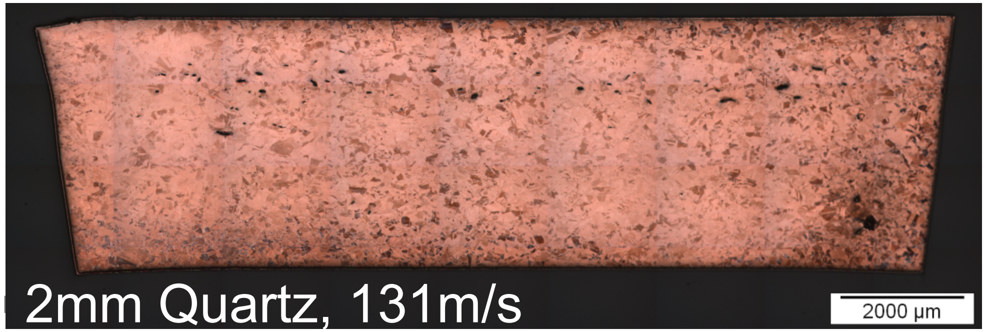


Model Driven Experiments Used to Identify Drive Conditions for Early Stage Damage

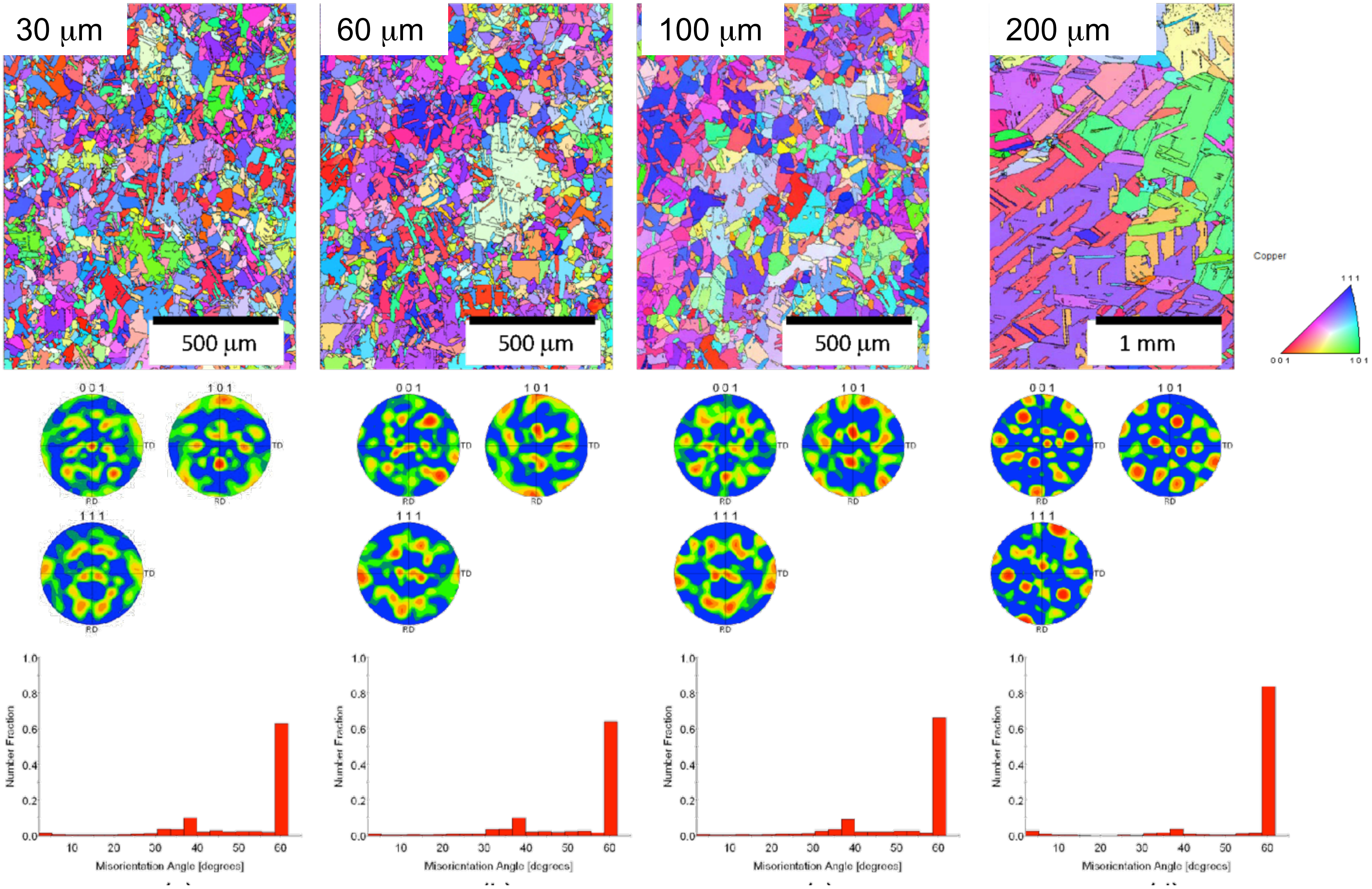



3mm Quartz, 110m/s

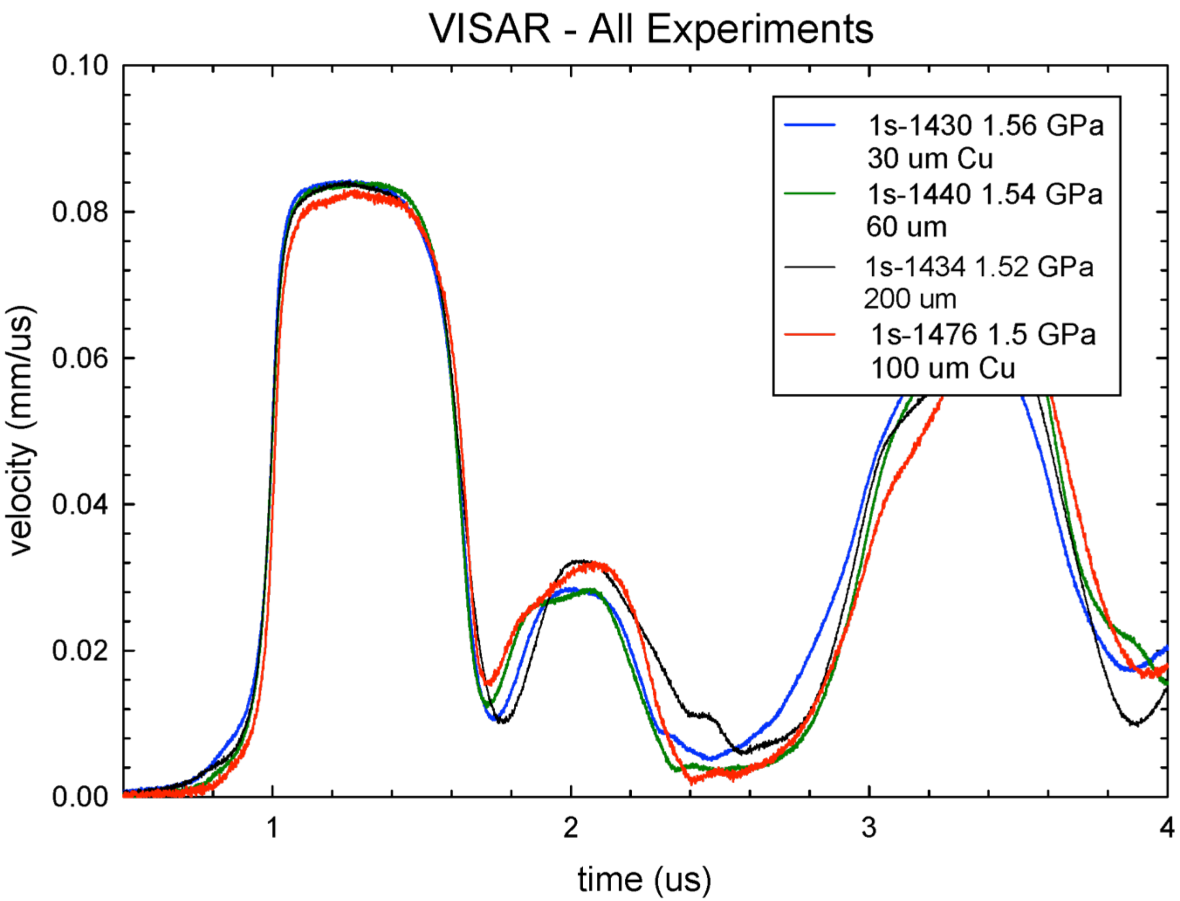

3mm Quartz, 171m/s


2mm Quartz, 131m/s

Four Microstructures Chosen for this Study



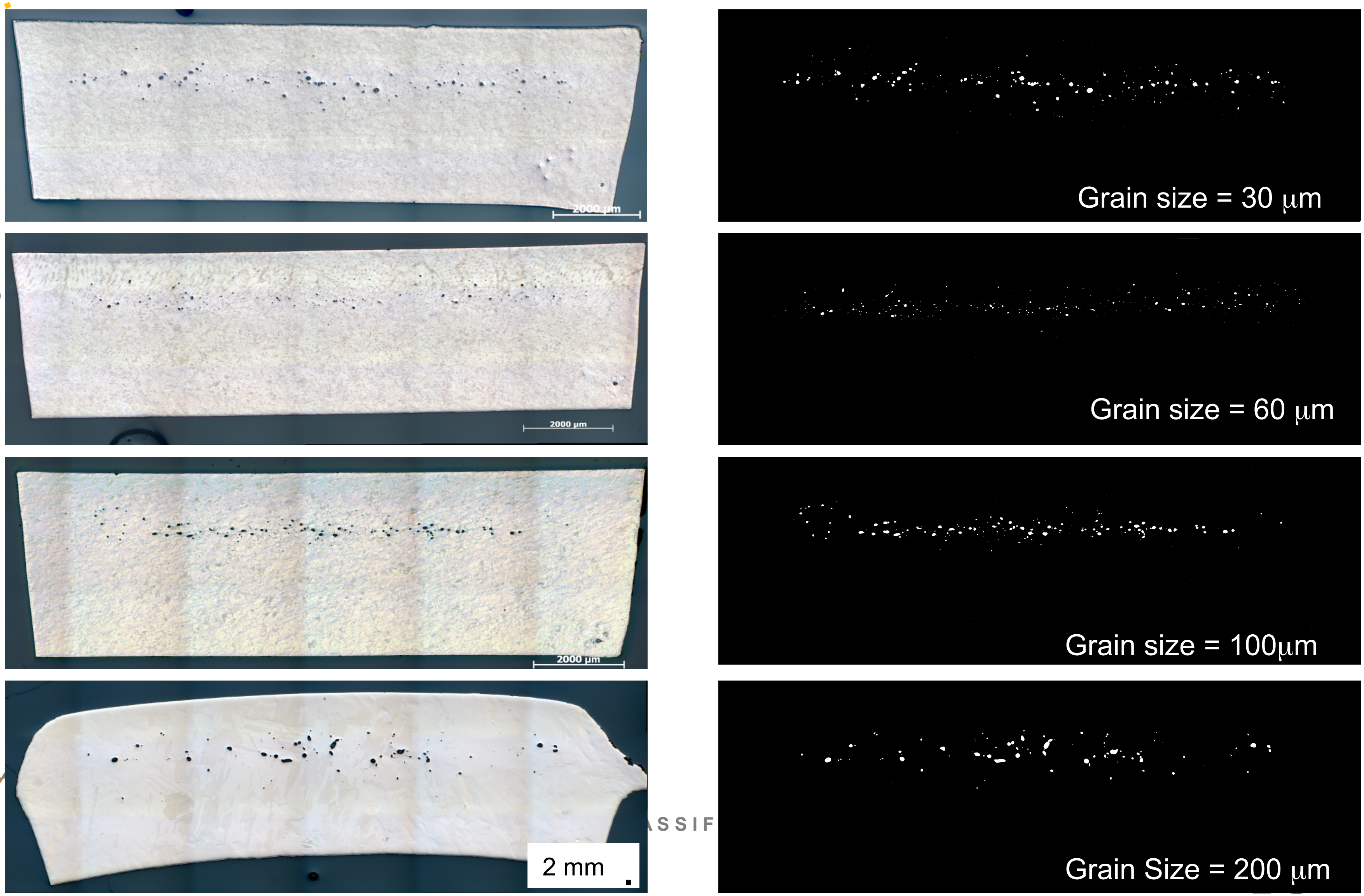
Continuum Level Measurement Suggests Similarities in Failure of the Specimens



Escobedo, et al., *Journal of Applied Physics*, 2011

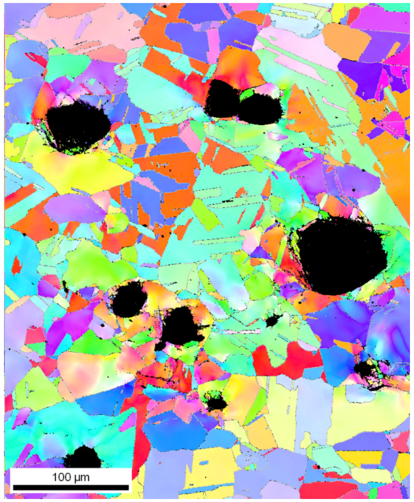
Macroscopic Damage Depends of Spatial Effect: Grain Size

Increasing Grain Size

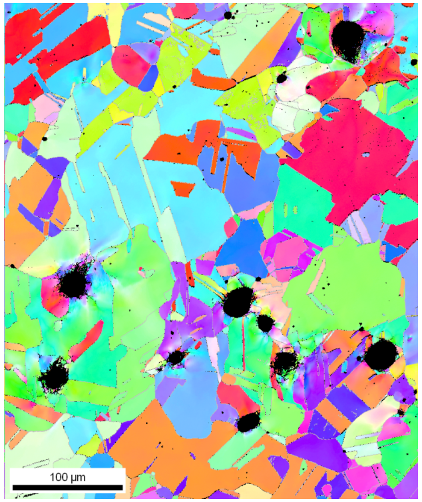


Damage Statistics are Dependent on Grain Size

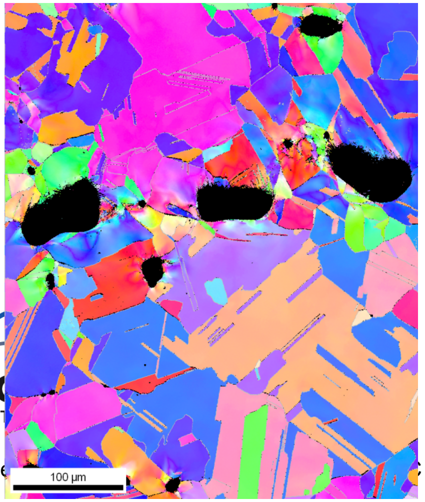
30μm



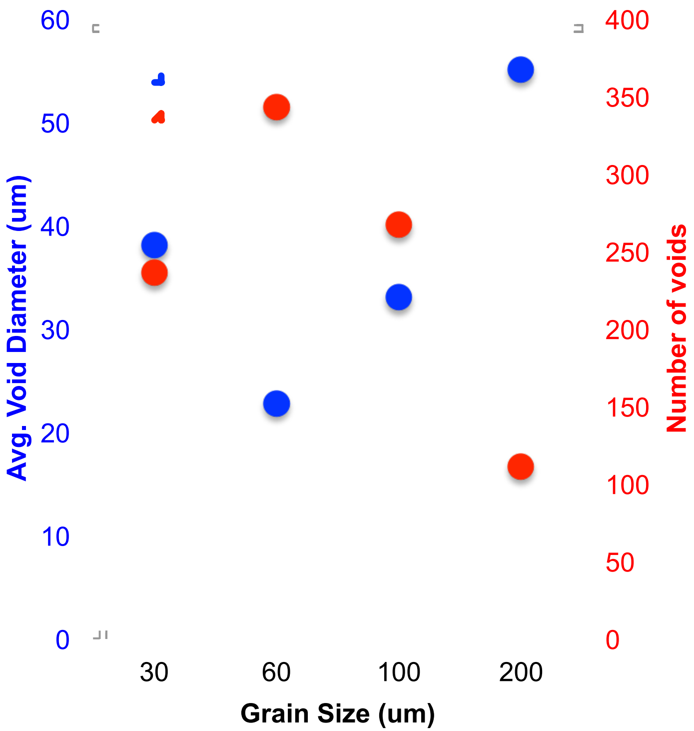
60μm



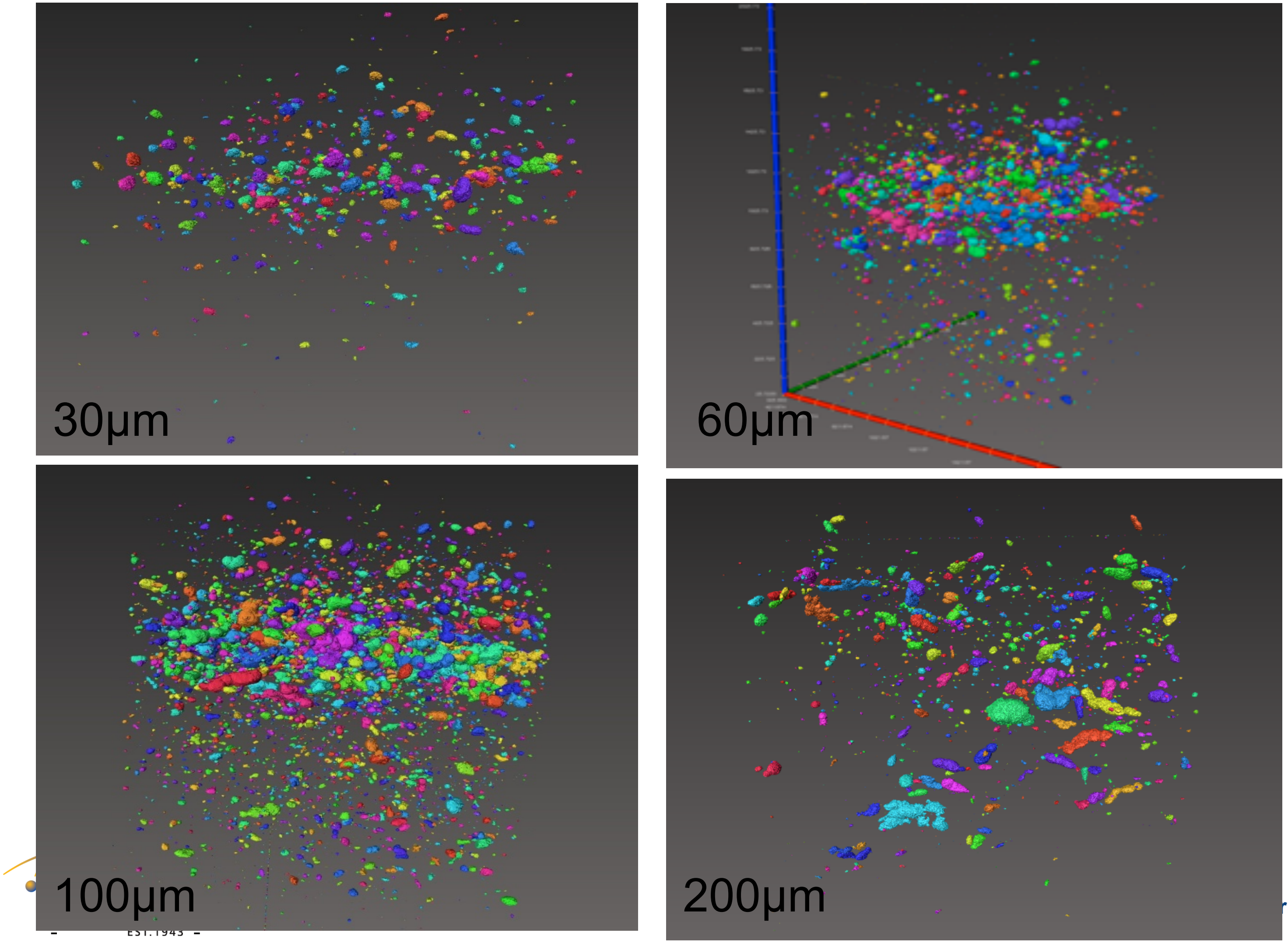
100μm



200μm

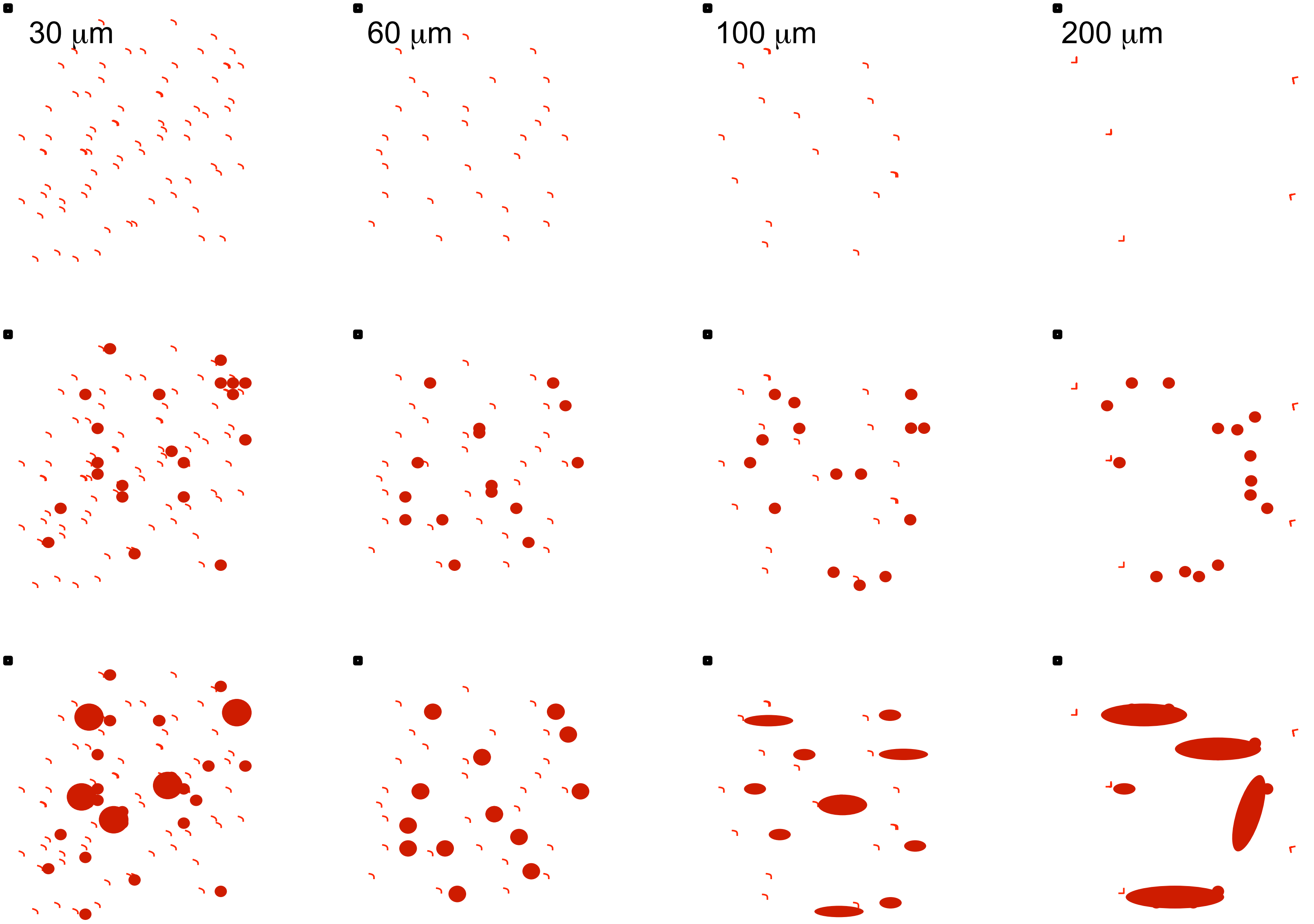


Void Growth Vs. Nucleation Controlled Growth Linked to Microstructural Length Scales



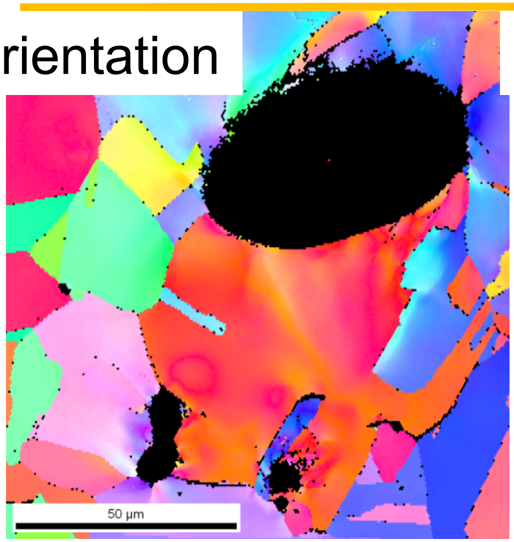
Patterson, et al. *Microscopy and Microanalysis*, in press.

Nucleation and Growth Controlled Damage Related to Boundary/Damage Proximity

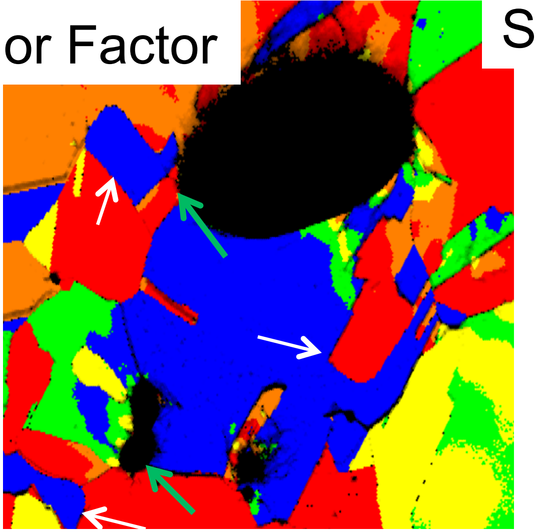


Grain Boundary Type Linked with Damage Nucleation

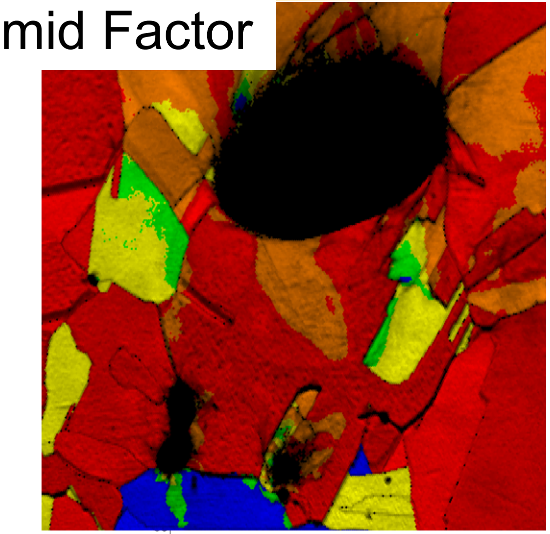
Orientation



Taylor Factor

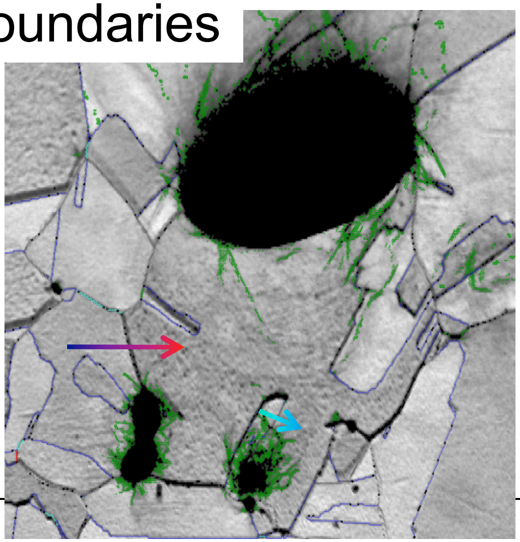


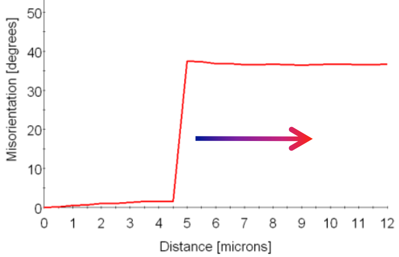
Schmid Factor

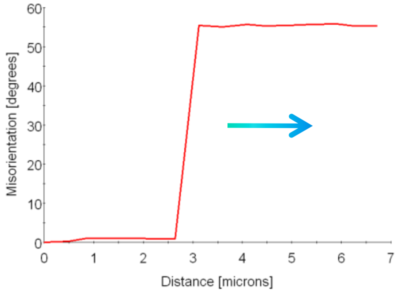


Elastic Stiffness

Boundaries

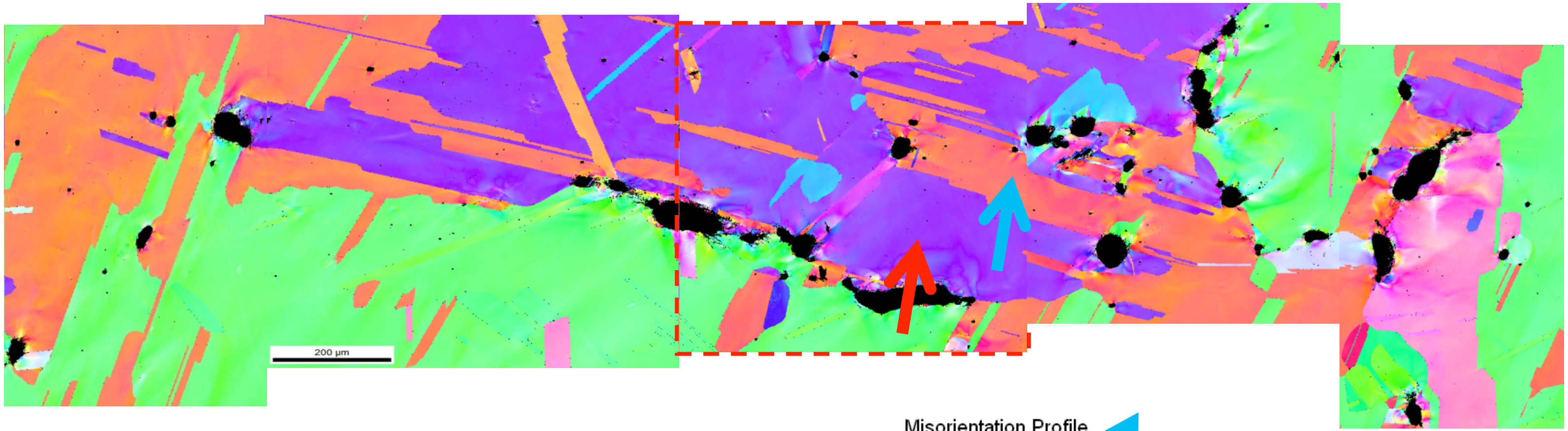


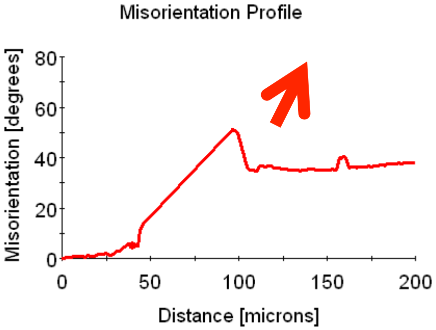


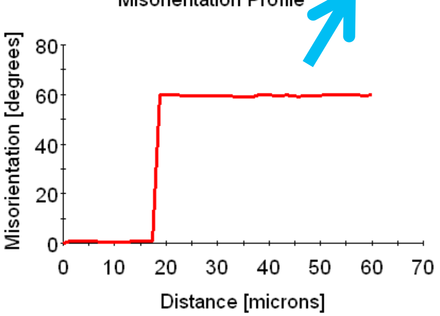


Grain Boundary Character is Critical to Damage Nucleation– Deterministic Contribution

200 μm





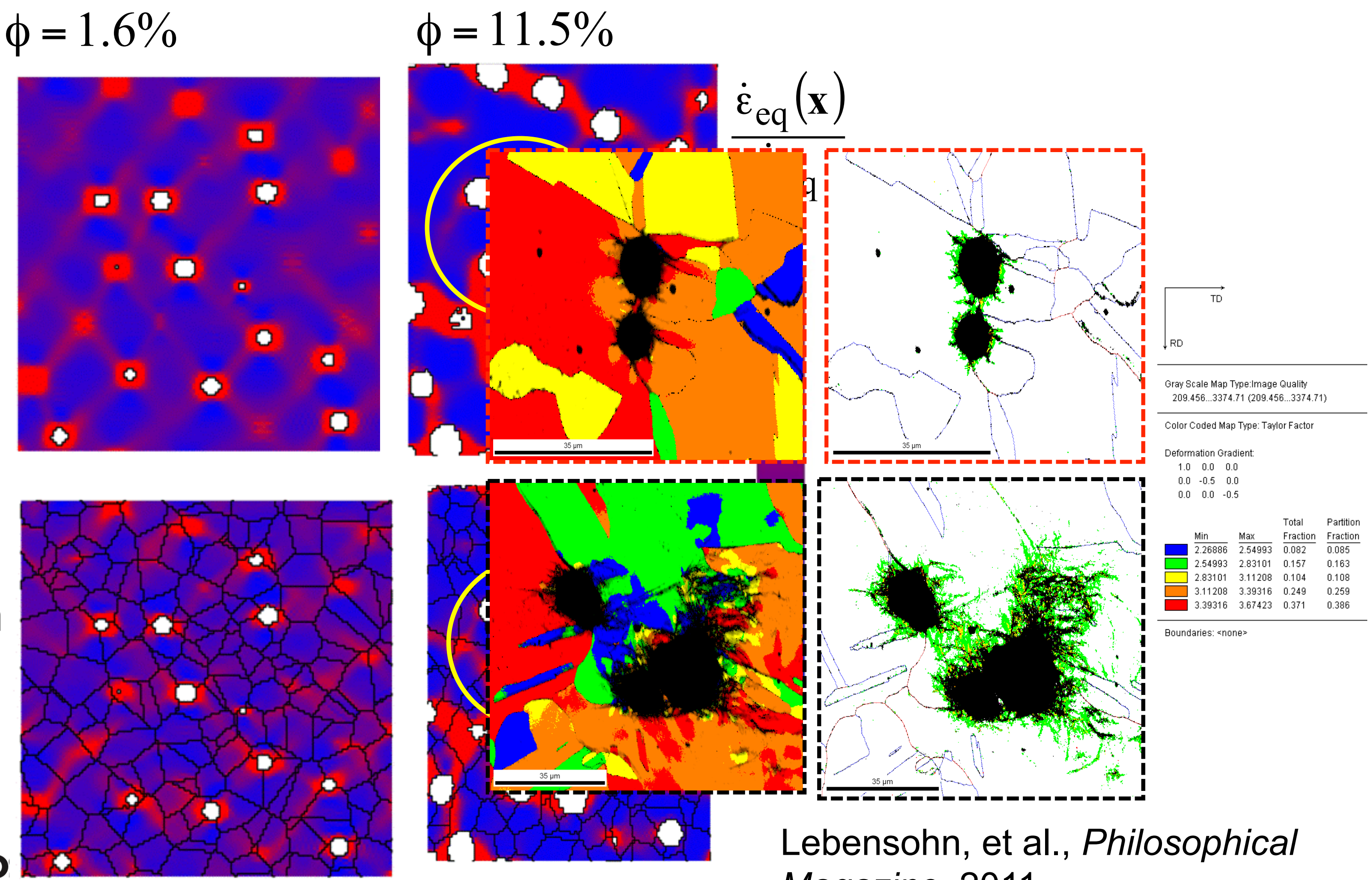


Cerreta, et al.,
Scripta Materialia.,
in press

Experiments & Simulation Reveal Microstructure (Grain Boundary Type & Orientation Neighborhoods) Control Nucleation & Growth

isotropic matrix

fcc random polycrystal



Gray Scale Map Type:Image Quality
209.456...3374.71 (209.456...3374.71)

Color Coded Map Type: Taylor Factor

Deformation Gradient:

$$\begin{matrix} 1.0 & 0.0 & 0.0 \\ 0.0 & -0.5 & 0.0 \\ 0.0 & 0.0 & -0.5 \end{matrix}$$

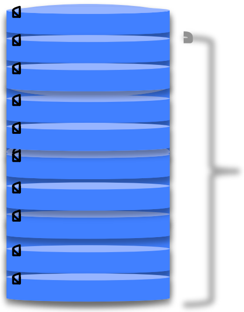
	Min	Max	Total Fraction	Partition Fraction
🟦	2.26886	2.54993	0.082	0.085
🟩	2.54993	2.83101	0.157	0.163
🟨	2.83101	3.11208	0.104	0.108
🟧	3.11208	3.39316	0.249	0.259
🟥	3.39316	3.67423	0.371	0.386

Boundaries: <none>

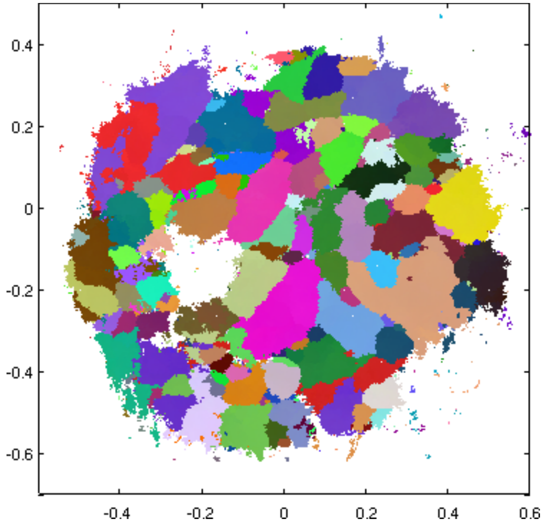
Lebensohn, et al., *Philosophical Magazine*. 2011.

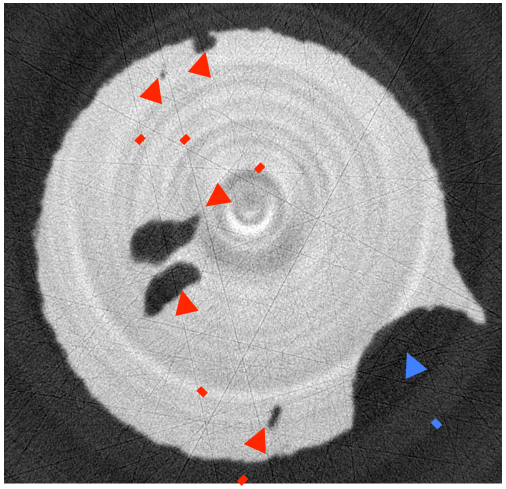
Challenges of 3D Data and Analysis Approached with Reserve Money

- **APS HEDM Experiments performed on Beam line 1-ID in collaboration with CMU and APS staff**
- **First of their kind to examine shock induced damage, largest data set collected at time of collection**



Layers assembled to form the 3D reconstruction

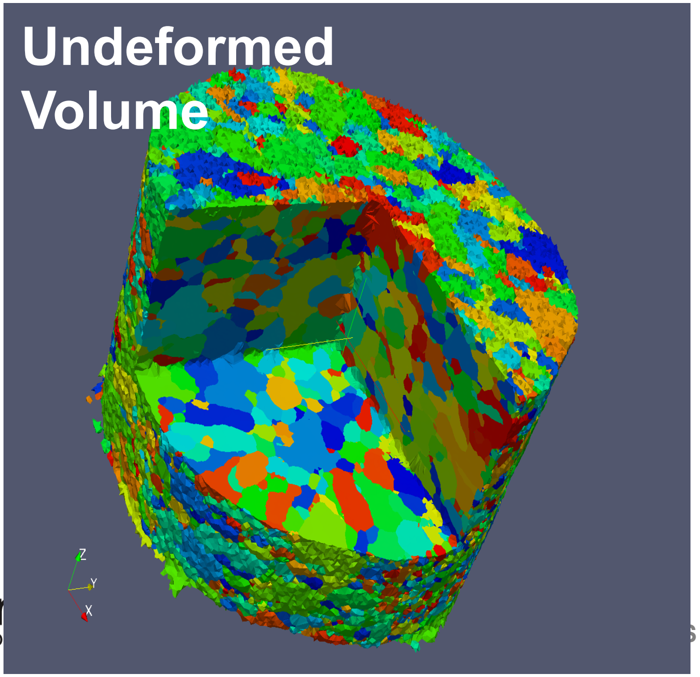




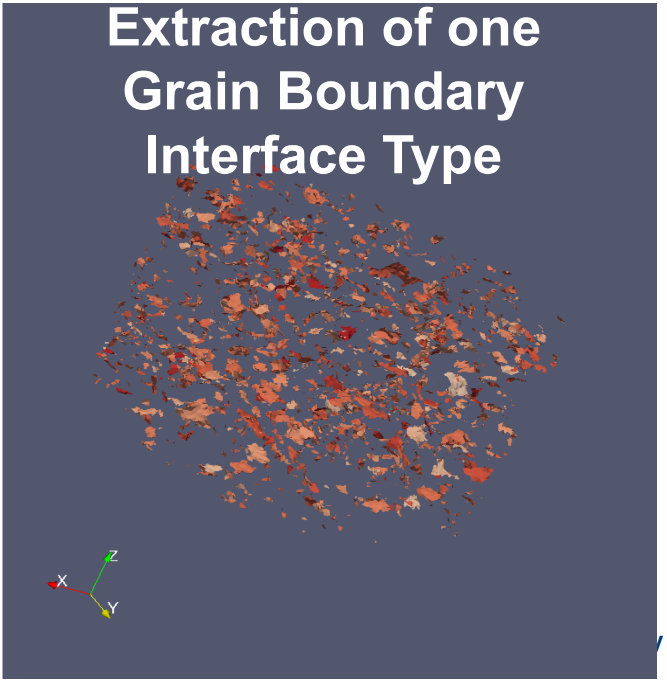
Tool Development for 3D data Correlation has Begun and Continues in Related Projects

The grain boundary network and grains have a complex structure, how do we extract features to explain relationships between structure & damage?

Approach: Use hierarchical representations of 3D data sets to capture multi-length scale nature of microstructure-damage relationships



Undeformed Volume



Extraction of one Grain Boundary Interface Type

Task 2: Influence of Kinetics on Damage Evolution

What are we doing?

Examine the role of tensile rate on damage nucleation while holding spatial distribution of defects constant

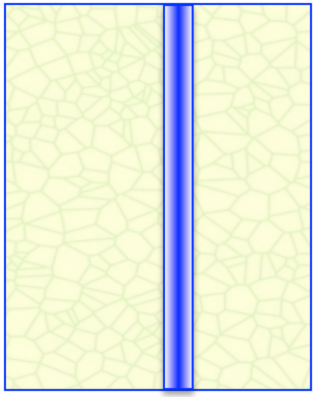
Why do it? (Goal)

Quantify the unique role of kinetics on damage to capture transitions between nucleation vs. growth dominated damage

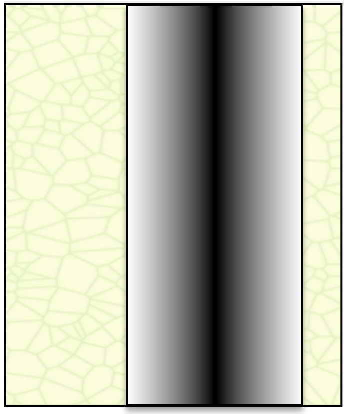
How?

- Utilize numerical simulation to determine rate of tension and sampled volume for a specific drive condition
- Alter microstructure to hold the number of defects in the sampled volumes constant

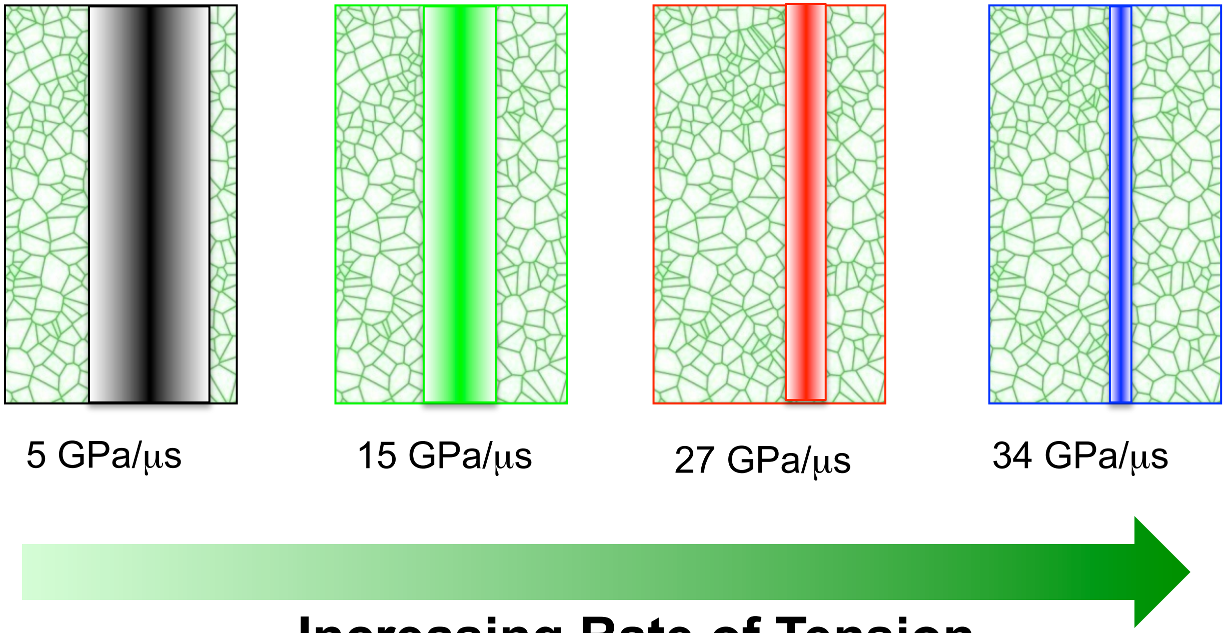
34GPa/μs



5 GPa/μs



Tensile Pulse Rate Experiments Require Control of Defect Density



5 GPa/μs

15 GPa/μs

27 GPa/μs

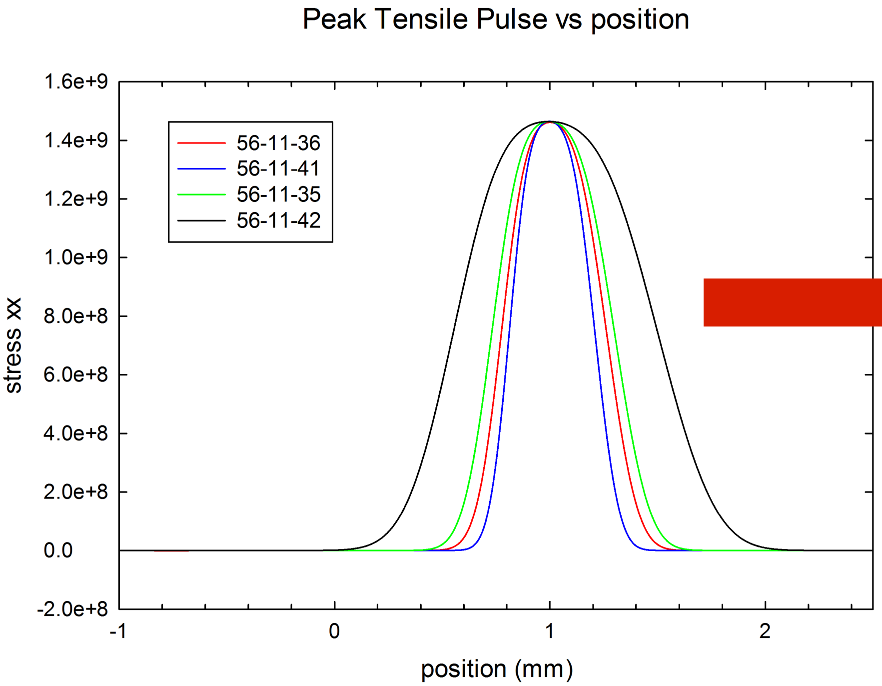
34 GPa/μs

Increasing Rate of Tension

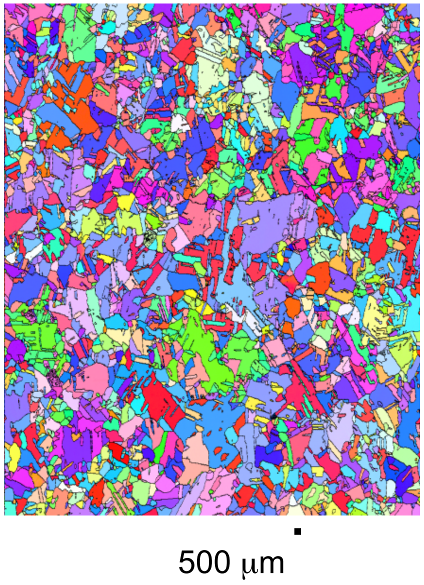
We rely on theoretical tools to design experiments that limit the parameters changed between experiments

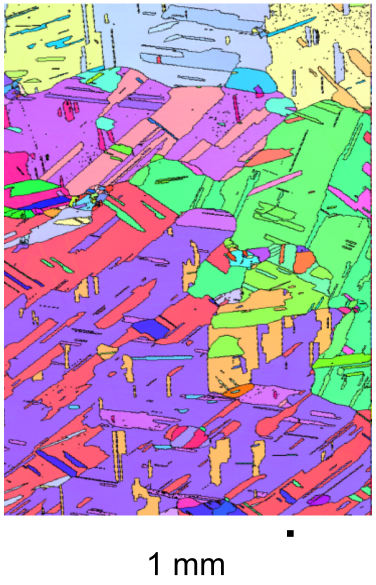
Experiments that Mimic Calculated Tensile Rate, Display Differing Compressive Pulse Durations

Calculation Used to Design the Experiment


Peak Tensile Pulse vs position

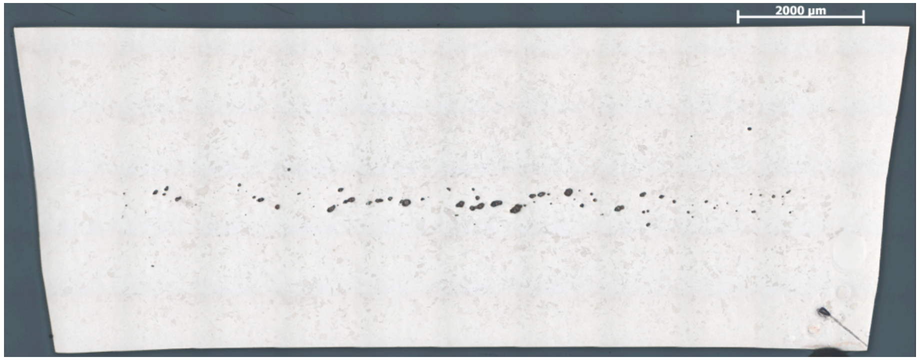
Microstructural Processing





Tensile Rate Affects Damage Evolution

Increasing Rate



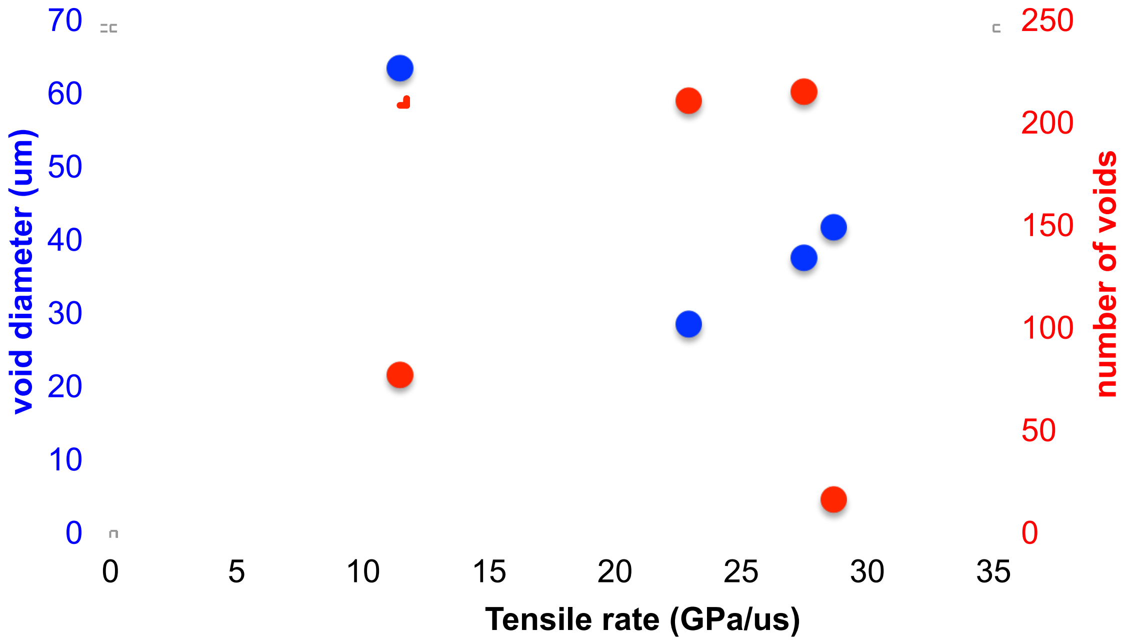
11.47 GPa/μs, 150 μm, **V_A = 0.698%**

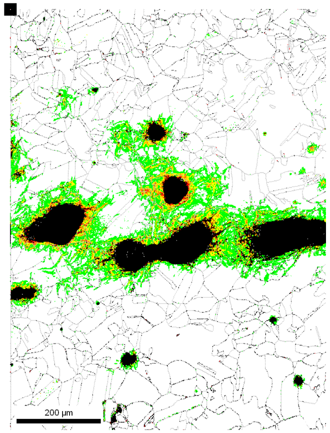
27.50 GPa/μs, 100 μm, **V_A = 0.819%**

22.94 GPa/μs, 100 μm, **V_A = 1.306%**

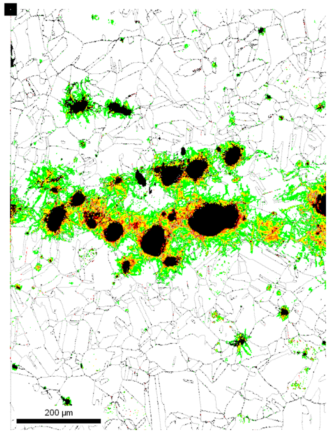
28.68 GPa/μs, 60 μm, **V_A = 0.148%**

Kinetics Effects on Plasticity Are Important to Damage Nucleation and Growth

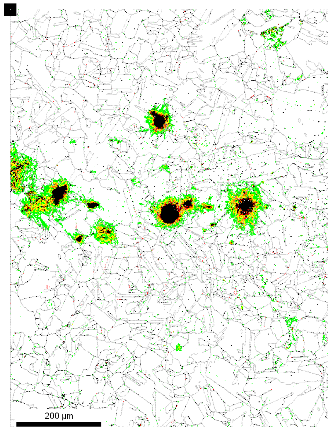




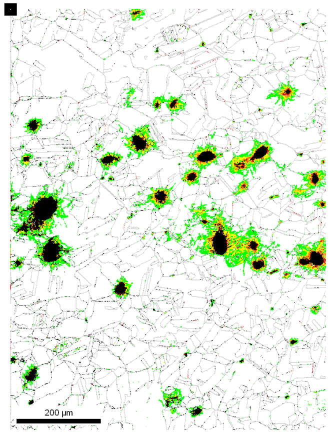
11.47 GPa/µs
V_A = 0.698%



22.94 GPa/µs
V_A = 1.306%



28.68 GPa/µs
V_A = 0.148%



27.50 GPa/µs
V_A = 0.819%

Task 3: Computational Tool Development

What are we doing?

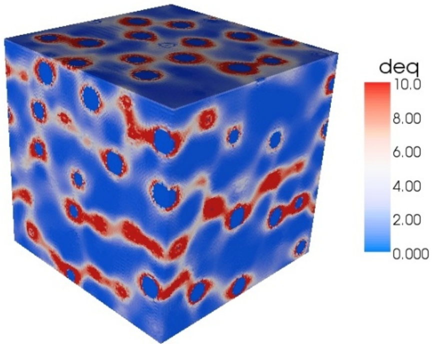
Develop the framework for capturing meso-scale phenomenon with continuum simulations in a computationally efficient manner

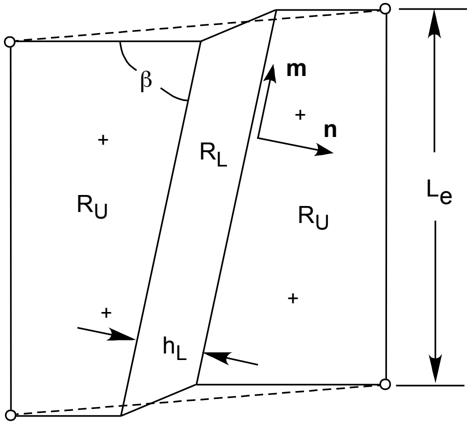
How?

- High rate single crystal plasticity model must be developed
- Framework for subgrid accounting of meso-scale processes must be developed

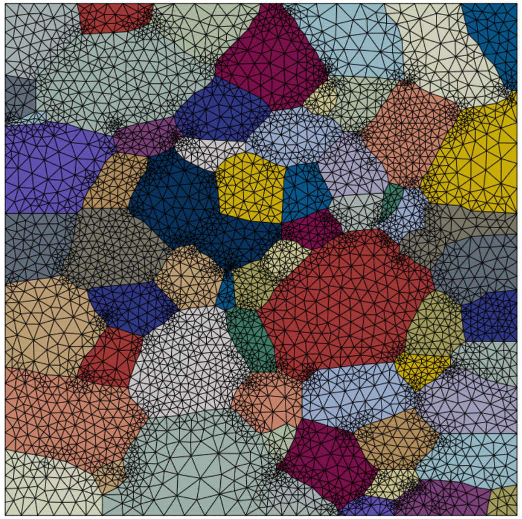
Why do it? (Goal)

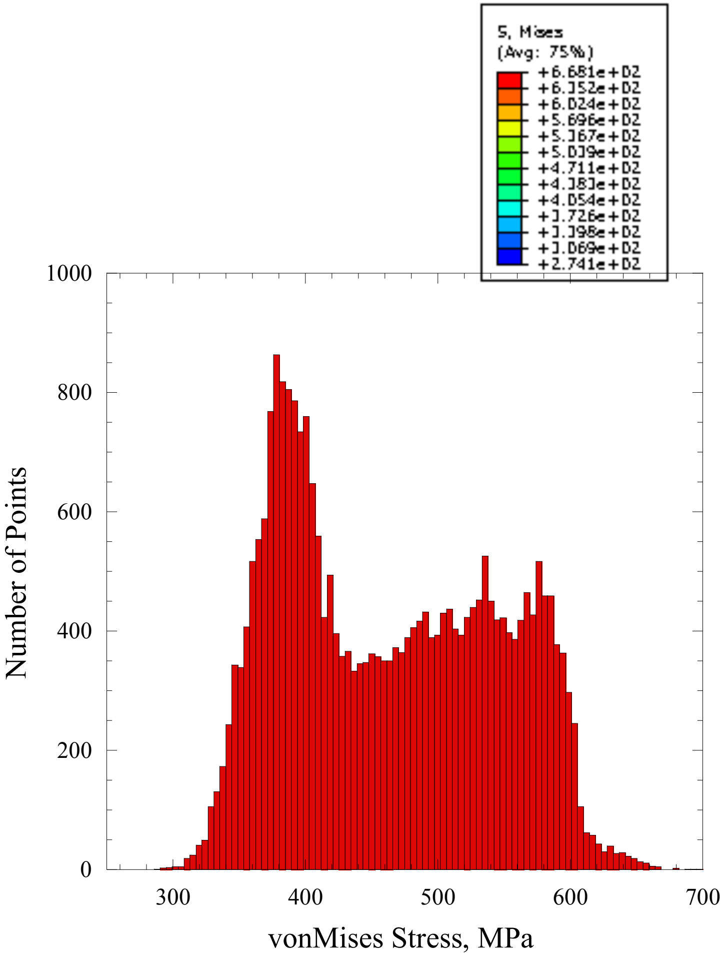
The physics of meso-scale processes drives failure but current continuum level frameworks need to readily incorporate this

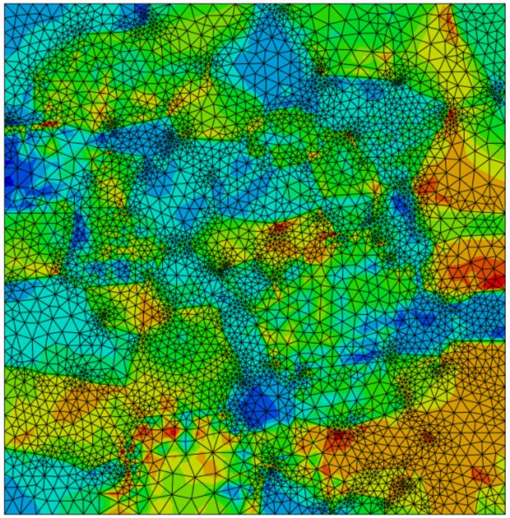




Meso-Scale Models Link Experiments and Macro-Scale Model Representation







New Single Crystal Model for High Rates has been Developed

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \exp\left[-\frac{F_0}{k\theta}\left\langle 1-\left\langle \frac{\left|\tau^{\alpha}\right| - s^{\alpha}\frac{\mu}{\mu_0}}{s_l^{\alpha}\frac{\mu}{\mu_0}} \right\rangle^{p} \right\rangle^{q}\right] \operatorname{sgn}\left(\tau^{\alpha}\right)$$

Previous model valid 10^4/s or less

New single crystal model developed for strain rates exceeding the thermally activated range, model valid through 10^6/s and higher

$$\dot{\gamma}_{\alpha} = b\rho_{\alpha}^{M} v_{\alpha} \qquad v_{\alpha} = \frac{\tau_{\alpha} b}{B}$$

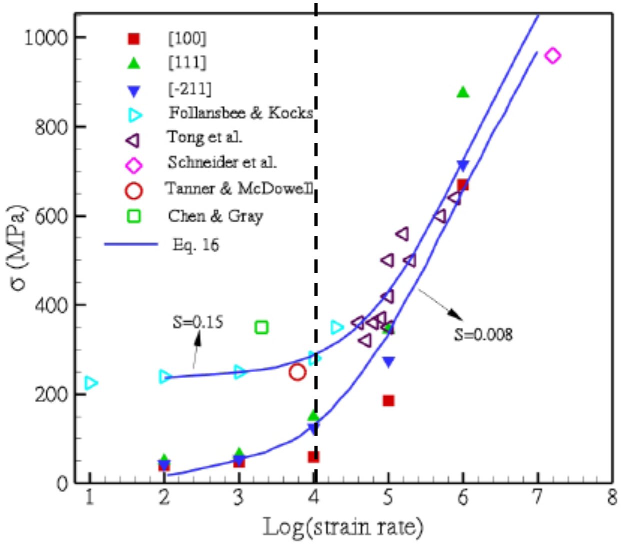
$$\dot{\rho}_{\alpha}^{M} = \dot{\rho}_{\alpha}^{gen} + \dot{\rho}_{\alpha}^{prop} + \dot{\rho}_{P\alpha}^{esc} - \sum_{inter} \dot{\rho}_{M\alpha}^{inter}$$

Thermal Activation Dominated

10^4

Drag Dominated

Plastic flow behavior changes at a strain rate of ~10^4 sec^{-1}



Based on modeling direct interaction of dislocations which improves validation.

-Wang and Beyerlein

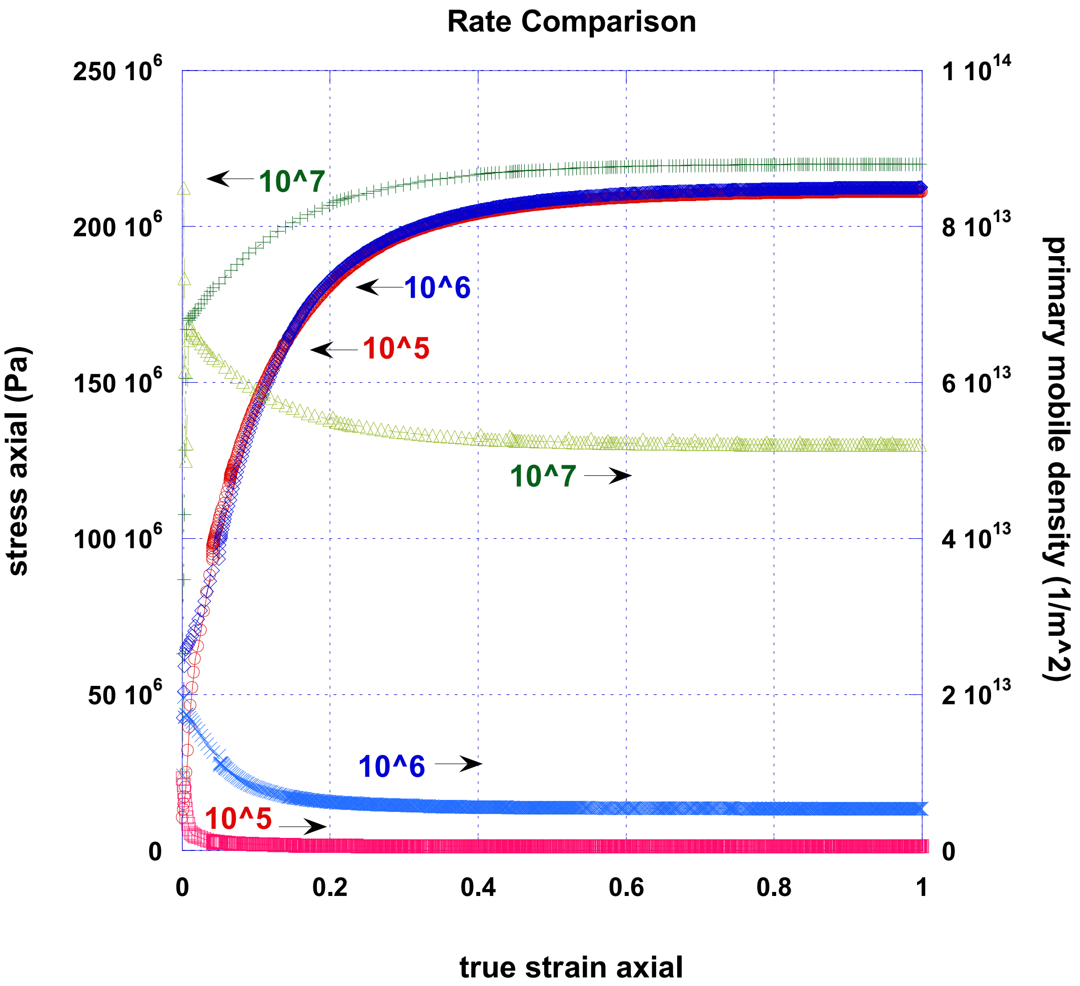
Highlights of New Dislocation-based Plasticity Model

- Dislocation densities modeled directly for comparison to experimental quantities.
- Includes latent hardening, thermal softening and kinetic effects
- Easily adjustable dislocation populations interactions – for varying materials.
- Inherent transition from high-rate drag-dominated to low-rate thermally activated dislocation motion.
- Statistical representation of dislocation evolution
  - Physical parameters such a dislocation densities and interaction distances modeled.

Current focus on FCC materials

Single Crystal Model Yields Dislocation Densities as a Function of Strain Rate

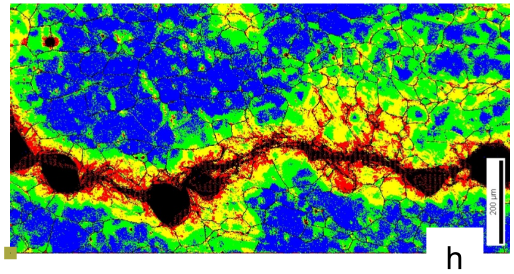
Cu 001 Single Crystal

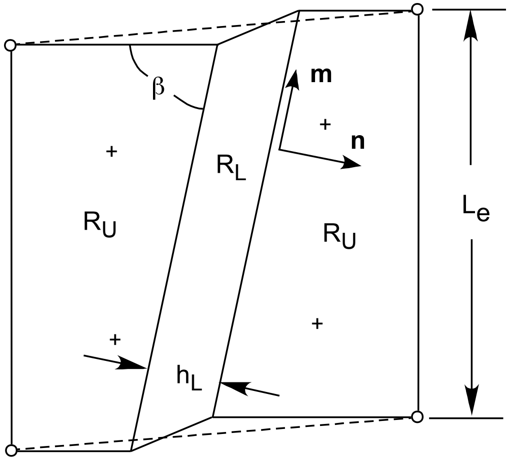


Void Growth And Coalescence Can be Dominated By Localization Behaviors

- Failing to represent localization behavior correctly leads to mesh-dependent results
- Conventional finite element tools must explicitly resolve localization bands
  1. a priori knowledge of the band location and orientation
  2. a prohibitive level of mesh refinement

- To circumvent this:
  1. a material stability analysis is used to detect the onset of strain localization
  2. localization bands are embedded within larger computational elements.





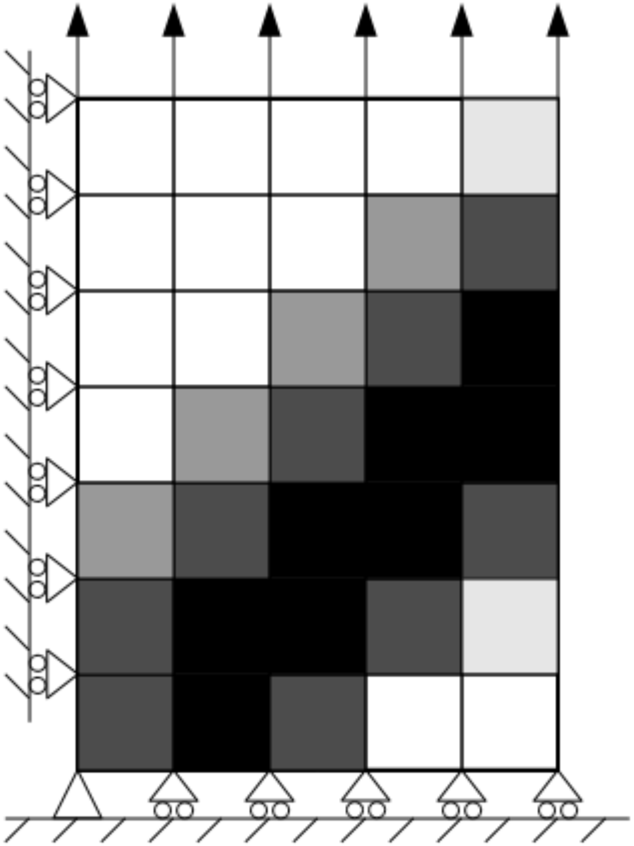
Material Stability Analysis, Hill 1962

Thus, the band width and the element size are separate parameters.

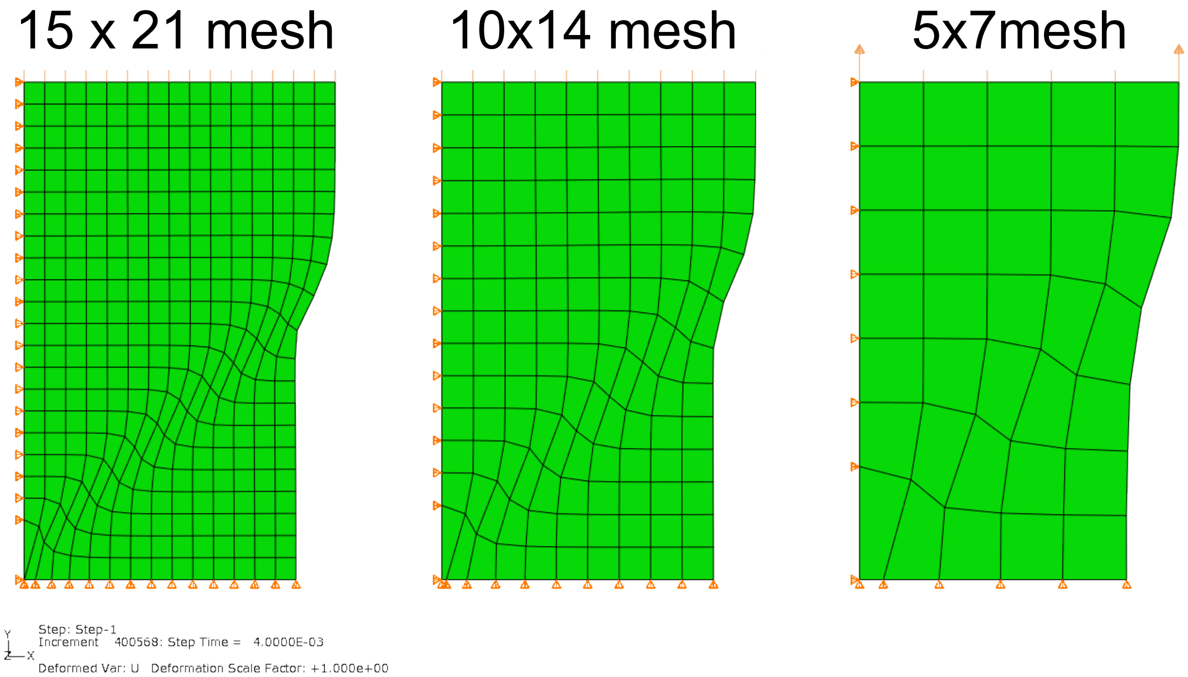
Modeling Failure in FEM Framework: Extension of Rectangular Steel Block

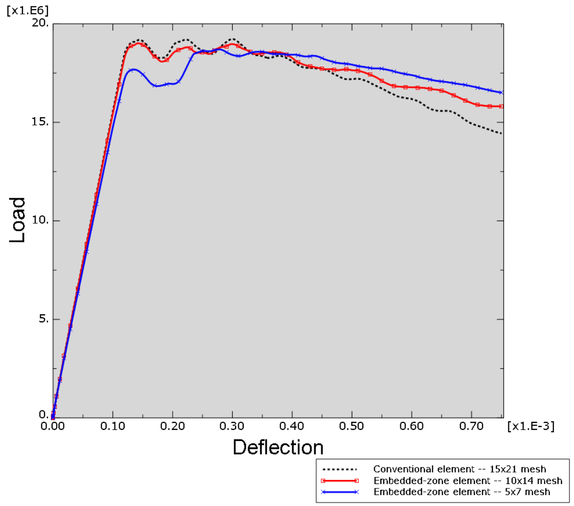
Model System: A rectangular steel block subjected to plane strain extension.

- A localization band forms as the block deforms, and is represented by shaded elements.
    - Darker shades signify instability at a larger number of Gauss points
- The material follows an elasto-plastic constitutive law
- A material imperfection is assumed in the bottom-left element leading to reduced strength



Framework is Mitigating Mesh Sensitivity Problems





- **Location and orientation of band, and its effect on overall deformation, are captured well, even by very coarse mesh.**
- **Correct structural response is captured throughout the loading process**
- **Useful for representation of adiabatic shear banding, slip line representation in single crystals, coalescence localization.**

Results to Date

1. **Microstructural length scales are critically important to damage evolution - nucleation vs. growth of voids**
    1. Deterministic feature of damage nucleation identified: function of boundary type– **mechanism determined through EFRC MD**
    2. Deterministic feature for void growth– **models reflect this**
2. **Damage evolution is sensitive to tensile rate**
    1. Partitioning of plasticity, void nucleation and growth mechanism depend on these rates
    2. Models must capture evolution of rarefaction waves during shock to model this process physically
3. **Development of a Fundamentally New High Rate Single Crystal Model**
4. **New Methodology for Experimental Design of Shock Experiments**

Results, Cont.

5. **Two new capabilities established at the lab**
    1. Drop tester
    2. Nano tomography unit – **leveraged against this and other LDRD and Weapons programs**
6. **A unified data set – Already have requests for this set by LLNL**
7. **Work has helped to drive considerations for future work**
    1. Meso-scale charge call
    2. Future signature facility requirements

Broader Implications of this Work

- **Advanced Damage model needs driven directly by concerns from the weapons program**
    - Future work in materials with increasingly more engineering defects represents the stepped approach for physically based, phase aware, process aware damage models
- **Identification of deterministic features of dynamic damage critical to "Materials-By-Design" and "Process-Aware" drivers in Materials Community**
- **Focus on linkage of the meso-scale to the continuum ties directly to laboratory response to OBES Meso-scale Charge**
- **3D damage quantification and kinetic studies help set parameters for design of future signature facilities like MaRIE**
- **Unified data sets are of broad interest to the strength and damage communities – LLNL has already asked for the data**

Publications

1. Abeele, K. Van Den, T. J. Ulrich, P. Le Bas, M. Griffa, B. Anderson, and R. Guyer. Vector Component Focusing in Elastic Solids using a Scalar Source in Three Component Time Reversal. 2010. In *International Congress on Ultrasonics ; 20090111 - 20090117 ; Univ. Santiago Chile, Santiago, CHILE.* Vol. 3, 1 Edition, p. 685.
2. Barton, N. R., J. V. Bernier, J. Knapp, A. J. Sunwoo, E. K. Cerreta, and T. J. Turner. A Call to Arms for Task Parallelism in Multi-scale Materials Modeling. 2011. *International Journal for Numerical Methods in Engineering.* **86**: 744.
3. Bronkhorst, C. A., A. R. Ross, B. L. Hansen, E. K. Cerreta, and J. F. Bingert. Modeling and Characterization of Grain Scale Strain Distribution in Polycrystalline Tantalum . 2010. *Computers, Materials, and Continua.* **17**: 149.
4. Bronkhorst, C. A., P. J. Maudlin, G. T. Gray III, E. K. Cerreta, E. N. Harstad, and F. L. Addessio. Accounting for Microstructure in large Deformation Models of Polycrystalline Metallic Materials. 2010. In *Computational Methods for Microstructure-Property Relationships.* Edited by Ghosh, S., and D. Dimiduk. Vol. 1, First Edition, p. -. Norwell: Springer.
5. Bronkhorst, C. A., S. R. Kalidindi, and S. R. Zavaliangos. Editorial - Special Issue in Honor of Lallit Anand. 2010. *International Journal of Plasticity.* **26**: 1071.
6. Cao, F., I. J. Beyerlein, F. L. Addessio, B. H. Sencer, C. P. Trujillo, E. K. Cerreta, and G. T. Gray III. Orientation Dependence of Shock Induced Twinning and Substructures in a Copper Bi-Crystal. 2010. *Acta Materialia.* **59**: 549.
7. Dennis-Koller, D., E. Cerreta, J. Escobedo-Diaz, and C. Bronkhorst. "Controlled Shock Loading Conditions for Microstructural Correlation of Dynamic Damage Behavior" . in *17th Biennial International Conference of the American Physical Society Topical Group on Shock Compression in Condensed Matter.* (Chicago, Ill, June 26 - July 1, 2011).
8. Escobedo, J. P., D. D. Koller, E. K. Cerreta, B. M. Patterson, C. A. Bronkhorst, B. L. Hansen, D. Tonks, and R. A. Lebensohn. Effects of Grain Size and Boundary Structure on the Dynamic Tensile Response of Copper. 2011. *Journal of Applied Physics.* **110** (3): 033513.
9. Escobedo-Diaz, J., D. Dennis-Koller, E. Cerreta, B. Patterson, and C. Bronkhorst. Effects of Grain Size and Boundary Structure on the Dynamic Tensile Response of Copper. in The*17th Biennial International Conference of the American Physical Society Topical Group on Shock Compression in Condensed Matter.* (Chicago, IL, June 26 - July 1, 2011).
10. Hansen, B. L., C. A. Bronkhorst, and M. Ortiz. Dislocation Subgrain Structures and Modeling the Plastic Hardening of Metallic Single Crystals. 2010. *Modeling and Simulation Materials Science and Engineering.* **18**: 055001.

Publications, Cont.

11. Lebensohn, R. A., A. D. Rollett, and P. Suquet. Fast Fourier Transform Based Modeling for the Determination of Micro-Mechanical Fields in Polycrystals. 2011. *Journal of Minerals, Metals and Materials Society.* **63**: 13.
12. Lebensohn, R. A., M. I. Idiart, P. Ponte Castaneda, and P. G. Vincent. Dilatational Viscoplasticity of Polycrystalline Solids with Intergranular Cavities. 2011. *Philosophical Magazine.* **91**: 3038.
13. Lebensohn, R., C. Hartley, C. Tome, and O. Castelnau. Modeling the mechanical response of polycrystals deforming by climb and glide. 2010. *Philosophical Magazine.* **90** (5): 567.
14. Luscher, D. J., D. L. McDowell, and C. A. Bronkhorst. A Second Gradient Theoretical Framework for Hierarchical Multi-scale Modeling of Materials. 2010. *International Journal of Plasticity.* **26**: 1248.
15. Patterson, B. M., J. Campbell, and G. J. Havrilla. Integrating 3D Images Using Laboratory-based micro x-ray computed tomography and confocal x-ray fluorescence techniques. 2010.
16. *X-ray Spectrometry.* **39** (3): 184.
17. Patterson, B. M., and C. E. Hamilton. Dimensional Standard for Micro-CT for the Quantification of 3D Voids Structures. 2010. *Analytical Chemistry.* **82** (20): 8537.
18. Patterson, B. P., J. P. Escobedo-Diaz, D. D. Koller, and E. K. Cerreta. Dimensional Quantification of Embedded Voids of Objects in Three Dimensions Using X-Ray Tomography. *Microscopy and Microanalysis, (2012) accepted.*
19. Perez-Bergquist, A. G., E. K. Cerreta, C. P. Trujillo, and F. Cao. Orientation Dependence of Void Formation and Substructure Deformation in a Spalled Copper Bicrystal. *Scripta Materialia* (2012) accepted..
20. Preston, D. L., V. I. Levitas, and D. W. Lee. Interface Propagation and Microstructure Evolution in Phase Field Models of Stress-Induced Martensitic Phase Transformations. 2010.I*nternational Journal of Plasticity.* **26**: 395.
21. Rollett, A. D., R. A. Lebensohn, M. Groeber, Y. Choi, J. Li, and G. S. Rohrer. Stress hot spots in viscoplastic deformation of polycrystals. 2010. *Modelling and Simulation in Materials Science and Engineering.* **18** (7): 074005 (16 pp.).
22. Tonks, D. L., and J. Bingert. Mesoscale Polycrystal Calculations of Damage in Shock Loaded Copper. 2010. *European Physics Journal, Web of Conference.* **10**: 6.
23. E.K. Cerreta, J.P. Escobedo, A. Perez-Bergquist, D.D. Koller, C.P. Trujillo, G.T. Gray III, C. Brandl, and T.C. Germann, “Early Stage Dynamic Damage and the Role of Grain Boundary Type”, *Scripta Materialia,* (2012) *accepted*.

Symposia Organized

1. <u>Minerals, Metals and Materials Under Pressure II</u>, Co-Organizers: D. Trinkle, R. Hening, and E. K. Cerreta, TMS Annual Meeting 2012, Orlando, Fl.
2. <u>Materials Science Session</u>, Organizer: E. Cerreta, APS Shock Compression of Condensed Matter Meeting 2011, Chicago, Il.
3. <u>Dynamic Behavior of Materials</u>, Co-organizers: C.A. Bronkhorst and G.T. Gray III, Plasticity 2011, Puerto Vallarta, Mexico.
4. <u>LDRD Review for DR-20100026</u>, Co-organizers: D.D. Koller, E.K. Cerreta, and C.A. Bronkhorst, 2011, Los Alamos, NM

Co-Design at Los Alamos National Laboratory

A. Redondo (T-DO)

This presentation will give an overview of co-design at Los Alamos National Laboratory. Part of the history of the co-design efforts will be discussed as well as how these efforts fit in various Laboratory strategies. We will also discuss how co-design is related to materials work at Los Alamos.

Co-Design
at Los Alamos National Laboratory

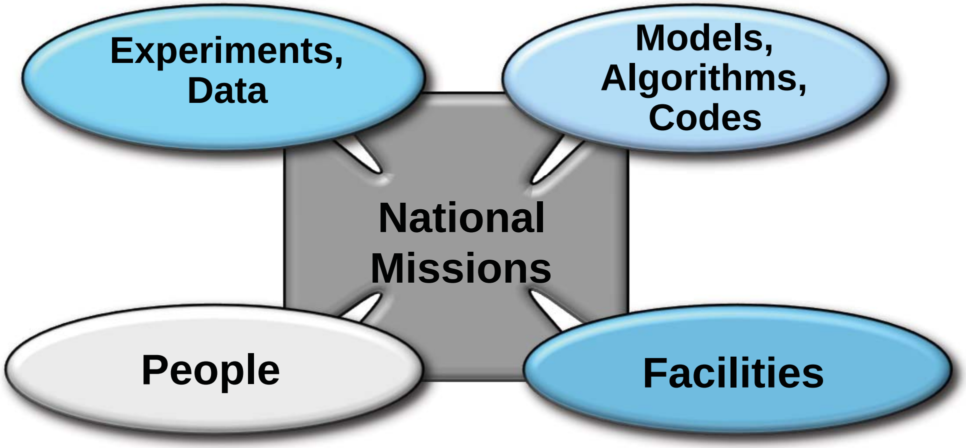
Antonio Redondo

Theoretical Division

Co-Design Theme Area

- **What you will see later:**
  - Technical talks:
    - Tim Germann: “Exascale Co-Design Center for Materials in Extreme Environments”
    - Deniece Korzekwa: “A Co-Design Approach to Plutonium Casting Development” (classified session)
  - Posters:
    - Irene Beyerlein: “A Multi-mesoscale predictive capability for interface-driven behavior”
    - Duan Zhang and Virginie Dupont: “Computational codesign for multi-scale application in the natural sciences”
    - Stephan Eidenbenz: “Optimization principles for computational co-design with applications to molecular dynamics”
    - Turab Lookman: “Co-design for materials: Confluence of MaRIE and Exascale”
    - Danny Perez: “Increasing the timescale of atomistic simulations through co-designed accelerated molecular dynamics methods”
    - Quanxi Jia: “Understanding, exploiting and controlling competing interactions in complex oxides”
    - Marc Cawkwell: “Co-design modeling of reactions behind a shock front”
  - This talk: what co-design is at Los Alamos

A national science/technology management challenge: How we do business to impact national-scale imperatives?



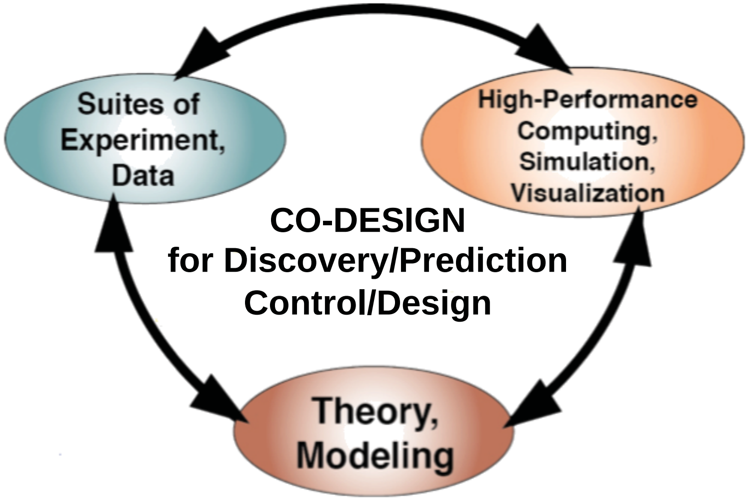
Experiments, Data

Models, Algorithms, Codes

National Missions

People

Facilities



Suites of Experiment, Data

High-Performance Computing, Simulation, Visualization

CO-DESIGN
for Discovery/Prediction
Control/Design

Theory, Modeling

- **A new framework for transformational ST&E at Science & Mission Frontiers**
  Integration and collaboration (DOE: EFRCs, SciDAC, Hubs, Co-Design Centers…)
  (OSTP: Adv. Manufacturing, Materials Genome…Initiatives)

- **LANL opportunities being developed: NW predictive capability framework, energy-climate, informatics, environmental management, cyber, … , materials, MaRIE**

- **DOE (SC, NNSA, App. Energy) has a full spectrum of assets for this future**
  - Integrating National Assets for Discovery, Prediction, Control, Design

Los Alamos National Laboratory and the Next Decade of Supercomputing

Mission Critical

Nuclear Weapons Stewardship

Nuclear Non-proliferation, Energy, Climate, Environment, Cyber, ….

Technology Transfer and US Economic Competitiveness

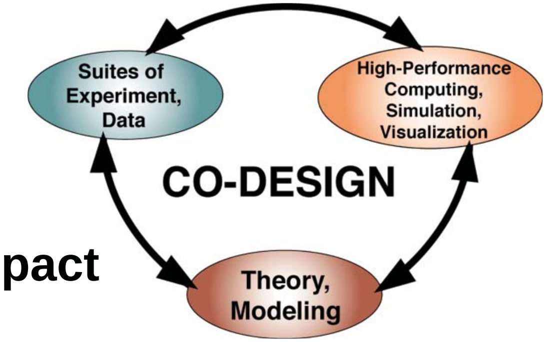
Simulation Science and the Century of Complexity

Advanced computing now a mature element in the “Scientific Method” for Complex Systems

- Multiscale, Multiphysics, External Events, UQ, …
- Component and Integral (System) Codes
- Compute- and Data-Intensive Computing

LANL must maximize mission and discipline impact

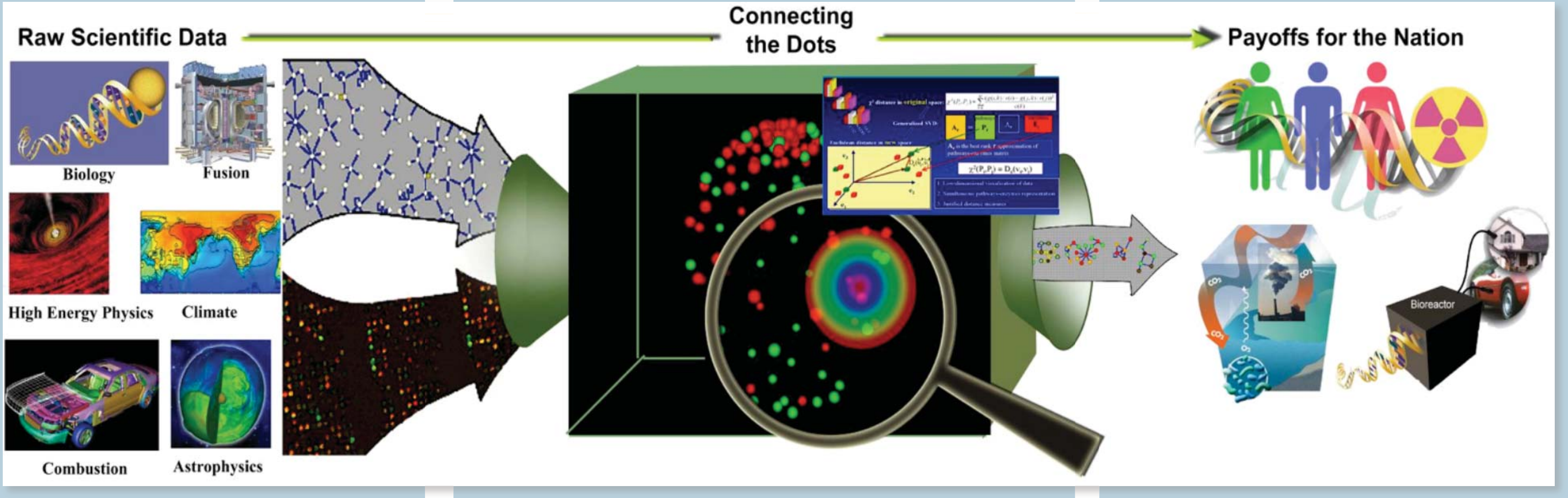
Coordination across PADWP, PADGS, and PADSTE



LANL must provide the infrastructure for “Connecting the Dots”

Finding the Dots

Understanding the Systems



New Worlds of High-Resolution, High-Precision

Data

Observations
Computations

Co-designing Algorithms, Architectures, Applications

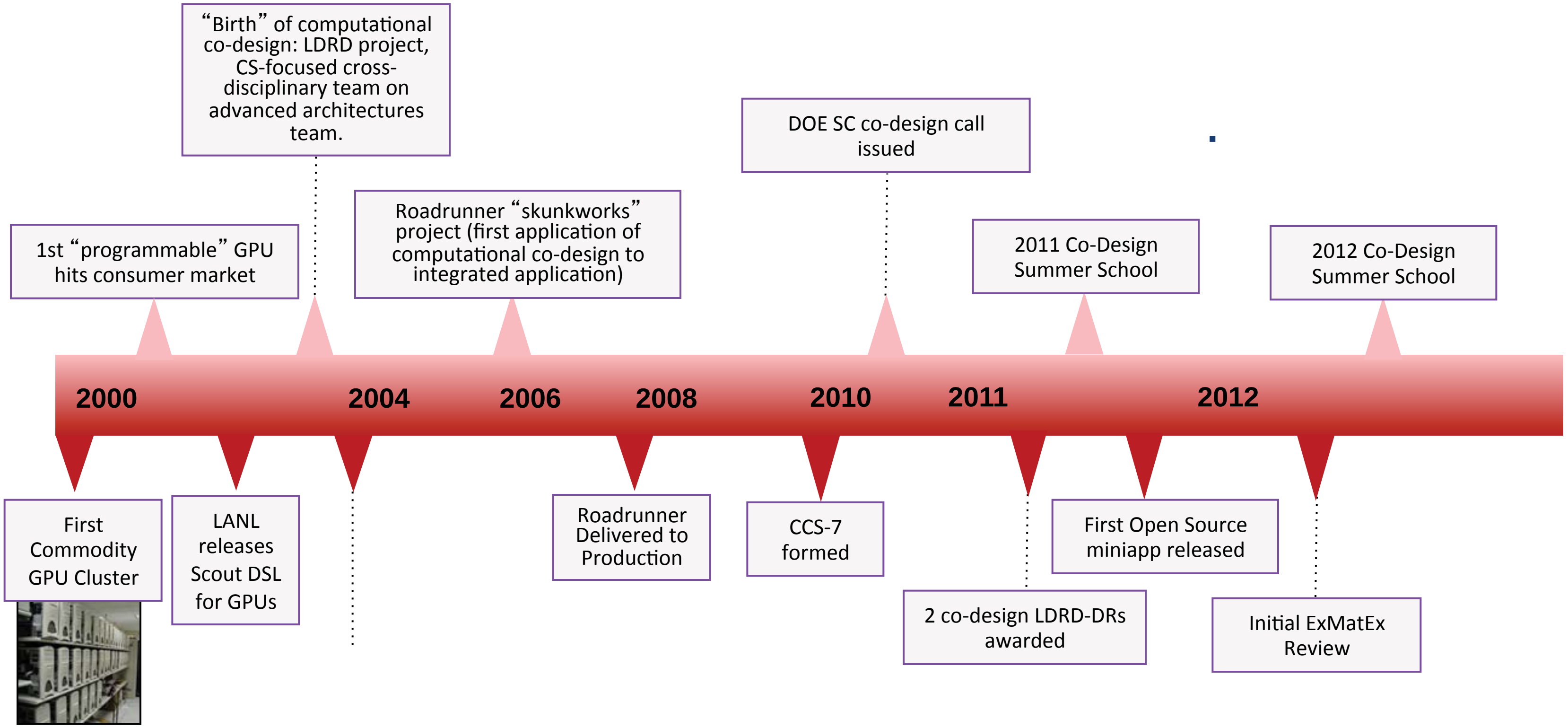
- Huge dimensional space
- Combinatorial challenge
- Noisy data, external events
- Requires advanced CS, HPC, theory, modeling, uncertainty quantification, data curation

Providing Predictive Understanding

- Nuclear Security
- Produce hydrogen-based energy
- Stabilize carbon dioxide
- Clean/dispose toxic waste
- Cyber Security

Adapted from: Raymond L. Orbach, DOE Undersecretary for Science
2006 AAAS Annual Meeting

LANL defined and has led they way in computational co-design

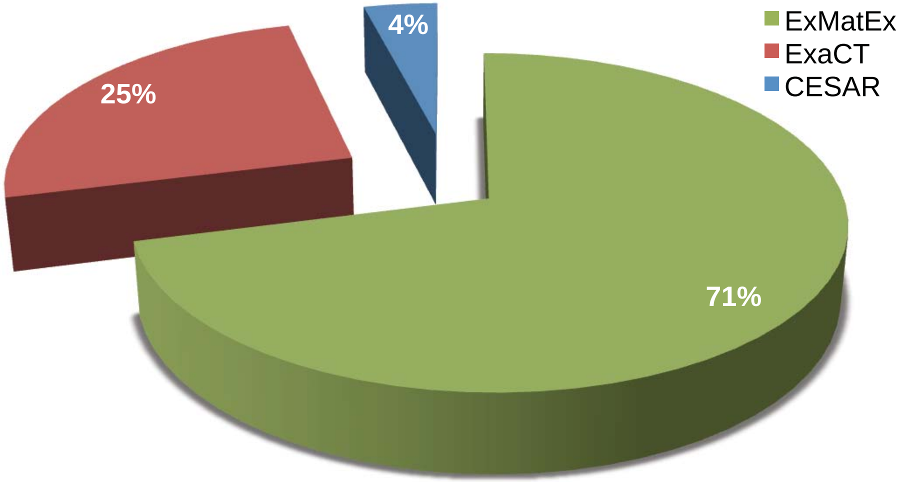


- 1st "programmable" GPU hits consumer market
- "Birth" of computational co-design: LDRD project, CS-focused cross-disciplinary team on advanced architectures team.
- Roadrunner "skunkworks" project (first application of computational co-design to integrated application)
- DOE SC co-design call issued
- 2011 Co-Design Summer School
- 2012 Co-Design Summer School
- First Commodity GPU Cluster
- LANL releases Scout DSL for GPUs
- Roadrunner Delivered to Production
- CCS-7 formed
- 2 co-design LDRD-DRs awarded
- First Open Source miniapp released
- Initial ExMatEx Review

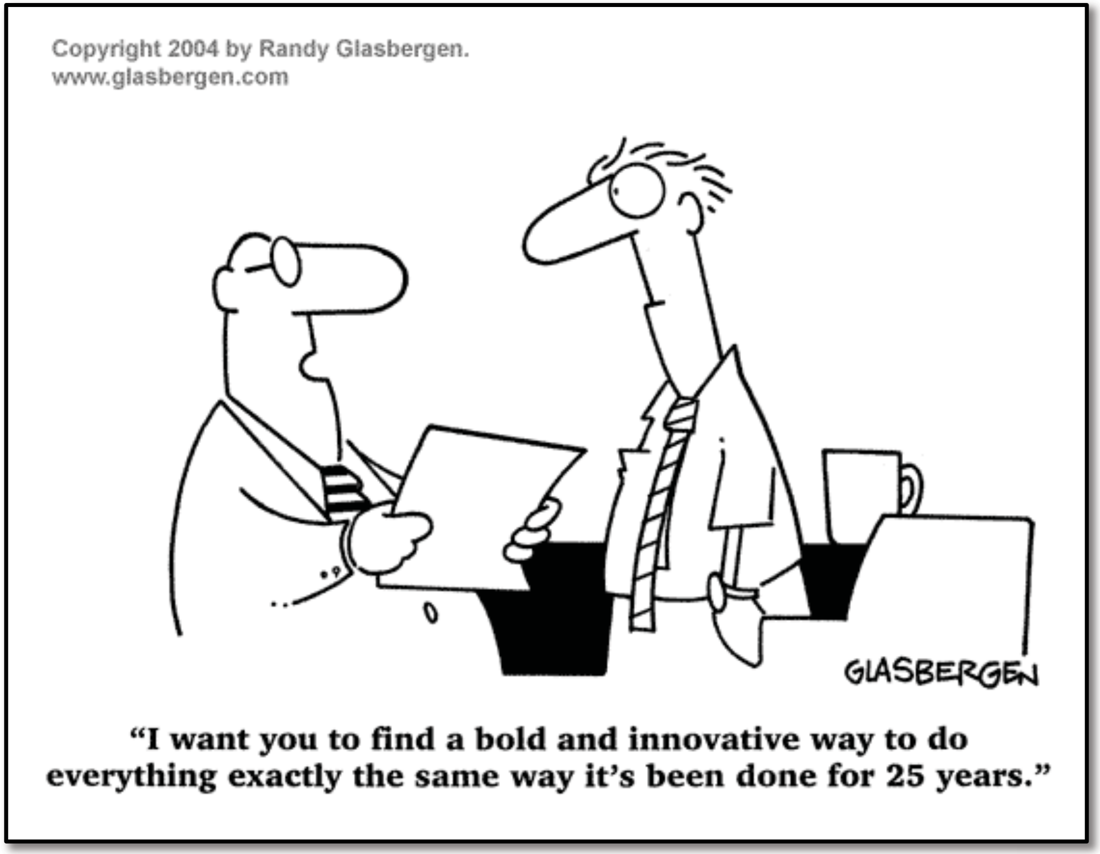
LANL Plays a Role in ASCR-funded Co-Design Centers

- **Co-Design Centers**
  - ExMatEx – Lead institution
    - (LANL Lead: Germann)
  - ExaCT – Programming Models
    - (LANL Lead: McCormick)
  - CESAR – Zero-copy for visualization and analysis
    - (LANL Lead: Ahrens)

Breakdown by Co-Design Center Participation



Advanced and Emerging Architectures Efforts Combined with Hands-On Application Redesign Forced us to Rethink our Approach



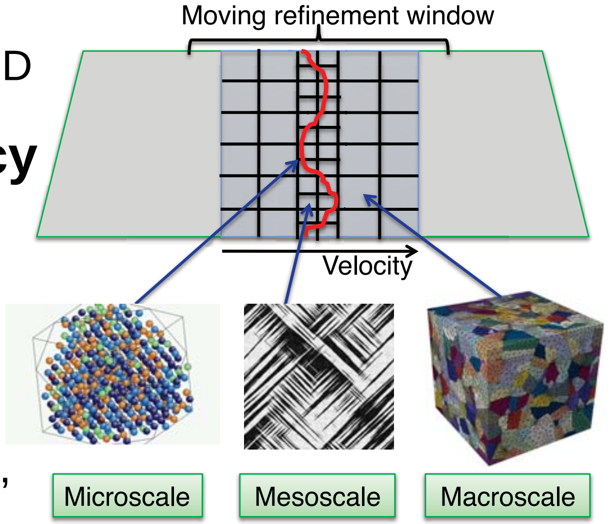
"I want you to find a bold and innovative way to do everything exactly the same way it's been done for 25 years."

Computational Co-design for Multi-scale Applications in the Natural Sciences (CoCoMANS)

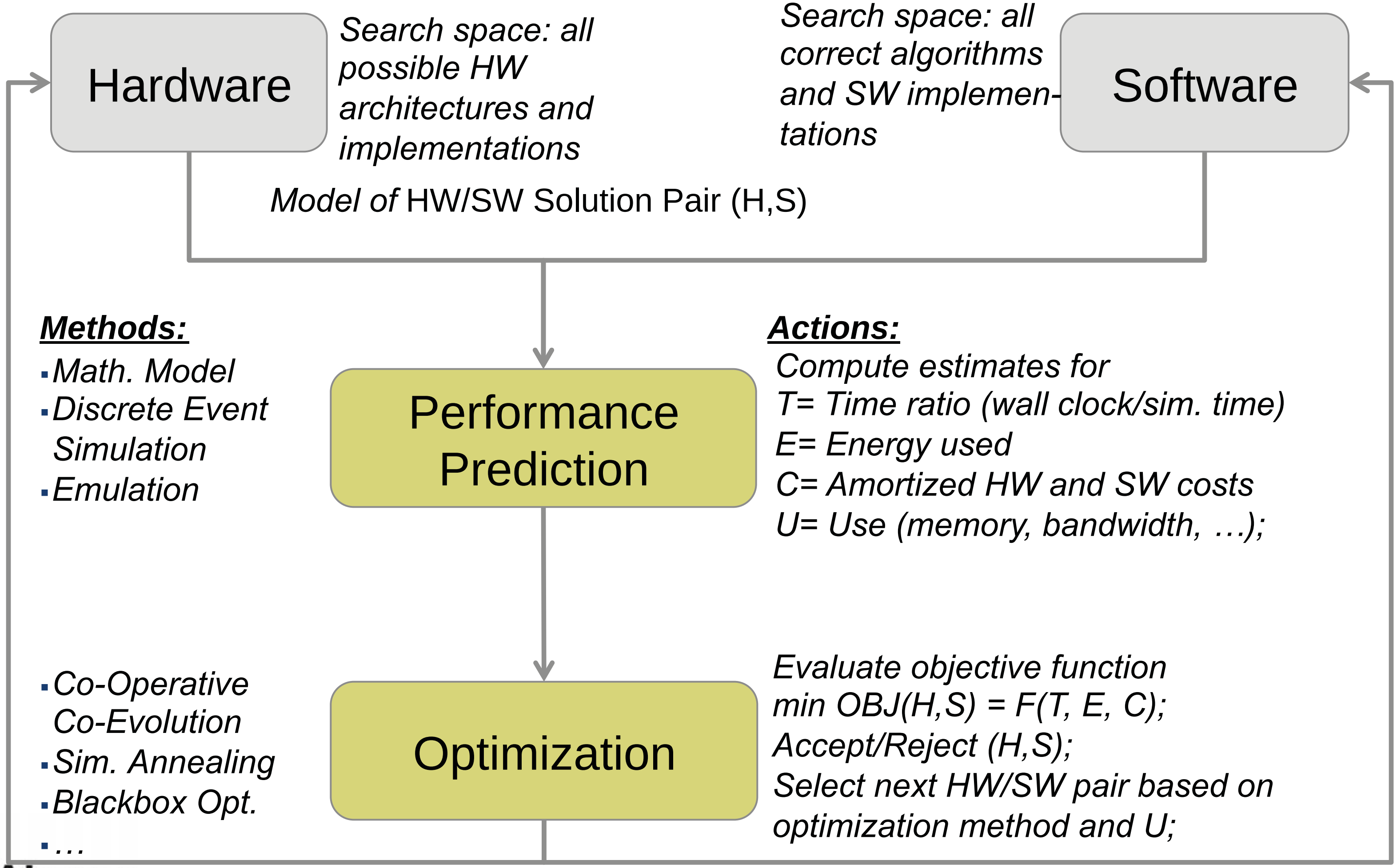
- **Applications + Algorithms + Architectures**
  - Plasma Physics, Materials Science, Climate (all multi-scale)
  - Moment-based, scale-bridging algorithms (heterogeneous with focus on data movement and asynchronous)
  - Emerging architectures (strong connections to industry partners)
- **Goals are:**
  - Demonstrate a paradigm shift in simulation on advanced architectures
  - Deliver a documented co-design knowledge-base (a process)
  - Strengthen and foster broad, long-term, industry research collaborations
  - Advance two-way scale-bridging algorithms
- **Moment-based scale-bridging algorithms**
  - High Order (HO) problem is discretized version of the fine-scale equations
  - Low Order (LO) problem (Engineering / System scale) is small number of phase space (or spatial) moments of the HO problem.
  - Both the LO problem and the HO problem can be solved over the entire geometry, or HO problem solved locally with adaption.

ExMatEx Co-Design Center

- **DoE ASCR funded ($4M/yr, 5 years)**
  - Led by Los Alamos (Tim Germann)
  - Partners: LLNL, ORNL, SNL, Stanford, Caltech
  - Vendor collaboration: IBM, nVidia, HP, Intel, Cray, AMD
- **Goal: Exploit massive exascale concurrency**
  - Embedded scale-bridging algorithms
  - Adaptively launch lower length scales a needed
  - Asynchronous task based approach
    - Escape bulk synchronous model
  - Co-Design of algorithms, codes, programming models, middleware, hardware
- **Deliverables**
  - Open source proxies, peta-scale materials code, et. al.
  - Documented process and exascale *specification*



Optimization Principles in HW/SW CoDesign: Generic Optimization Loop for Given Problem Instance



Hardware

Search space: all possible HW architectures and implementations

Search space: all correct algorithms and SW implementations

Software

Model of HW/SW Solution Pair (H,S)

Methods:

- *Math. Model*
- *Discrete Event Simulation*
- *Emulation*

Performance Prediction

Actions:

Compute estimates for
T= Time ratio (wall clock/sim. time)
E= Energy used
C= Amortized HW and SW costs
U= Use (memory, bandwidth, …);

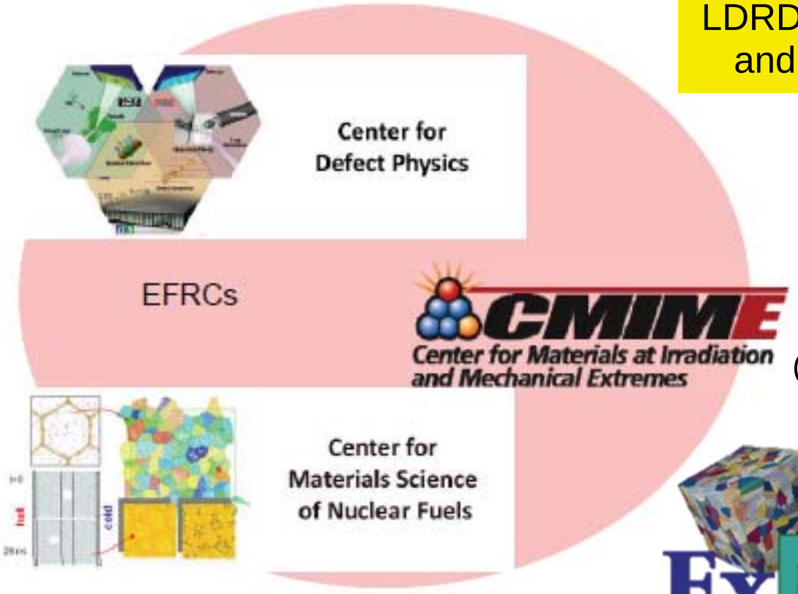
- *Co-Operative Co-Evolution*
- *Sim. Annealing*
- *Blackbox Opt.*
- *…*

Optimization

Evaluate objective function
min OBJ(H,S) = F(T, E, C);
Accept/Reject (H,S);
Select next HW/SW pair based on optimization method and U;

Recent efforts to integrate theory and experiment through co-design for materials in extremes are succeeding and build on LDRD investments

LDRD (Dennis-Koller) Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage Evolution



(w/MIT)

CASL

NE (ORNL, INL, LANL, MIT, et al.)

MaRIE

ExMatEx

ASCR(LANL, LLNL, et al.)

LDRD (Germann) Spatial-temporal frontiers of atomistic simulations in the petaflop computational world

LDRD (Beyerlein) Innovative & Validated Sub-micron to Meso-scale Modeling of the Evolution of Interface Structure and Properties Under Extreme Strains

OSTP “Materials Genome Initiative”

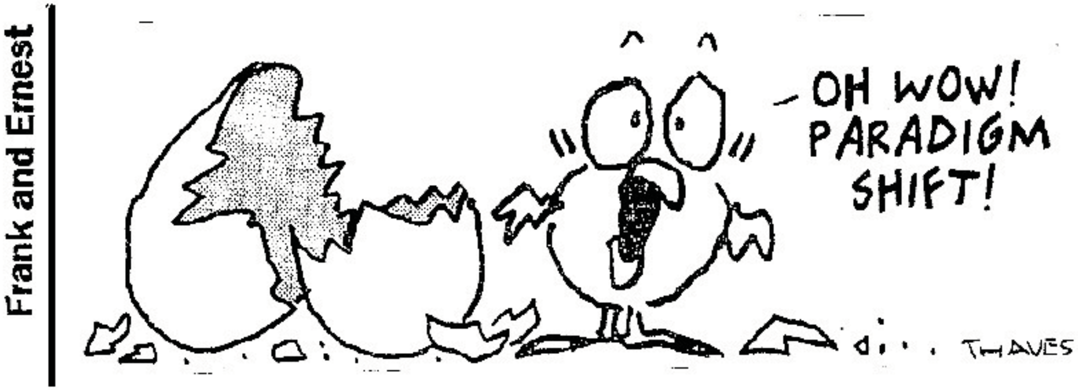
Materials in Extremes/Irradiation Resistant Materials (BES/FES/ASCR)/NNSA/NE

Co-Design: rough estimate of funding associated with materials

- **FY11 ASCR call: ExMatEx – $4M/year for 5 years (LANL lead)**
- **Special FY11 LDRD Call – ~$1.5M/year for 3 years**
  - "Computational Co-Design for Multi-scale Applications in the Natural Sciences" (CoCoMANS)
  - "Optimization Principles in Computational Co-Design Applied to Molecular Dynamics"
- **MaRIE – ~$1.5M/year**
  - LANL G&A and LDRD investment
  - Theory Modeling and Computation planning and support
- **LANL a key partner in CASL (Consortium for Advanced Simulation of Light water reactors)**
  - 10 principal partners, ORNL (lead), LANL, INL, SNL, MIT, NC State, TVA, UMich, WEC, EPRI
  - ~$22M/yr for 5 years; LANL funding $2.7M FY11, $3.25M FY12 (MST, CCS, and T; LANL leads: Lowrie, CCS, and Stanek, MST)
- **Other LDRD – ~$1.5M/year each**
  - Dennis-Koller: Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage Evolution
  - Germann: Spatial-temporal frontiers of atomistic simulations in the petaflop computational world
  - Beyerlein: Innovative & Validated Sub-micron to Meso-scale Modeling of the Evolution of Interface Structure and Properties Under Extreme Strains

Co-Design will continue to be a critical aspect of how we do science, technology and engineering in the future

- **We will continue to be forced to take advantage of potentially game-changing trends within the computer industry**
- **Adapting to and taking unique advantage of these technologies will be critical to success**



[Science is a] "series of peaceful interludes punctuated by intellectually violent revolutions" [where] "one conceptual world view is replaced by another".

-- Thomas Kuhn

Exascale Co-Design Center for Materials in Extreme Environments

T.C. Germann (T-1)

Computational materials scientists have been among the earliest and heaviest users of leadership-class supercomputers. The codes and algorithms which have been developed span a wide range of physical scales, and have been useful not only for gaining scientific insight, but also as testbeds for exploring new approaches for tacking evolving challenges, including massive (nearly million-way) concurrency, an increased need for fault and power management, and data bottlenecks. Multiscale, or scale-bridging, techniques are attractive from both materials science and computational perspectives, particularly as we look ahead from the current petascale era towards the exascale platforms expected to be deployed by the end of this decade. In particular, the increasingly heterogeneous and hierarchical nature of computer architectures demands that algorithms, programming models, and tools must mirror these characteristics if they are to thrive in this environment. Given the increasing complexity of such high-performance computing ecosystems (architectures, software stack, and application codes), computational "co-design" is recognized to be critical as we move from current petascale (10^{15} operations/second) to exascale (10^{18} operations/second) supercomputers over the next 5-10 years. The Exascale Co-design Center for Materials in Extreme Environments (ExMatEx) is an effort to do this by initiating an early and extensive collaboration between computational materials scientists, computer scientists, and hardware manufacturers. Our goal is to develop the algorithms for modeling materials subjected to extreme mechanical and radiation environments, and the necessary programming models and runtime systems (middleware) to enable their execution; and also influence potential architecture design choices for future exascale systems.

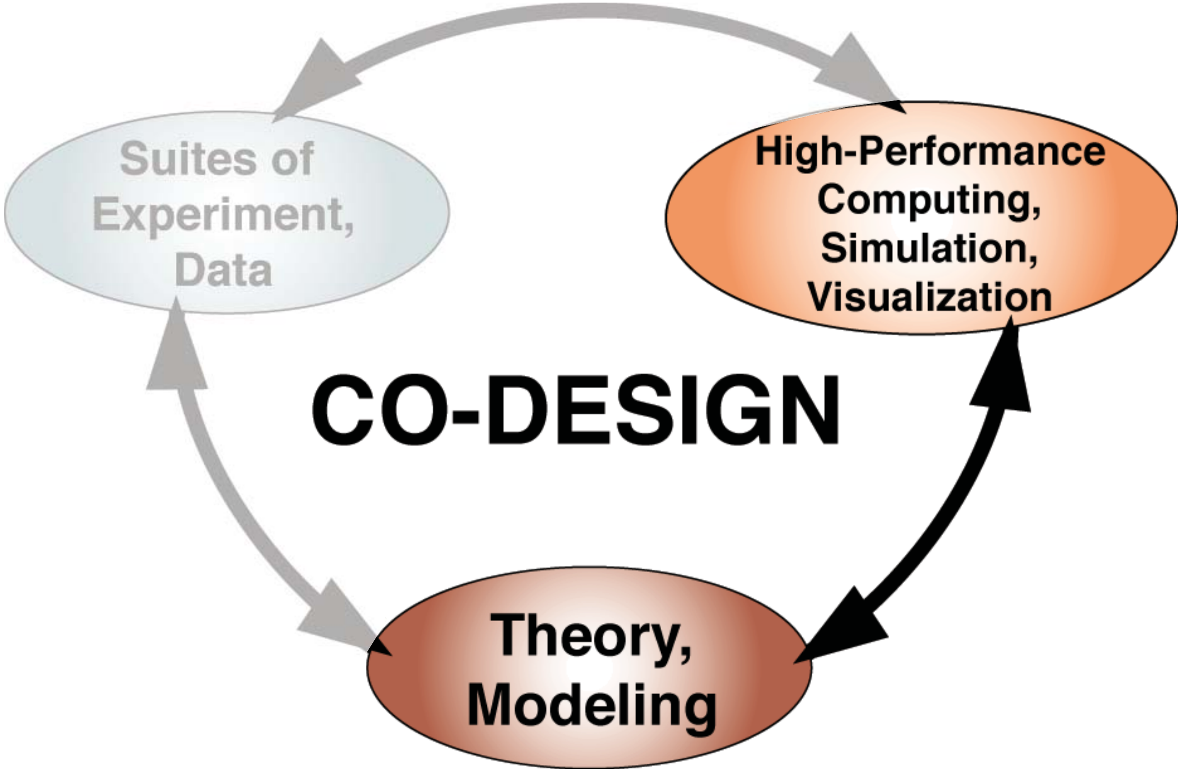
Exascale Co-Design Center for Materials in Extreme Environments

Timothy C. Germann

Physics and Chemistry of Materials (T-1)

Theoretical Division

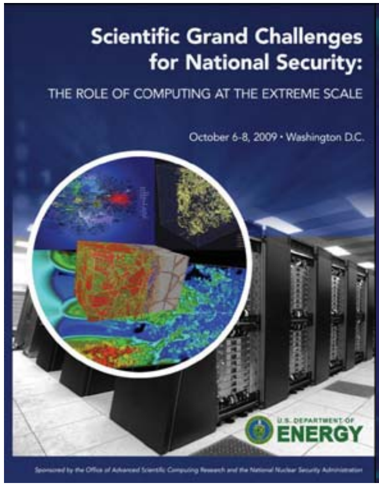
Computational co-design is focused on the interaction between applications, algorithms, and architectures



Executive Summary

- **The Exascale Co-design Center for Materials in Extreme Environments (ExMatEx) is one of three DOE Office of Science, Advanced Scientific Computing Research (ASCR) co-design centers.**
  - Each funded at $4M/year for 5 years (Aug 2011 – Aug 2016)
  - Others: nuclear energy (Rosner, Argonne) and combustion (Chen, Sandia-CA)
- **Computer architectures are undergoing dramatic changes.**
  - Increased concurrency
  - Increased heterogeneity and hierarchy (Roadrunner Opteron/Cell, GPGPUs)
  - Greatly increased flop/byte ratios
- **The complexity of emerging HPC systems, and opportunity to influence early architecture, software stack, and algorithm design choices for the exascale era (~2020), is being tackled via computational co-design.**
  - An early and extensive collaboration between domain scientists, computer scientists, and hardware manufacturers

A predictive understanding of the response of materials to extreme conditions (mechanical and/or irradiation) underpins many DOE missions



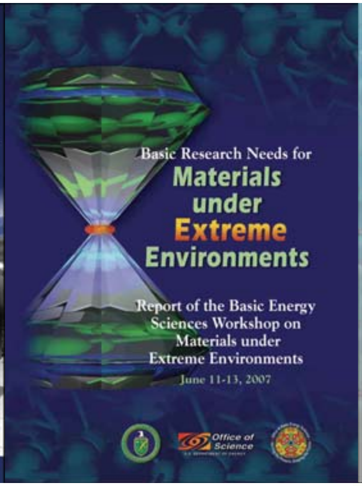
Scientific Grand Challenges for National Security:

THE ROLE OF COMPUTING AT THE EXTREME SCALE

October 6-8, 2009 • Washington D.C.

U.S. DEPARTMENT OF ENERGY

Sponsored by the Office of Advanced Scientific Computing Research and the National Nuclear Security Administration



Basic Research Needs for Materials under Extreme Environments

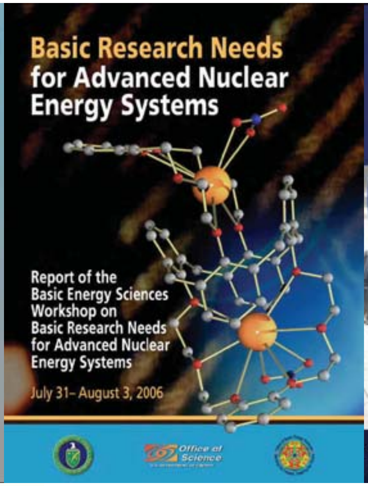
Report of the Basic Energy Sciences Workshop on Materials under Extreme Environments

June 11-13, 2007

Office of Science

COMPUTATIONAL MATERIALS SCIENCE AND CHEMISTRY

Accelerating Discovery and Innovation through Simulation-Based Engineering and Science

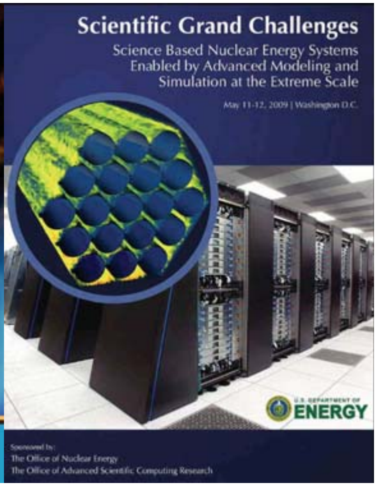


Basic Research Needs for Advanced Nuclear Energy Systems

Report of the Basic Energy Sciences Workshop on Basic Research Needs for Advanced Nuclear Energy Systems

July 31– August 3, 2006

Office of Science



Scientific Grand Challenges

Science Based Nuclear Energy Systems Enabled by Advanced Modeling and Simulation at the Extreme Scale

May 11-12, 2009 | Washington D.C.

U.S. DEPARTMENT OF ENERGY

Sponsored by:
The Office of Nuclear Energy
The Office of Advanced Scientific Computing Research

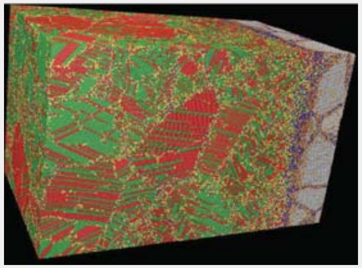
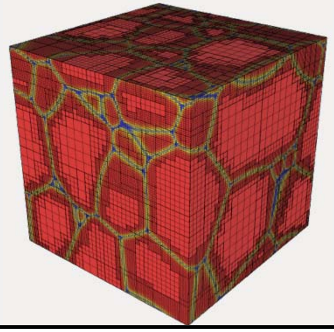
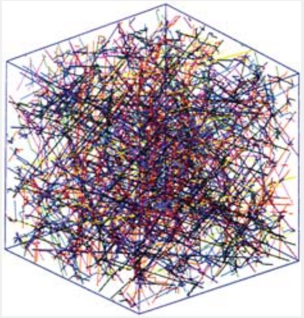
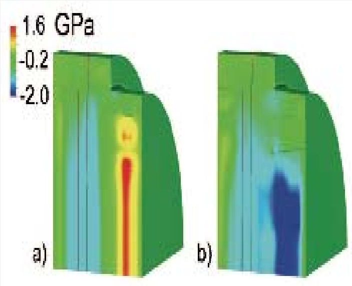
ADVANCED SIMULATION & COMPUTING™

CMIME
Center for Materials at Irradiation and Mechanical Extremes

CASL

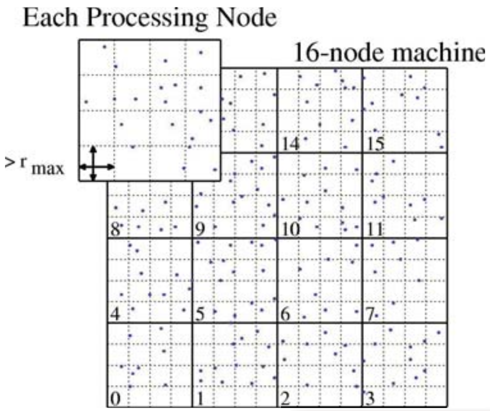
> **"With the advent of exascale computing, the possibility exists to achieve predictive capabilities to manipulate microstructure and interfaces, at the grain scale, to enable the design and development of extreme environment tolerant advanced materials."**
> **– *Scientific Grand Challenges for National Security* report**

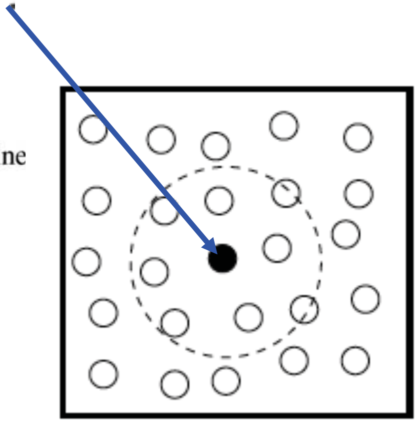
Computational materials science involves a hierarchy of length/time scales

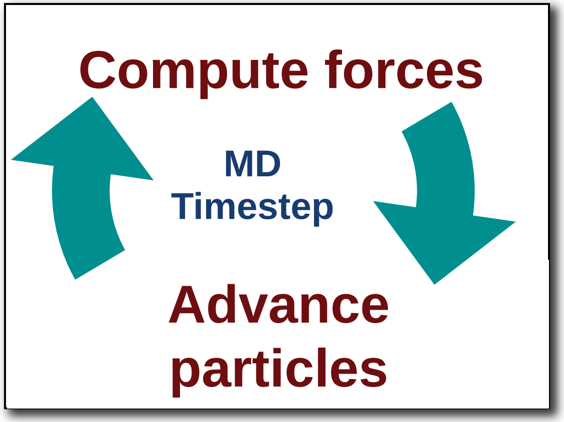
Ab-initio	**MD**	**Phase Field**	**Dislocation**	**Continuum**
Inter-atomic forces, equation of state	**Defects and interfaces, nucleation**	**Meso-scale multi-phase evolution**	**Meso-scale strength**	**Maco-scale material response**
				
Code: Qbox/LATTE Motif: Particles and wavefunctions, plane wave DFT with nonlocal norm-conserving, ScaLAPACK, BLACS, and custom parallel 3D FFTs Prog. Model: MPI + CUBLAS/CUDA	Code: SPaSM/ ddcMD Motif: Particles, explicit time integration, neighbor and linked lists, dynamic load balancing, parity error recovery, and *in situ* visualization Prog. Model: MPI + Threads	Code: AMPE/GL Motif: Regular and adaptive grids, implicit time integration, real-space and spectral methods, complex order parameter (phase, crystal, species) Prog. Model: MPI	Code: ParaDis Motif: “segments” Regular mesh, implicit time integration, fast multipole method Prog. Model: MPI	Code: VP-FFT/ LULESH Motif: Regular and irregular grids, implicit time integration, 3D FFTs, polycrystal and single crystal plasticity. Prog. Model: MPI + Threads

State-of-the-art molecular dynamics: SPaSM

$$\mathbf{F}_i(t) = m_i \ddot{\mathbf{r}}_i(t) = -\frac{\partial \Phi}{\partial \mathbf{r}_i}$$







Compute forces

MD Timestep

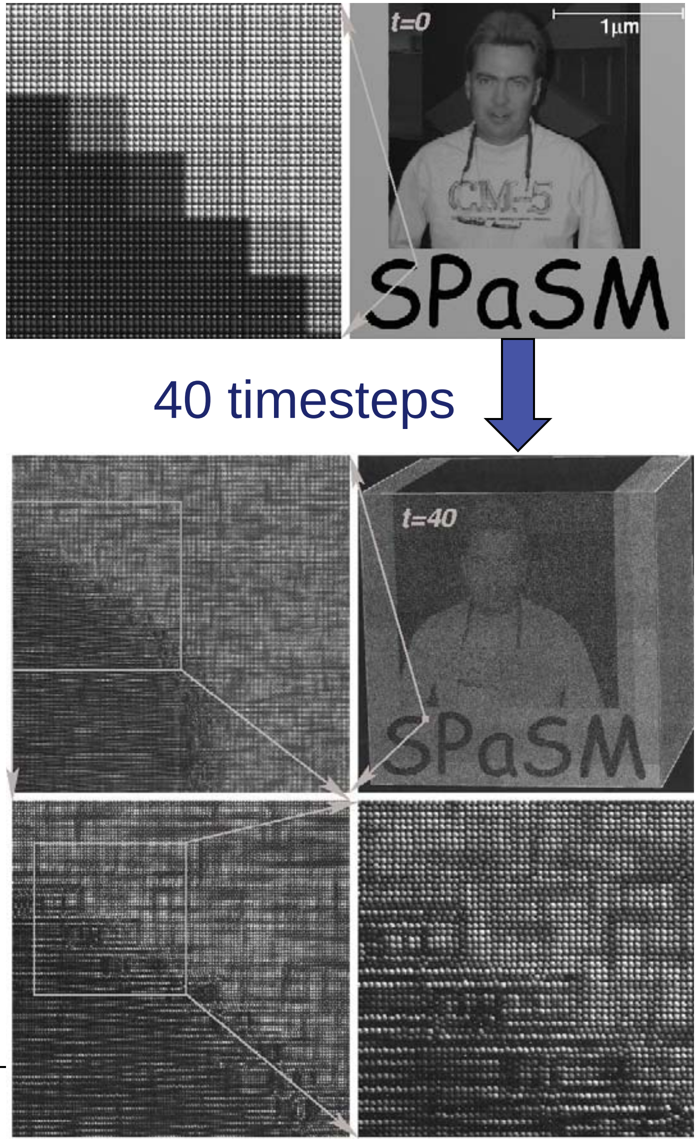
Advance particles

- Scalable Parallel Short-range Molecular dynamics
- Finite-range (r_{max}) interactions ⇒ $O(N)$ computational scaling
- Spatial decomposition on shared and distributed memory architectures
- 1993 Gordon Bell Prize (CM-5)[*]
- 1998 Gordon Bell Prize (Avalon)
- 2005, 2008 GB Finalist (BG/L, RR)
- First (only) trillion-atom simulation
- Object-oriented scripting language with parallel in situ visualization and analysis libraries (runtime “steering”)

[*] David Beazley, Peter Lomdahl, Niels Grønbech-Jensen, Pablo Tamayo

In situ analysis and visualization is frequently a necessity, not an option

- **Portable and scalable graphics library implemented in C / MPI, arbitrary resolution images**
- **Parallelization strategy**
  - Each processor renders only objects assigned to it (spatial decomposition)
  - Binary-tree reduction of partial images into one picture (depth buffer)
- **BG/L demonstration (in 2007)*:**
  - $10^4 \times 10^4 \times 10^4$ = 1 trillion atoms in a metastable simple cubic lattice
  - Initial velocities assigned from bitmap image
  - Single precision
  - ~90 sec per timestep, 5 – 30 sec per image (800x800 – 1500x1500 pixels) on full machine (212,992 CPUs)



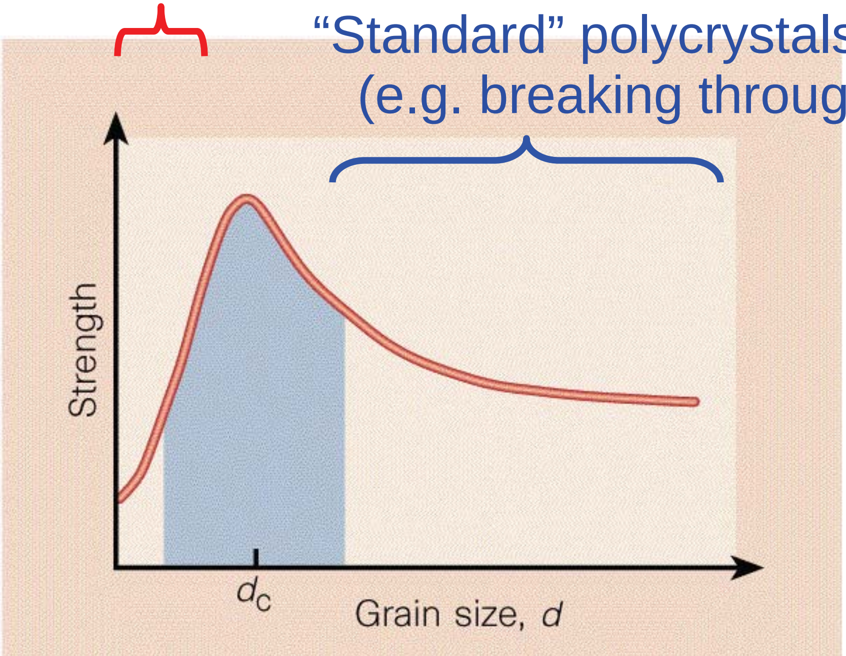
*T.C. Germann and K. Kadau, *Int. J. Modern Phys. C* (2008)

A wide range of applications have been studied with SPaSM: 1993-2010

Beyond the “Hall-Petch Peak:” Polycrystal Plasticity and Mechanical Response

Nanocrystalline metals: grain boundary (GB) sliding dominates

“Standard” polycrystals: dislocation pileups within grains
(e.g. breaking through GBs or other obstacles) dominates



S. Yip, *Nature* **391**, 532 (1998)

The predicted d_c ranges from 2-3 nm (Ni, Fe) to 20 nm (Cu) for most metals.

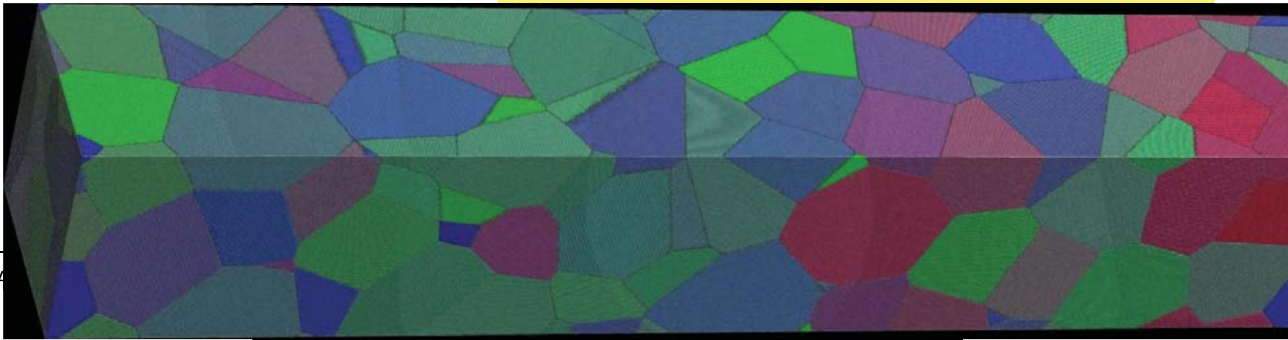
To model a polycrystal exhibiting a “standard” response requires ~100 grains with diameter ~50 nm

10^8 - 10^9 atoms

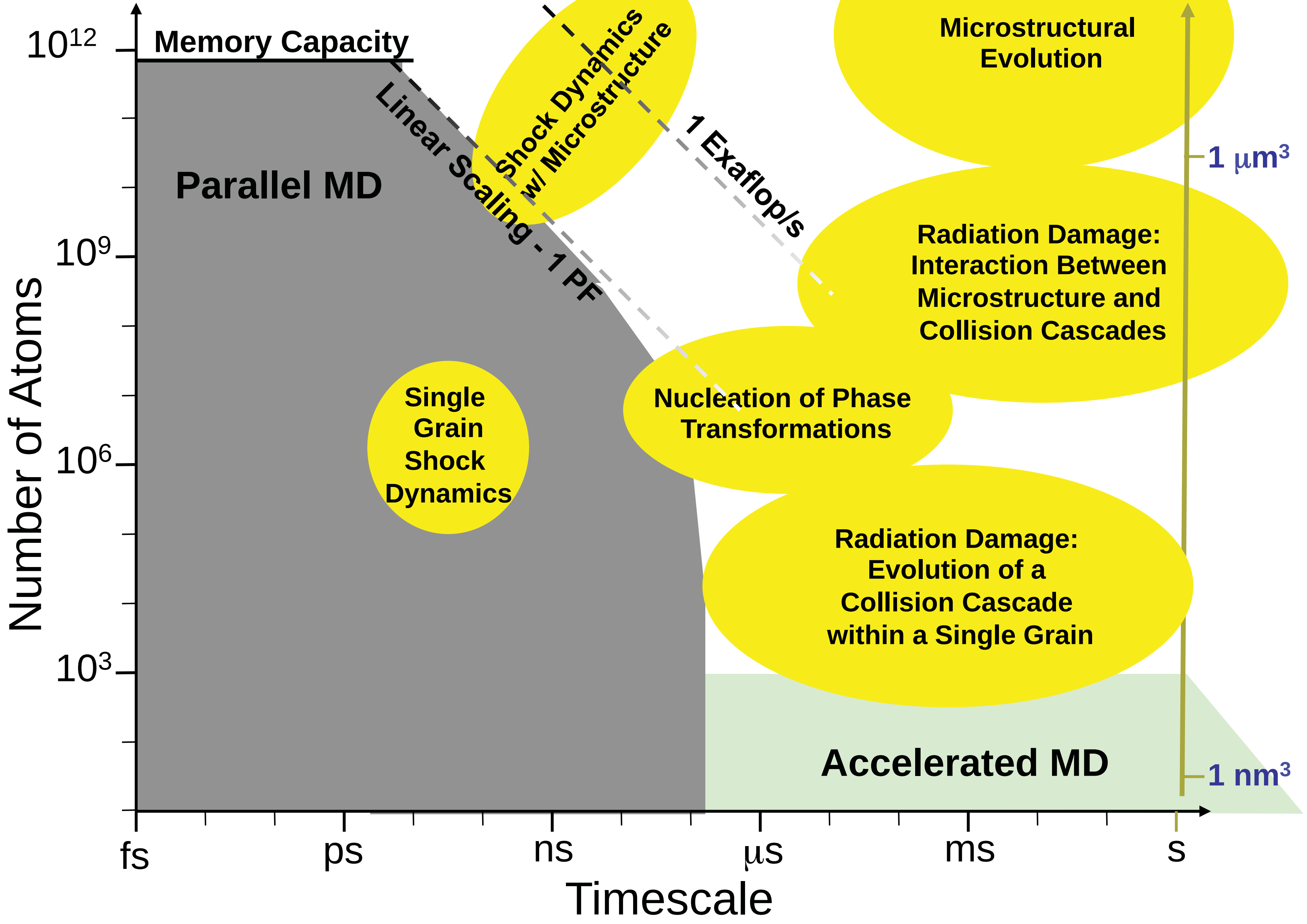
for timescales of ns - μs

10^6 - 10^9 timesteps

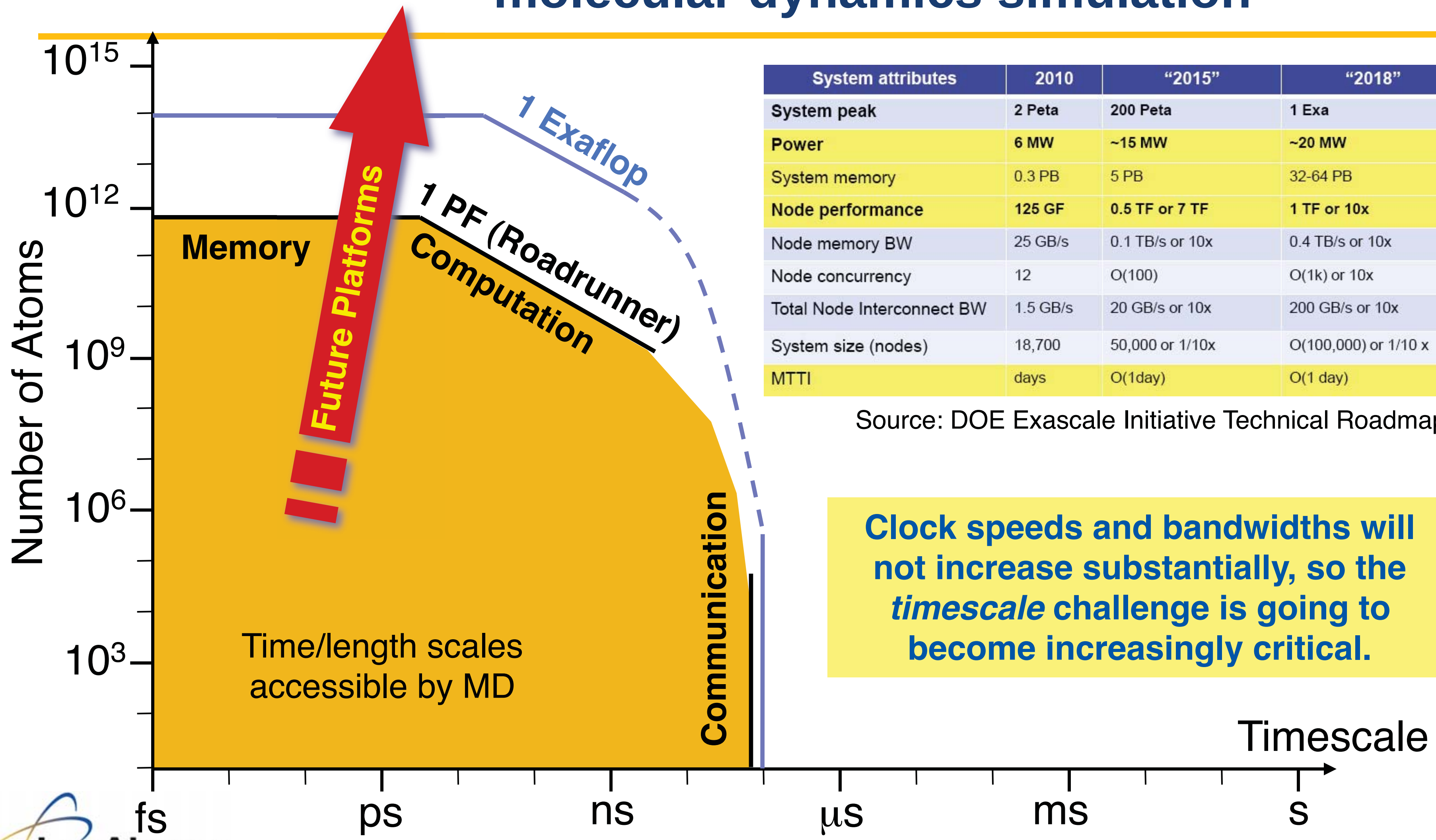
Shocked nc-Ta
~100 M atoms
(Ramon Ravelo)



Current and future capabilities of classical MD simulations



Current HPC trends will increase the *length*, but not *time*, scales accessible by molecular dynamics simulation



System attributes	2010	"2015"	"2018"
System peak	**2 Peta**	**200 Peta**	**1 Exa**
Power	**6 MW**	**~15 MW**	**~20 MW**
System memory	0.3 PB	5 PB	32-64 PB
Node performance	**125 GF**	**0.5 TF or 7 TF**	**1 TF or 10x**
Node memory BW	25 GB/s	0.1 TB/s or 10x	0.4 TB/s or 10x
Node concurrency	12	O(100)	O(1k) or 10x
Total Node Interconnect BW	1.5 GB/s	20 GB/s or 10x	200 GB/s or 10x
System size (nodes)	18,700	50,000 or 1/10x	O(100,000) or 1/10 x
MTTI	days	O(1day)	O(1 day)

Source: DOE Exascale Initiative Technical Roadmap

Clock speeds and bandwidths will not increase substantially, so the *timescale* challenge is going to become increasingly critical.

Preparing for exascale: issues to confront

- **Computer architectures are becoming increasingly heterogeneous and hierarchical, with greatly increased flop/byte ratios.**
- **The algorithms, programming models, and tools that will thrive in this environment must mirror these characteristics.**
- **Bulk synchronous (10^9-way) parallelism will no longer be viable.**
- **Power, energy, and heat dissipation are increasingly important.**
- **Traditional global checkpoint/restart is becoming impractical.**
  - Local flash memory?
- **Fault tolerance and resilience**
  - Recovering from soft and hard errors, and anticipating faults
  - MPI/application ability to drop or replace nodes
  - The curse of silent errors
- **Analysis and visualization**
  - *In situ*, e.g. “active storage” using I/O nodes?

Everything Must Change

news

Technology | DOI:10.1145/1978542.1978549

Supercomputing's Exaflop Target

The twin challenges of parallelism and energy consumption are enlivening supercomputers' progress.

ASIA HAS COME out swinging at the top of June 2011's Top500 list, which rates the world's fastest computers based on the LINPACK benchmark. Leading the list is the K Computer, which achieved 8.2 quadrillion floating-point operations per second (petaflops) to give Japan its first appearance in the much-coveted number-one position since November 2004. It knocks China's Tianhe-1A, at 2.6 petaflops, to second place. The U.S.'s Jaguar (1.75 petaflops) was pushed from second to third place. China's Nebulae (1.27 petaflops) dropped from third to fourth, and Japan's Tsubame 2.0 (1.19 petaflops) slipped from fourth to the fifth position.

Asia's success comes at a time when national governments are reconsidering the value of these ratings—and what defines supercomputing success. The U.S. President's Council of Advisors on Science and Technology (PCAST) recently warned that a focus on such rankings could "crowd out … fundamental research in computer science and engineering." Even Jack Dongarra, the list's founder and a computer science professor at the University of Tennessee, believes the rankings need to be seen in a larger context. "You can't judge a car solely by how many RPMs its engine can do," he says, pointing to the Graph500 list and
Challenge Benchmark as other sou
of comparative supercomputing da

Computer scientists are also skep
cal about the value of such ranking
Petaflops are not the same as usefu
work; practical applications need to
both preserve and take advantage of
their power. Xuebin Chi, director of
the Supercomputing Center at the Chinese Academy of Sciences, points out
that "programming [for the CPU/GPU

**The Top500's leading su
competitors combined.**

combinations now po
computing] is more di
commodity CPUs," and
ing from sequential to p
not easy." He predicts tha
sition would take three t
But even with super
real-world

enators cited Tianhe-1A
letter to President Obama warni
that "the race is on" to develop super
computers capable of 1,000 petaflops

Communications of the ACM, Aug 2011

NEWSFOCUS

What It'll Take To Go Exascale

Scientists hope the next generation of supercomputers will carry out a million trillion operations per second. But first they must change the way the machines are built and run

USING REAL CLIMATE DATA, SCIENTISTS AT LAWRENCE BERKELEY National Laboratory (LBNL) in California recently ran a simulation on one of the world's most powerful supercomputers that replicated the number of tropical storms and hurricanes that had occurred over the past 30 years. Its accuracy was a landmark for computer modeling of global climate. But Michael Wehner and his LBNL colleagues have their eyes on a much bigger prize: understanding whether an increase in cloud cover from rising temperatures would retard climate change by reflecting more light back into space, or accelerate it by trapping additional heat close to Earth.

To succeed, Wehner must be able to model individual cloud systems on a global scale. To do that, he will need supercomputers more powerful than any yet designed. These so-called exascale computers would be capable of carrying out 10^{18} floating point operations per second, or an exaflop. That's nearly 100 times more powerful than today's biggest supercomputer, Japan's "K Computer," which achieves 11.3 petaflops (10^{15} flops) (see graph), and 1000 times faster than the Hopper supercomputer used by Wehner and his colleagues. The United States now appears poised to reach for the exascale, as do China, Japan, Russia, India, and the European Union.

It won't be easy. Advances in supercomputers have come at a steady pace over the past 20 years, enabled by the continual improvement in computer chip manufacturing. But this evolutionary approach won't cut it in getting to the exascale. Instead, computer scientists must first figure out ways to make future machines far more energy efficient and tolerant of errors, and find novel ways to program them.

"The step we are about to take to exascale computing will be very, very difficult," says Robert Rosner, a physicist at the University of Chicago in Illinois, who chaired a recent Department of Energy (DOE)
mmittee charged with exploring whether exascale computers would
ble. Charles Shank, a former director of LBNL who recently
separate panel collecting widespread views on what it would
uild an exascale machine, agrees. "Nobody said it would be
ble," Shank says. "But there are significant unknowns."

ng support

ext generation of powerful supercomputers will be used to
n high-efficiency engines tailored to burn biofuels, reveal the
es of supernova explosions, track the atomic workings of cata-
lysts in real time, and study how persistent radiation damage might affect the metal casing surrounding nuclear weapons. "It's a tech-

Online
sciencemag.org
Podcast by author Robert F. Service.

On fire. More powerful supercomputers now in the design stage should make modeling turbulent gas flames more accurate and revolutionize engine designs.

CREDIT: J. CHEN/CENTER FOR EXASCALE SIMULATION OF COMBUSTION IN TURBULENCE, SANDIA NATIONAL LABORATORIES

ed by AAAS

Science, 27 Jan 2012

---

the 451 group
Analyzing the Business of Enterprise IT Innovation

system to the next can often be described as "more of the same, but bigger and faster." The move to exascale systems is different, however – everything has to change.

ICE | INFRASTRUCTURE COMPUTING FOR THE ENTERPRISE

4 FINDINGS

- The high power consumption of current high-end systems cannot extend to exascale systems. **PAGE 7**

5 IMPLICATIONS

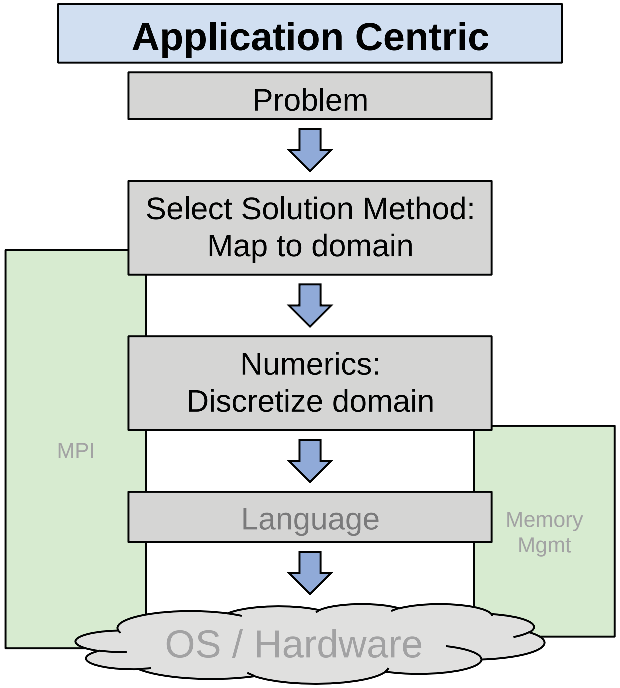
- Tomorrow's high-end systems will use different memory technologies to deliver low power, including 3D stacking. **PAGE 16**

1 BOTTOM LINE

- The huge changes required to build exascale systems are such that all of the HPC community must work together to design

Current science application development strategies are difficult to sustain

An air gap has been encouraged between application developers & system / OS developers and the hardware



Application Centric

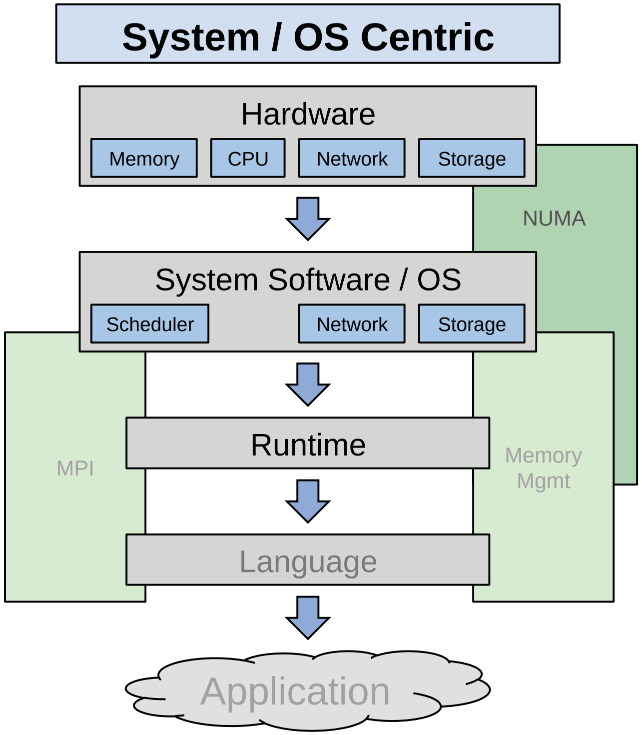
Problem

Select Solution Method:
Map to domain

Numerics:
Discretize domain

Language

OS / Hardware



System / OS Centric

Hardware
Memory | CPU | Network | Storage

System Software / OS
Scheduler | Network | Storage

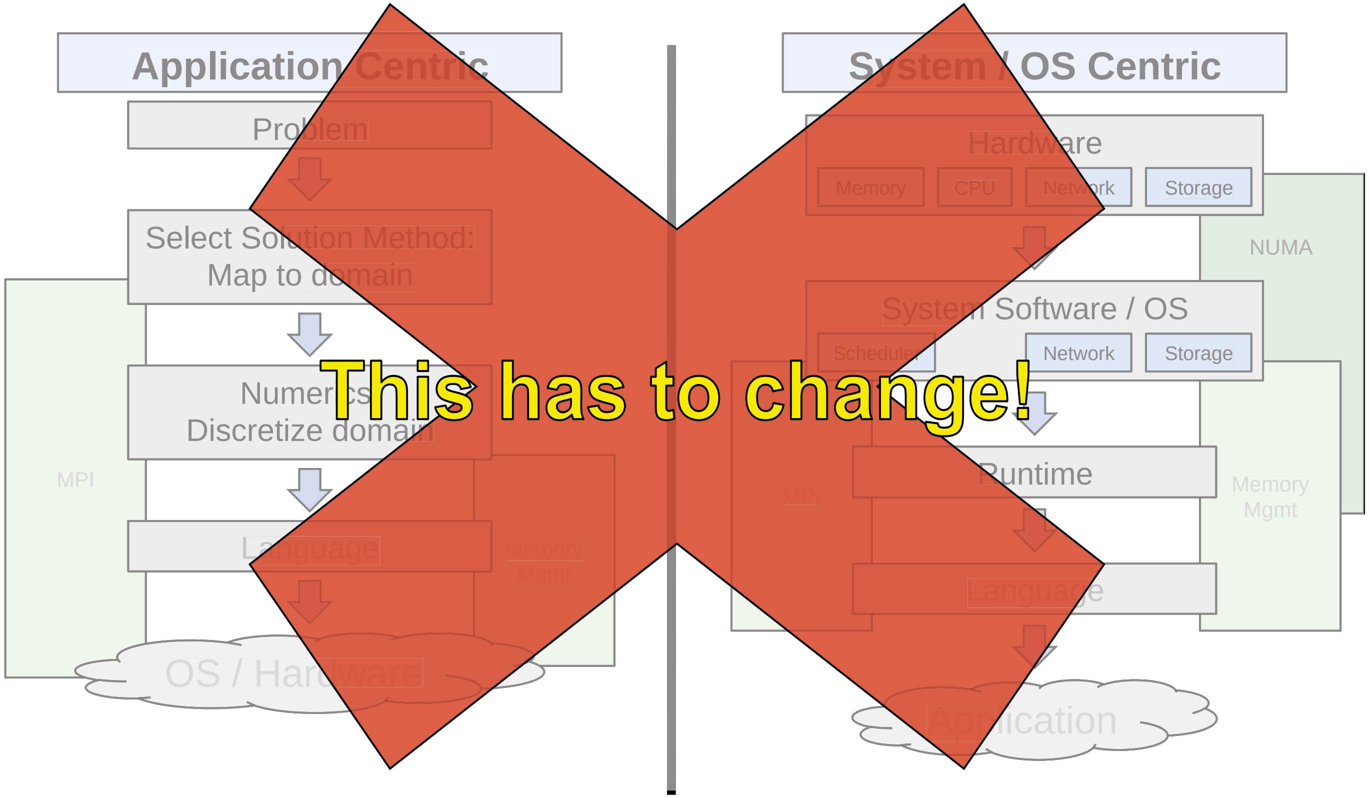
Runtime

Language

Application

Current science application development strategies are difficult to sustain

An air gap has been encouraged between application developers & system / OS developers and the hardware



Application Centric

Problem

Select Solution Method: Map to domain

Numerics Discretize domain

Language

OS / Hardware

MPI

Memory Mgmt

System / OS Centric

Hardware

Memory CPU Network Storage

NUMA

System Software / OS

Scheduler Network Storage

Runtime

MPI

Memory Mgmt

Language

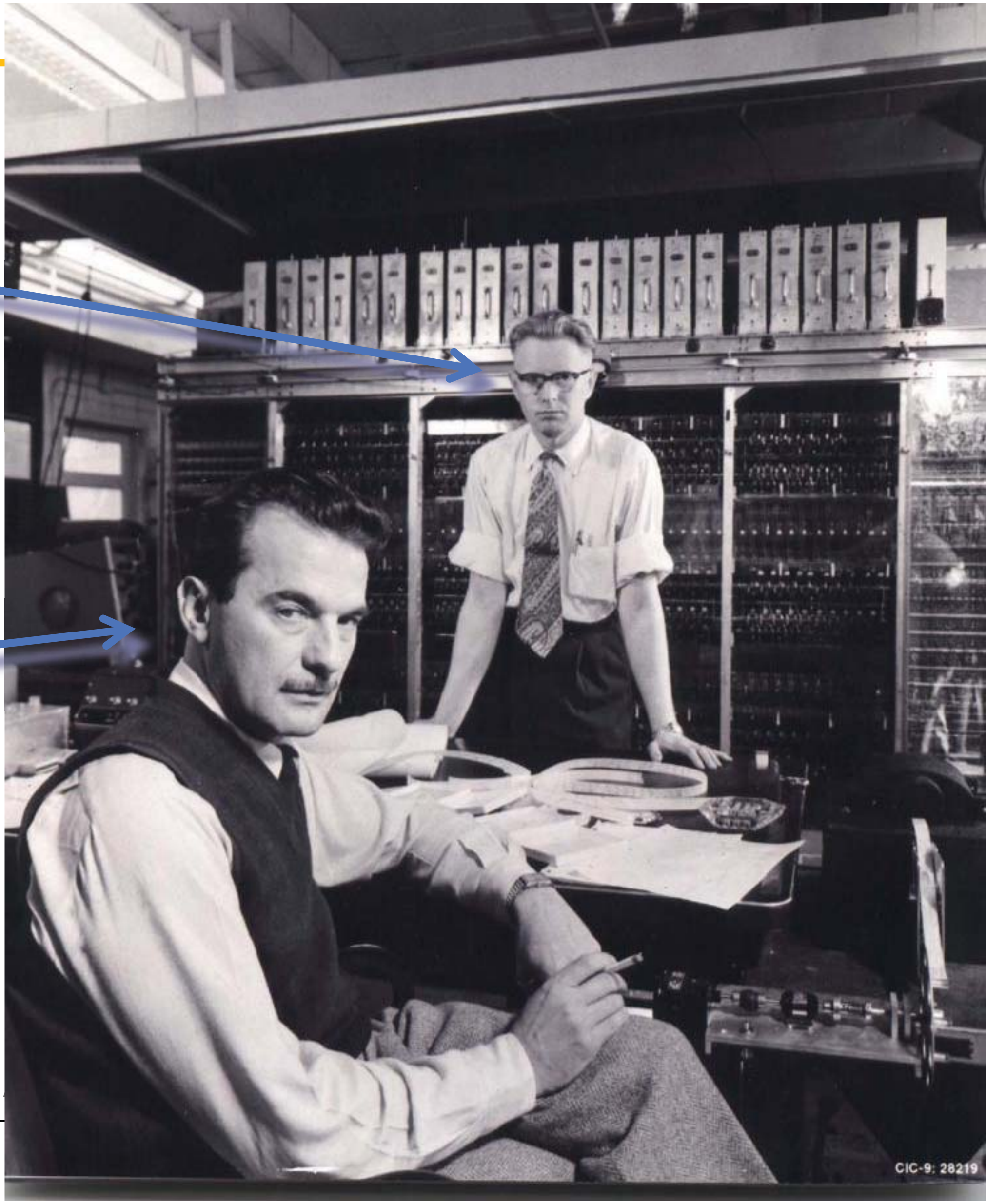
Application

This has to change!

Co-design is a process by which computer science, applied math, and domain science experts work together to enable scientific discovery

- **Hardware is changing dramatically**
  - Comparable to the transition from vector to parallel supercomputers
- **Algorithms and methods will have to be rethought / revisited**
  - It isn't just "porting" code
  - Flops are (almost always) free
  - Memory is at a premium
  - Power is a constraint for large scale systems
  - Resiliency is a challenge
- **Few domain scientists have the extended expertise "from hardware to application" to enable applications to run at exascale.**
- **Success on the next generation of machines will require extensive collaboration between domain scientists, applied mathematicians, computer scientists, and hardware manufacturers.**

Los Alamos computational co-design, circa 1950



Hardware architect (Richardson)

Application scientist (Metropolis)

H. L. Anderson,
“Metropolis, Monte Carlo, and the MANIAC,”
Los Alamos Science **14**, 96-107 (1986).

Los Alamos computational co-design, circa 2008

- **Roadrunner was a leap into the future**
  - First computer to reach a petaflop
  - First *heterogeneous* supercomputer
  - First *accelerated* supercomputer
  - Demonstrated that accelerated supercomputing was possible
  - 96% of compute power concentrated in accelerators
- **Success required domain scientists, applied mathematicians, and computer scientists working together to identify the correct abstractions for domain science, applied mathematics, programming models, and hardware**
- **Many successful applications, including**
  - Large Scale MD*
  - Long time MD
  - Roadrunner Universe
  - DNS of turbulence
  - VPIC laser backscatter
  - VPIC magnetic reconnection
  - Supernova simulations
  - HIV phylogenetics

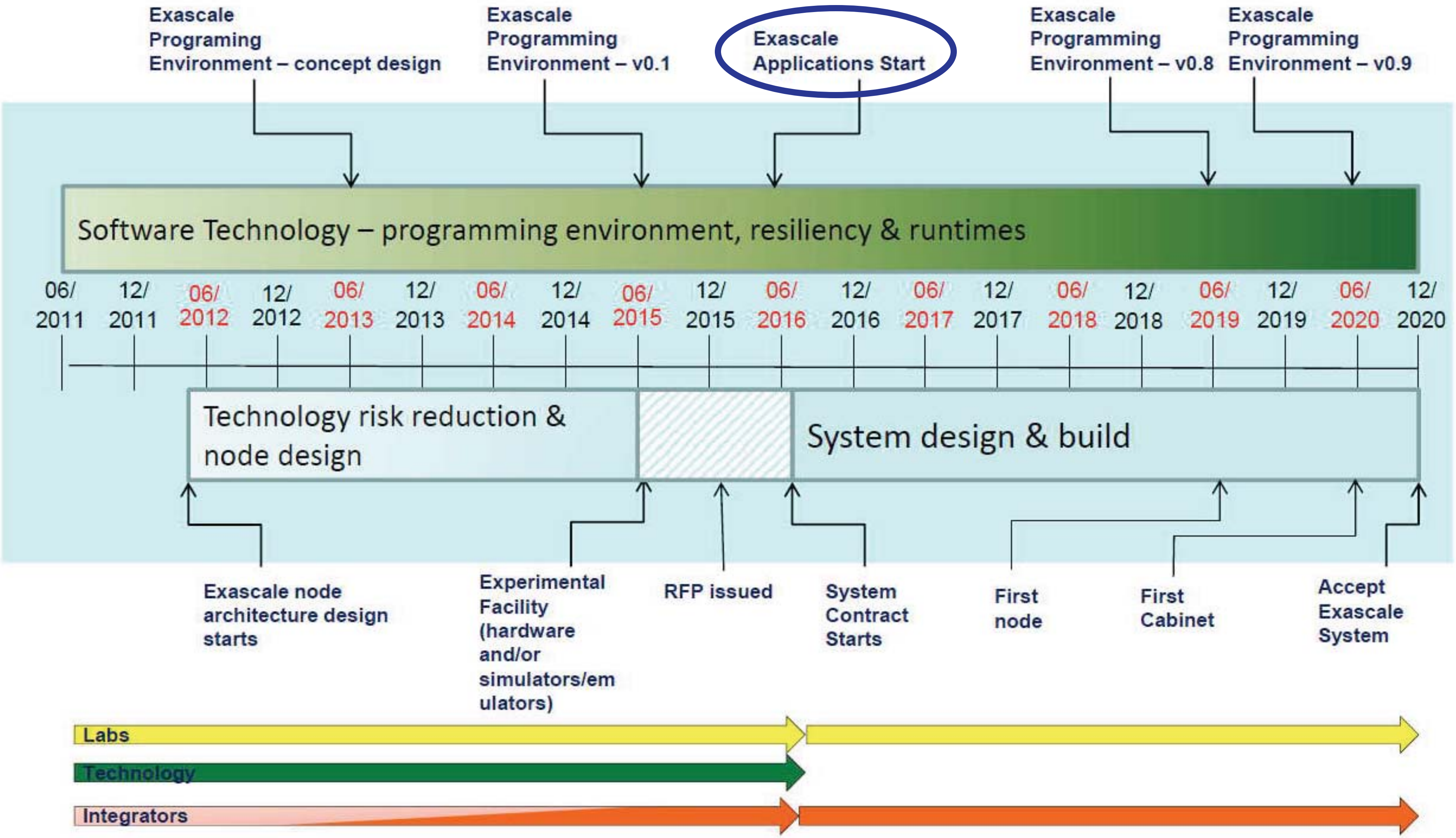
UNCLASSIFIED

*T.C. Germann, K. Kadau, and S. Swaminarayan, *Concurrency Comput.: Pract. Exper.* **21**, 2143 (2009)

U.S. DEPARTMENT OF ENERGY

Exascale Reverse Timeline

(from Arch I Workshop, Stanford, August 2-3, 2011)



Exascale Programing Environment – concept design

Exascale Programming Environment – v0.1

Exascale Applications Start

Exascale Programming Environment – v0.8

Exascale Programming Environment – v0.9

Software Technology – programming environment, resiliency & runtimes

06/ 2011 | 12/ 2011 | 06/ 2012 | 12/ 2012 | 06/ 2013 | 12/ 2013 | 06/ 2014 | 12/ 2014 | 06/ 2015 | 12/ 2015 | 06/ 2016 | 12/ 2016 | 06/ 2017 | 12/ 2017 | 06/ 2018 | 12/ 2018 | 06/ 2019 | 12/ 2019 | 06/ 2020 | 12/ 2020

Technology risk reduction & node design

System design & build

Exascale node architecture design starts

Experimental Facility (hardware and/or simulators/emulators)

RFP issued

System Contract Starts

First node

First Cabinet

Accept Exascale System

Labs

Technology

Integrators

Three Exascale Co-Design Centers Awarded

Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx)

Director: Timothy Germann (LANL)

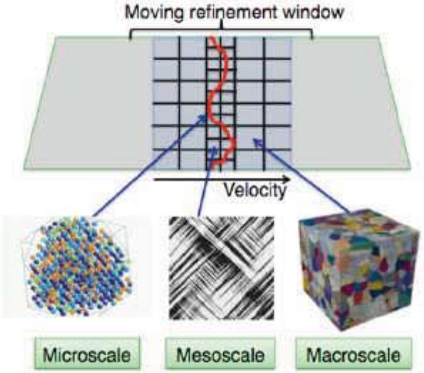
Center for Exascale Simulation of Advanced Reactors (CESAR)

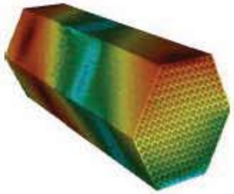
Director: Robert Rosner (ANL)

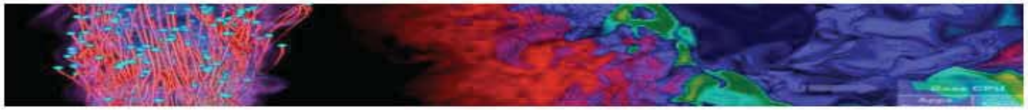
Combustion Exascale Co-Design Center (CECDC)

Director: Jacqueline Chen (SNL)

	ExMatEx (Germann)	CESAR (Rosner)	CECDC (Chen)
National Labs	LANL	ANL	SNL
	LLNL	PNNL	LBNL
	SNL	LANL	LANL
	ORNL	ORNL	ORNL
		LLNL	LLNL
			NREL
University & Industry Partners	Stanford	Studsvik	Stanford
	CalTech	TAMU	GA Tech
		Rice	Rutgers
		U Chicago	UT Austin
		IBM	Utah
		TerraPower	
		General Atomic	
		Areva	

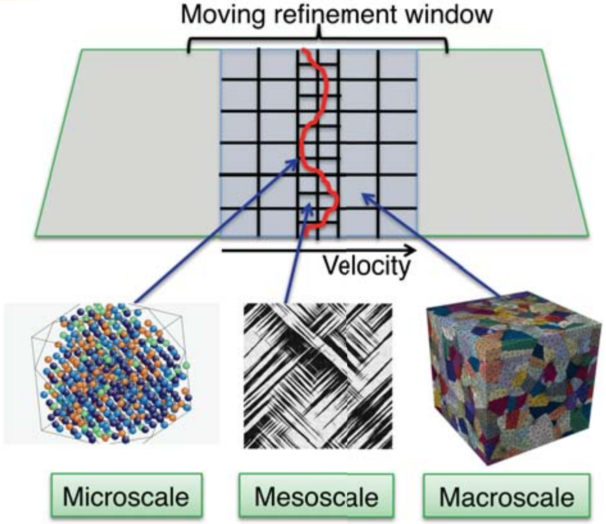






Exascale Co-design Center for Materials in Extreme Environments (ExMatEx)

- **One of three DOE/SC/ASCR co-design centers**
- **Large scale collaboration between national labs, industry and academia**
- **Goal: Establish relationship between algorithms, software stack, and architectures to enable exascale-ready materials science apps in ~2020**
- **Strategy: Exploit hierarchical, heterogeneous architecture to achieve more realistic large-scale simulations with adaptive physics refinement**



ExMatEx

Los Alamos National Laboratory EST. 1943

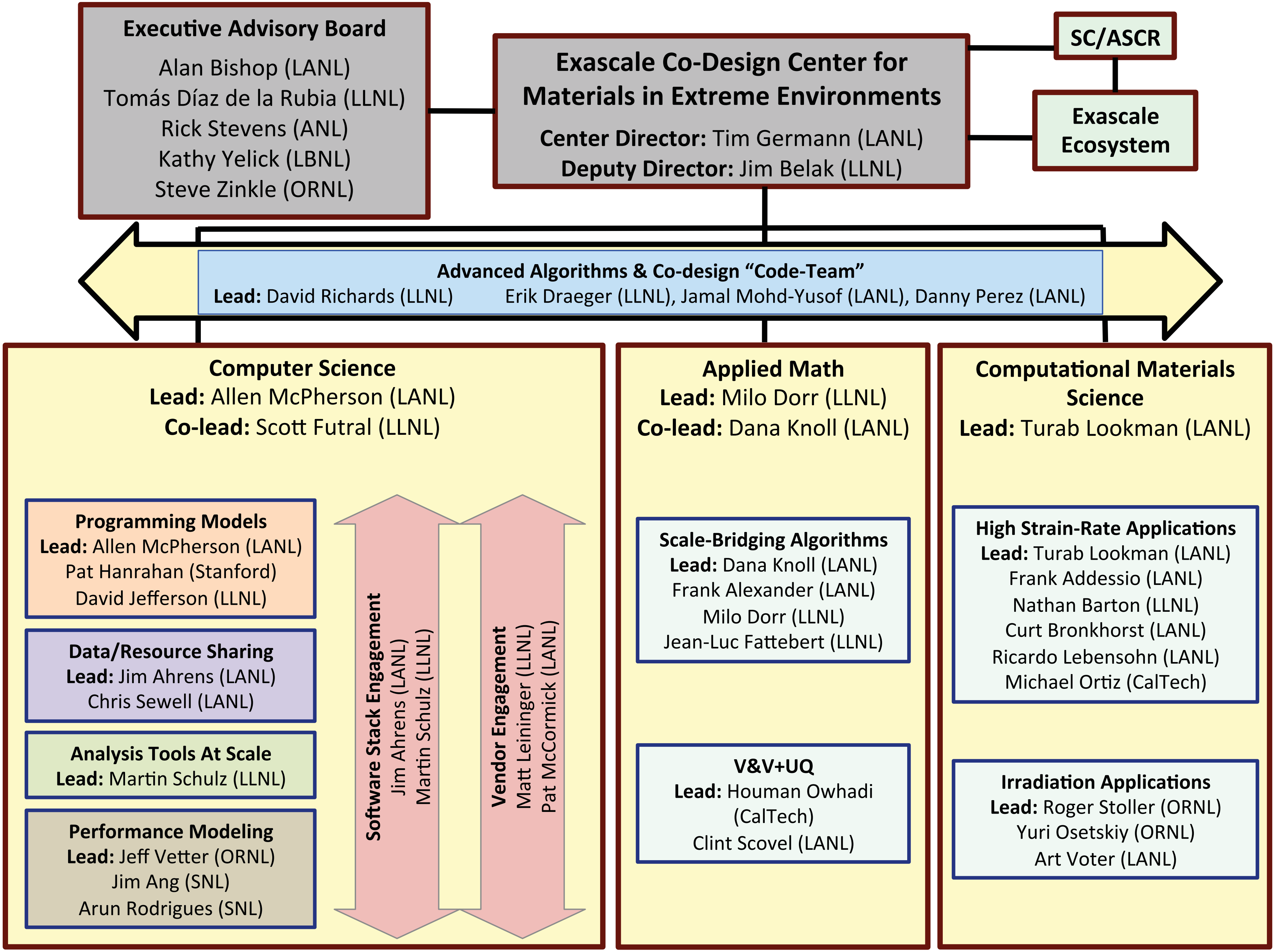
Lawrence Livermore National Laboratory

Oak Ridge National Laboratory

Stanford University

Sandia National Laboratories

California Institute of Technology 1891



Executive Advisory Board
Alan Bishop (LANL)
Tomás Díaz de la Rubia (LLNL)
Rick Stevens (ANL)
Kathy Yelick (LBNL)
Steve Zinkle (ORNL)

Exascale Co-Design Center for Materials in Extreme Environments
Center Director: Tim Germann (LANL)
Deputy Director: Jim Belak (LLNL)

SC/ASCR

Exascale Ecosystem

Advanced Algorithms & Co-design "Code-Team"
Lead: David Richards (LLNL) Erik Draeger (LLNL), Jamal Mohd-Yusof (LANL), Danny Perez (LANL)

Computer Science
Lead: Allen McPherson (LANL)
Co-lead: Scott Futral (LLNL)

Programming Models
Lead: Allen McPherson (LANL)
Pat Hanrahan (Stanford)
David Jefferson (LLNL)

Data/Resource Sharing
Lead: Jim Ahrens (LANL)
Chris Sewell (LANL)

Analysis Tools At Scale
Lead: Martin Schulz (LLNL)

Performance Modeling
Lead: Jeff Vetter (ORNL)
Jim Ang (SNL)
Arun Rodrigues (SNL)

Software Stack Engagement
Jim Ahrens (LANL)
Martin Schulz (LLNL)

Vendor Engagement
Matt Leininger (LLNL)
Pat McCormick (LANL)

Applied Math
Lead: Milo Dorr (LLNL)
Co-lead: Dana Knoll (LANL)

Scale-Bridging Algorithms
Lead: Dana Knoll (LANL)
Frank Alexander (LANL)
Milo Dorr (LLNL)
Jean-Luc Fattebert (LLNL)

V&V+UQ
Lead: Houman Owhadi (CalTech)
Clint Scovel (LANL)

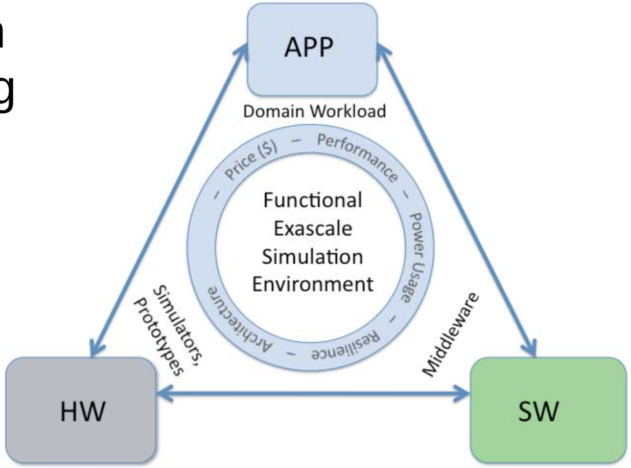
Computational Materials Science
Lead: Turab Lookman (LANL)

High Strain-Rate Applications
Lead: Turab Lookman (LANL)
Frank Addessio (LANL)
Nathan Barton (LLNL)
Curt Bronkhorst (LANL)
Ricardo Lebensohn (LANL)
Michael Ortiz (CalTech)

Irradiation Applications
Lead: Roger Stoller (ORNL)
Yuri Osetskiy (ORNL)
Art Voter (LANL)

ExMatEx Co-Design Project Goals

- Our **goal** is to establish the interrelationship between hardware, middleware (software stack), programming models, and algorithms required to enable ***a productive exascale environment*** for multiphysics simulations of materials in extreme mechanical and radiation environments.
- We will exploit, rather than avoid, the greatly increased levels of concurrency, heterogeneity, and flop/byte ratios on the upcoming exascale platforms.



- Our **vision** is an uncertainty quantification (UQ)-driven adaptive physics refinement in which meso- and macro-scale materials simulations spawn micro-scale simulations as needed.
  - This *task-based* approach leverages the extensive concurrency and heterogeneity expected at exascale while enabling fault tolerance within applications.
  - The programming models and approaches developed to achieve this will be broadly applicable to a variety of multiscale, multiphysics applications: astrophysics, climate and weather prediction, structural engineering, plasma physics, radiation hydrodynamics, etc.

Agile proxy application development

- Petascale single-scale and scale-bridging proxy apps will be used to explore algorithm and programming model design space with domain experts, hardware architects and system software developers.
- Proxy apps communicate the application workload to the hardware architects and system software developers, and are used in models/ simulators/emulators to assess performance, power, and resiliency.
- These are not "toy models", but realistically encapsulate the workload, data flow and mathematical algorithms of the full applications.

1998 GORDON BELL PRIZE

Perform

Michael S. Warren, Timothy

John K. Sal

For Th

Avalon: An Alpha/Linu

COMPUTER SOCIETY

SC07

Reno-Sparks Convention Center • November 10-16, 2007

Gordon Bell Prize

James N. Glosli, Kyle J. Caspersen,
David F. Richards, Robert E. Rudd,
Frederick H. Streitz,
Lawrence Livermore National Laboratory
John A. Gunnels, IBM Corporation

Extending Stability Beyond CPU-Millennium:
Micron-Scale Atomistic Simulation of Kelvin-Helmholtz Instability

Becky Verastegui, Conference Chair

David H. Bailey, Gordon Bell Prize Chair

SC06

POWERFUL BEYOND IMAGINATION

Gordon Bell Prize WINNER

Peak Performance Award

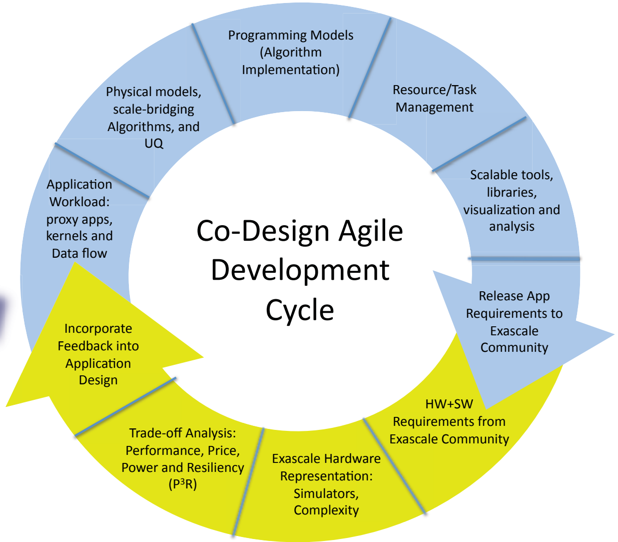
"Large-scale Electronic Structure Calculations of High-Z Metals on the BlueGene/L Platform"

Francois Gygi, *University of California, Davis;*
Erik W. Draeger, Martin Schulz, Bronis R. de Supinski, *Lawrence Livermore National Laboratory;*
John A. Gunnels, Vernon Austel, James C. Sexton, *IBM;*
Franz Franchetti, *Carnegie Mellon University;* and
Stefan Kral, Christoph W. Ueberhuber, Juergen Lorenz, *Vienna University of Technology*

SC06 GORDON BELL PRIZE CHAIR

Barbara Horner-Miller

SC06 GENERAL CHAIR



Agile proxy application development

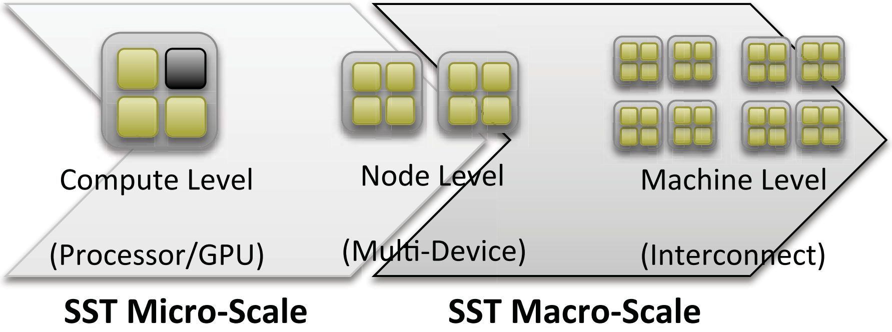
- **Proxy apps for single-scale applications (e.g. molecular dynamics) will be used to assess node-level issues including:**
  - Data structures
  - Hierarchical memory storage and access
  - Power management strategies
  - Node-level performance
- **Asynchronous task-based scale-bridging proxy apps will be used to optimize:**
  - System-level data movement
  - Resilience (fault management)
  - Load balancing techniques
  - Performance scalability
- **These proxy apps are not static entities, but the central mechanism for our co-design process.**
- **Application, software, and hardware communities must all analyze and respond to trade-offs with new requirements and capabilities.**

Single-scale proxy app: Co-designed Molecular Dynamics (CoMD)

- Available at https://github.com/exmatex/CoMD (LA-CC-11-119)
- (Analytic) Lennard-Jones and (tabular) embedded atom method potentials
- On-the-fly centrosymmetry analysis and Visualization Toolkit (VTK) library or pure OpenGL visualization
- On-node implementations in C, OpenCL, and OpenMP
- Both Structure-of-Arrays and Array-of-Structures data layouts
- OpenCL: ~10x speedup on a 12-core Xeon, ~100x speedup on graphics processor
- Following February workshop in Santa Fe, the compiler team at Intel is using CoMD to improve the performance of their MIC (many integrated core) compiler

Structural Simulation Toolkit (SST) Analysis of Proxy Apps

- **Understanding the potential performance of code at large scale and on alternative hardware architectures is particularly challenging for applications which will need to perform at Exascale.**
- **ExMatEx is using two flavors of the Structural Simulation Toolkit (Micro- and Macro-Scale) to provide insight in this area.**
- **Materials proxy apps are stressing SST capabilities.**


Compute Level

(Processor/GPU)

Node Level

(Multi-Device)

Machine Level

(Interconnect)

SST Micro-Scale

SST Macro-Scale

SST Micro simulating serial LULESH on an AMD A8 2.90 GHz (2011) Core

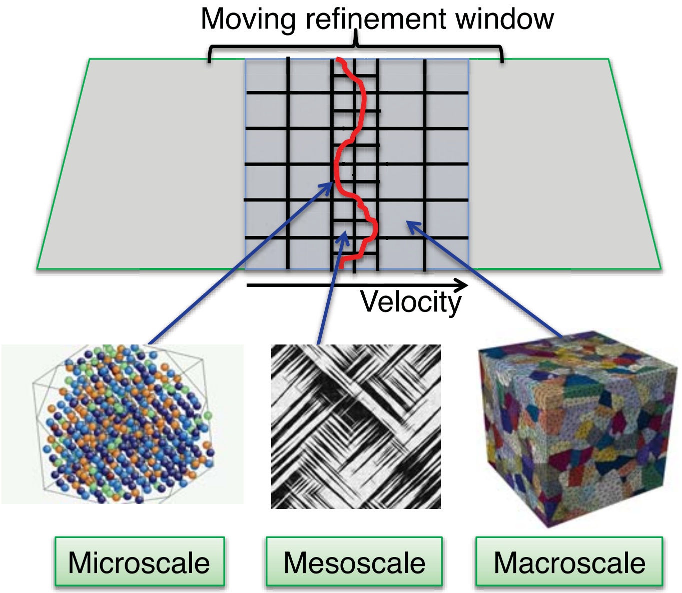
Iterations	Actual (s)	Predicted (s)	Error (%)
10	1.5060	1.6200	7.57
20	2.9360	3.3771	15.02
30	4.2480	5.2400	23.35
40	5.9110	6.7500	14.19

SST Macro simulating LULESH MPI on a cluster of 27 AMD A8 2.9GHz (2011) cores

Iterations	Actual (s)	Predicted (s)	Error (%)
4177	1065.77	811.77	23.83

Embedded Scale-Bridging Algorithms

- **Our goal is to introduce more detailed physics into computational materials science applications in a way which escapes the traditional synchronous SPMD paradigm and exploits the heterogeneity expected in exascale hardware.**
- **To achieve this, we are developing a UQ-driven *adaptive physics refinement* approach.**
- **Coarse-scale simulations dynamically spawn tightly coupled and self-consistent fine-scale simulations as needed.**
- **This *task-based* approach naturally maps to exascale heterogeneity, concurrency, and resiliency issues.**



Embedded Scale-Bridging Algorithms

- **Scale-bridging algorithms require a consistent two-way algorithmic coupling between temporally evolving distinct spatial levels; they are not "modeling", and not one-way information flow.**
- **Our focus is on coupling between macro (coarse-scale model) and meso (fine-scale model) scales with all unit physics being deterministic.**
- **We begin by building off of our adaptive sampling* success, but move to the use of temporally evolving mesoscale and spatial adaption.**
- **Similar concepts apply in the time domain, e.g. using *ab initio* techniques to compute activation energies for a rate theory or kinetic Monte Carlo model ("on-the-fly kMC") applied to radiation damage modeling.**

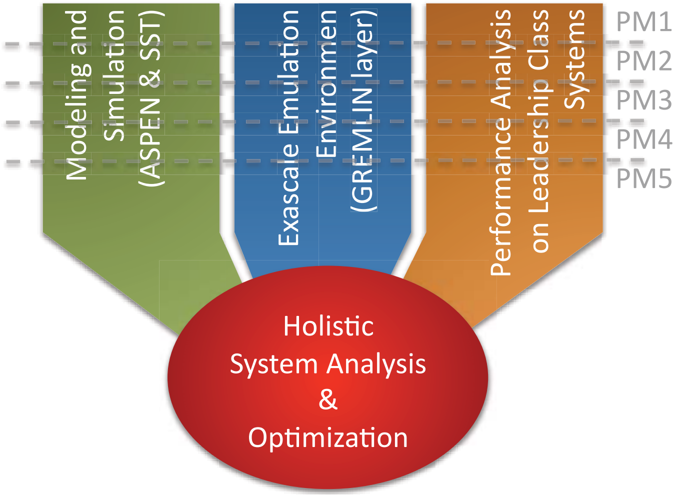
*N.R. Barton, J.V. Bernier, J. Knap, *et al*,
Int. J. Numer. Meth. Engng **86**, 744–764 (2011).

Application friendly programming models

- **A hierarchy of programming models exposes and exploits the architectural heterogeneity, while providing a transparent layer of abstraction that insulates the application programmer from the continuous flux and complexity of the underlying hardware.**
- **We implement abstractions…**
  - …on top of the technologies proven by the proxies
    - *Abstractions “compile” to underlying technology*
  - …as libraries, run-time systems, domain-specific languages
    - *Domain science abstractions, e.g. meshes, particles, halo communication, etc.*
    - *System-level abstractions, e.g. interoperability (resource sharing) for scale-bridging, in situ visualization, tools, scheduling, load-balancing, fault tolerance, etc.*

Holistic analysis and optimization

- **A hierarchy of performance models, simulators, and emulators are used to explore algorithm, programming model, and hardware design space and perform trade-off analysis between competing requirements and capabilities in a tightly coupled optimization loop.**
- **Node- to system-level models and simulators**
  - *ASPEN: Rapid exploration of design space using application skeletons*
  - *SST: Detailed simulation of data flow, performance and energy/power cost*



- **Exascale emulation layer (GREMLIN) to introduce perturbations similar to those expected on future architectures**
- **Performance analysis on hardware prototypes & leadership-class machines**
- **Trade-offs to co-optimize algorithms & architectures for price, performance, power (chiefly memory and data movement), and resilience (P^3R)**

Summary

- **Our objective is to establish the interrelationship between algorithms, system software, and hardware required to develop a multiphysics exascale simulation framework for modeling materials subjected to extreme mechanical and radiation environments.**

- **This effort is focused in four areas:**
  - Proxy applications
    - Communicate the application workload to the hardware architects and system software developers, and used in performance models/simulators/emulators
  - Scale-bridging algorithms
    - Uncertainty Quantification (UQ)-driven adaptive physics refinement
  - Programming models
    - Task-based multiple-program, multiple-data (MPMD) approaches to leverage concurrency and heterogeneity at exascale while enabling fault tolerance
  - Co-design analysis and optimization
    - Optimization of algorithms and architectures for performance, memory and data movement, power, and resiliency

A Multi-mesoscale Predictive Capability for Interface-driven Behavior

I. Beyerlein (T-3); K. Barros (CNLS); C. Bronkhorst (T-3); J. Carpenter (MST-6); H. Chu (MST-8); W. Han (CINT); B. Hansen K. Kang (T-3); T. Lookman (T-4); N. Mara (CINT); J. Mayeur (T-3); R. McCabe (MST-6); H. Mourad (T-3); J. Wang (MST-8); R. Zhang (T-3); S. Zheng (CINT); C. Zhou (T-3)

In bulk multi-phase composite metals containing an unusually high density of heterophase interfaces, the bi-metal interface controls all defect-related processes. Quite unconventionally, the constituent phases play only a secondary role. With the 'right' characteristics, these bi-material interfaces can possess significantly enhanced abilities to absorb and eliminate defects. Through their unparalleled ability to mitigate damage accumulation induced under severe loading and/or severe environments, they will provide their parent composite with a highly effective healing mechanism and consequently an unrivaled robustness not possible in existing advanced structural materials. Today's bulk synthesis techniques and materials models, however, are unprepared to treat materials that are dominated by bi-metal interfaces. In this program, we aim to develop and validate a new meso, multi-Scale (M2S) model in order to predict the evolution of the interfacial structure and behavior during bulk large strain deformation. To succeed in this effort, we are co-designing many new theoretical and simulation models that uniquely account for the special roles of bi-metal interfaces in plastic deformation. This multi-scale predictive capability will offer a tool to address materials falling within the new paradigm of interface dominance and to predict the synthesis routes needed for a targeted set of desired interfacial properties.

Computational Co-design for Multi-Scale Application in the Natural Sciences (CoCoMANS)

V. Dupont, T.C. Germann (T-1); S. Pakin, A.L. McPherson (CCS-7); S. Mao, D.Z. Zhang, D. Knoll (T-3)

Forge a qualitatively new capability exploiting evolving high-performance computer architectures for multiple national-security-critical application areas. Simultaneously evolving science, methods, software, and hardware in an integrated computational co-design process.

- Develop new "applications-based", self consistent, two-way, scale-bridging methods that have broad applicability to the targeted science.
- Map well to emerging heterogeneous computing models (while concurrently guiding hardware and software to maturity).
- Provide the algorithmic acceleration necessary to probe new scientific challenges at unprecedented scales.
- Foster broad, long-term research collaborations with appropriate hardware partners.

Optimization Principles for Computational Co-Design with Applications to Molecular Dynamics

S. Eidenbenz (PI, CCS-3); K. Davis (Co-PI, CCS-7); A. Voter (Co-PI, T-1); H. Djidjev, L. Gurvits (CCS-3); C. Junghans (T-1); S. Mniszewski (CCS-3); D. Perez (T-1); N. Santhi, S. Thulasidasan (CCS-3)

The objective of the research project *Optimization Principles for Codesign applied to Molecular Dynamics* at Los Alamos National Laboratory is to develop methodological and software frameworks for *hardware-software codesign as a formally posed optimization problem*. While the optimization framework will be applicable to multiple problem domains, for the target application we use *molecular dynamics (MD),* an exemplar for the need for computational scaling (weak, strong, and combinations of both), and archetypical of the obstacles thereof. We view codesign as search and selection from a vast space of hardware and software designs that map to performance metrics. The objective functions that we optimize for have components such as *run time (or computational rate), problem size, simulated time duration, energy use,* and *hardware cost.*

Our semi-formal codesign optimization framework relies on

1. **Efficient enumeration methods** for finding feasible hardware architectures and software designs;
2. **A multi-scale approach to performance prediction modeling**, where we use cycle-accurate virtual machine emulation, discrete event simulation, graph mapping, and constraint programming as different prediction methodologies; and
3. **Optimization methods with fast identification of new hardware-software pairs** to be tested with the more detailed performance prediction methods.

From our chosen applications domain, molecular dynamics, we will develop atomistic simulation tools that will enable the study of processes such as *ductile spall failure* under shock conditions and the *evolution of radiation damage*. Achieving this requires a two order of magnitude increase in simulated time over current state-of-the art petascale computing, and more importantly cannot be realized without this codesign approach, as direct implementation on an exascale platform cannot achieve this. These two applications address issues of the response of materials in extreme conditions and enabling the design of more effective and safe fission power plants, respectively.

Codesign for Materials: Confluence of MaRIE and Exascale

T. Lookman (T-4); F. Addessio, C. Bronkhorst (T-3); D. Brown, E. Cerreta (MST-8); X. Ding (T-4); D. Knoll (T-3); J. Scovel, M. Wall (CCS-3)

This poster captures ideas, as well as some work over the last couple of years, in extending the traditional paradigm of codesign to include domain sciences. In particular, it discusses a pilot project that includes theory, experiment and computation all focused on understanding the development and evolution of microstructure in a shocked phase transforming material. Theory makes certain predictions in given regimes of the phase diagram that experiments can probe. Simulations guide what experiments should see, which in turn inform simulations as well the theory. Ultimately with imaging and visualization tools the objective is to have quantitative information flow or feedback in real time. The work is an attempt at small steps towards the notion of constrained optimization and involving multiple domains, including the application area of materials dynamics.

Increasing the Timescale of Atomistic Simulations through Co-designed Accelerated Molecular Dynamics Methods

D. Perez, C. Junghans, A.F. Voter (T-1); T. Lelievre, C. Le Bris (École des Ponts); M. Luskin (U. of Minnesota); S. Eidenbenz (CCS-3) and LDRD-DR Team

Molecular Dynamics (MD) is one of the most important computational techniques to study the dynamical behavior of matter at the atomic scale. Timescales amenable to MD are however severely restricted, leaving important physical processes out of reach. Following pioneering work at LANL, Accelerated Molecular Dynamics (AMD) methods were developed to expand timescales amenable to MD simulations.

In *Parallel Replica Dynamics (ParRep),* one can parallelize the evolution of the system in the time domain. ParRep is extremely powerful at leveraging parallel computing resources, but its efficiency is ultimately limited by the fastest processes in the system.

We show that ParRep can be applied at a coarse-grained level so as to exploit *any* separation of timescale while maintaining arbitrary accuracy. We show how this extra algorithmic flexibility can be exploited in a co-design effort to develop the next generation of efficient AMD codes.

Understanding, Exploiting, and Controlling Competing Interactions in Complex Oxides

Q.X. Jia, J.H. Lee, Y.H. Lin, R. Prasankumar, J.B. Qi, Y.M. Sheu, L. Yan, D. Yarotski (MPA-CINT); A.V. Balatsky, J. Haraldsen, S. Trugman, J.X. Zhu (T-4); S. Singh, M. Fitzsimmons (LANSCE-LC)

Epitaxial nanocomposites, in which emergent behaviors can be achieved through interfacing different strongly correlated materials at the nanoscale, provide a new design paradigm to produce enhanced and/or novel functionalities that cannot be obtained in the individual constituents. We target to manipulate the competing interactions by designing and synthesizing complex oxide nanocomposites using ferroelectric, ferromagnetic, and high-temperature superconducting materials as the functional components. We pursue a conceptually new approach to design new architectures with entirely new or significantly improved functionalities, by understanding the emergent physics that evolves over multiple length and time scales in these systems. Our ultimate objective is to develop a framework for understanding and controlling the states that emerge from strong electronic correlations. The impact of this project is expected to reach well beyond these particular materials, as this study will enable the transition from “observation and validation” to “prediction and control.”

Co-design Modeling of Reactions Behind a Shock Front

M. Cawkwell, J. Coe, A. Niklasson (T-1); S. Mniszewski (CCS-3); S. McGrane and D. Dattelbaum (WX-9)

Chemical reactions induced by dynamic or shock compression occur over extremely short time scales. While recent time-resolved laser shock and plate impact experiments have provided convincing evidence for shock-induced reactions in organic liquids, the reactions themselves have not been identified unambiguously. Reactive molecular dynamics (MD) simulations access the time scales relevant to shock-induced chemistry but their utility depends strongly on the nature of the interatomic potential that is employed. We have pursued in the LANL-developed, open-source code LATTE the co-design of new algorithms and methods that enable highly accurate, explicitly quantum mechanical interatomic potentials to be used in large-scale MD simulations. We demonstrated recently the first energy conserving, linear scaling, O(N), Born-Oppenheimer MD simulations. Accurate O(N) methods are pivotal for accuracy at extended length and time scales. We have also developed and implemented algorithms that use general-purpose graphics processing units to reduce the computational bottlenecks that arise during the calculation of the interatomic forces. The application of these new theoretical and computational tools to the shock-induced polymerization of simple organic liquids will be illustrated.

Energetic Materials and High Pressure Science

D.J. Funk (WX-DO)

The Manhattan project required the capability to understand and utilize energetic materials (high explosives). This desire to harness the destructive potential of the atom also drove the need developing an understanding of the response of materials to dynamic loading and the extreme conditions of pressure and temperature provided by energetic materials. These same capabilities were used to develop an understanding of the geological implications of underground tests conducted at the Nevada Test Site. Much of the work of yesterday was at the continuum level, and provided enough information such that nuclear testing could be accomplished successfully (albeit in an Edisonian manner). Today, we require these capabilities, but we are conducting research with a different emphasis and focus. We are no longer satisfied with continuum level analysis: we are developing and utilizing new techniques and diagnostics to start to look inside materials, ultimately achieving process aware understanding. Static pressure techniques that were utilized principally for obtaining static Equation of State (EOS) information are being applied to actinide physics, modern studies of carbon sequestration, and understanding the storage and transport of water in the deep earth. Our dynamic material capabilities are being utilized in support of Global Security mission goals: principally Protecting Against Nuclear Threats, but also in a supporting role to mitigate other emerging threats, such as those posed by homemade explosives and other sources of IEDs. This talk will provide an overview of our capabilities in Energetic Materials and High Pressure Science, with detail about personnel, budget, and publications.

Energetic Materials and High Pressure Science

David J. Funk

Weapons Experiments Division Leader

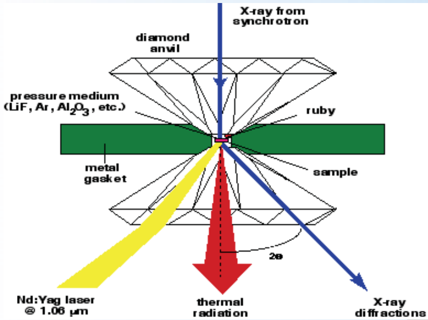
Los Alamos National Laboratory

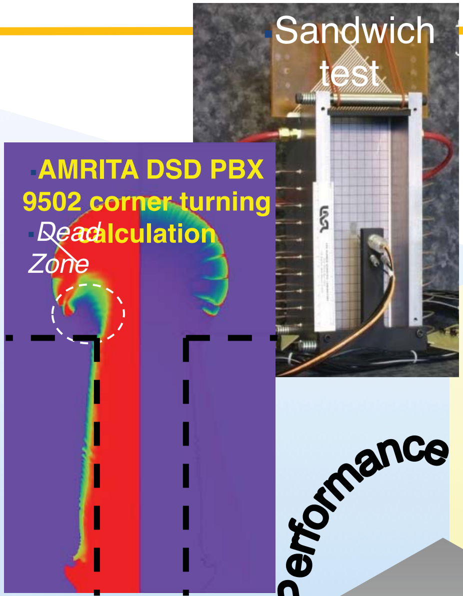
UNCLASSIFIED

Energetic Materials and High Pressure Science R&D are key capabilities needed to meet Nuclear Weapon and Global Security program deliverables

PERFORMANCE-primary physics certification, e.g. ***B61 Cold, W76 LEP & SFI resolution***

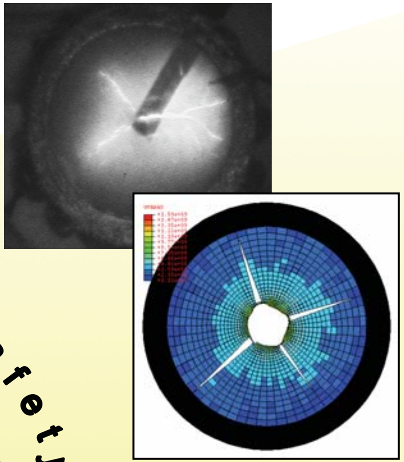
- HE Product and Metal EOS
- Detonation Shock Dynamics (DSD)
- Initiation




Sandwich test

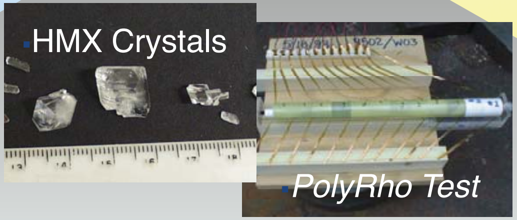
AMRITA DSD PBX 9502 corner turning calculation

PBX 9501 Mechanically Confined Cook-Off Test



SAFETY- ***Surety, SFI resolution, NESS & OSR***

- Thermal Behavior & response
- Shear initiation & response
- Constitutive model development for energetics and metals


HMX Crystals

PolyRho Test

MATERIALS DEVELOPMENT and CHARACTERIZATION

e.g. ***understanding materials for Life Extension Programs, Pit Re-use, new apps***

Small Scale Formulations & Characterization

Crystal Growth & Characterization

Micro & Mesoscale Characterization

Falling Man Pendulum Apparatus Demonstration

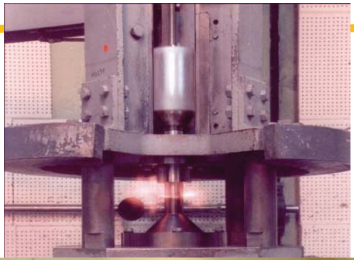
Providing Scientific and Engineering Solutions to meet Nuclear Weapon Complex Needs

Our Energetic Material and High Pressure Science portfolio has a broad customer base that leverages our historical capabilities in these areas

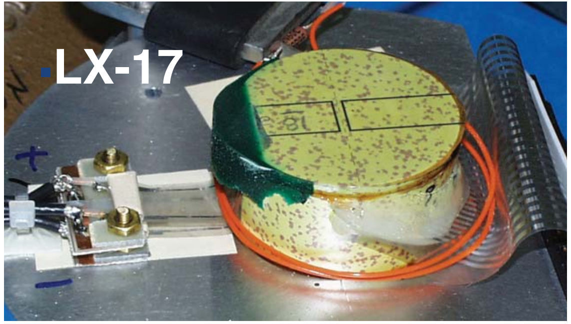
- Department of Defense
- Defense Threat Reduction Agency
- Office of Naval Research
- Department of Homeland Security
  - NEXESS
- Other classified projects and programs
- *Leverage is required in today's budget environment*

Department of Energy · United States of America

We require and maintain a full suite of “classic” energetic material research and development capabilities



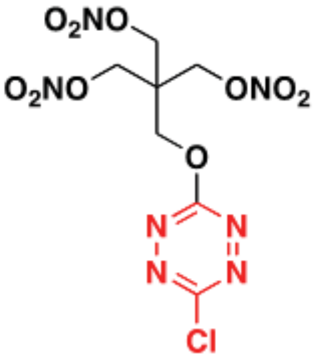
- CHNO synthesis: our specialty is high nitrogen compounds
- Analytical and small-scale sensitivity characterization
  - GPC, HPLC, IR, DSC, DMA, Henkin, Vacuum Stability
  - Small-scale safety: drop weight impact, spark, and friction
- Scaling and Formulation in our Pilot Plant(s)
- Mechanical Properties (Instron, Taylor Anvil)
- Combustion and Burn (including cook-off)
- Shock Initiation Sensitivity (embedded gauge)
- Detonation Properties (velocity, CJ pressure, EOS)

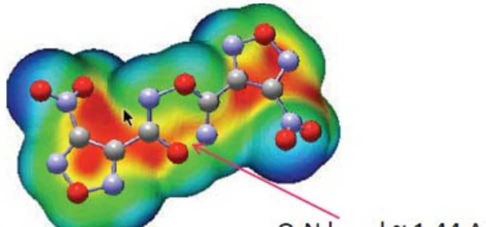


The Energetic Material Characterization Facility (EMCF) has risen in priority within the NNSA Construction Working Group

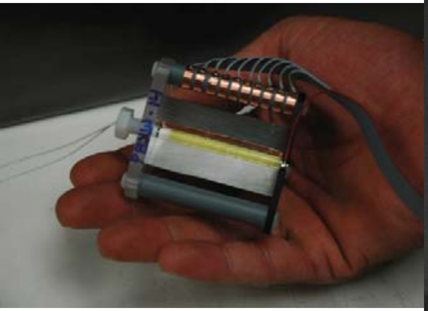
High Explosives Science & Technology: Synthesis and Small-scale Testing

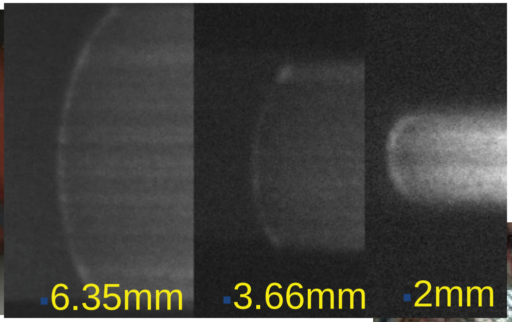
- Energetic material synthesis: Exploring new compounds with novel properties (BNDD, TAGBTMN), staying current with foreign efforts (BNFF, TNET), supporting DoD modeling efforts, derivatized PETN for DOI applications
- Novel testing development: Small scale performance and surface mapping detonation breakout
- Homemade Explosive (HME) Training
  - *Poster: "Los Alamos National Laboratory Homemade Explosive (HME) Afghanistan Training"*

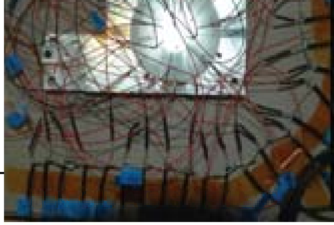


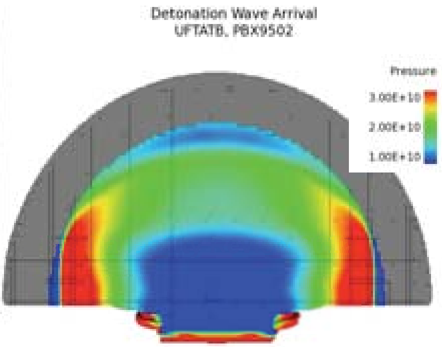


BNDD polymorph I
ρ(g/cc) = 1.914
ΔH_s (kcal/mol) = 145.1







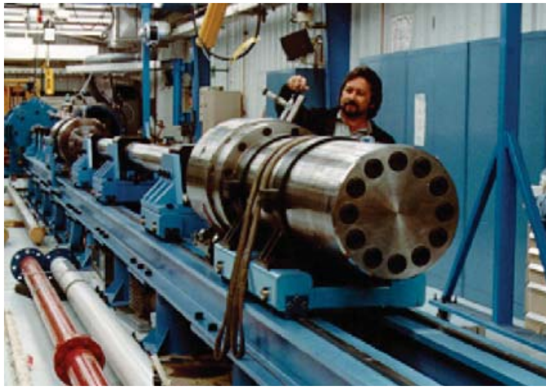


Our suite of gas guns (8) are used used to investigate a wide range of shock and detonation physics problems (SNM, inerts, HE)

- Supports designers' QMU requirements and predictive needs
  - Shock response:
    - Spall and strength
    - Shock initiation to detonation
    - EOS data
- Nuclear weapon HE requirements span a wide range of performance and safety issues from cradle-to-grave
  - *Poster: "Thwarting Chemistry in Dynamic Extremes: Multi-shock Compression of High Explosives"*
- We utilize these resources to understand the initiation and response of our weapon explosives and Home Made Explosives (HME)
  - *Poster: "EOS Development and Compaction Models for Porous Materials (U)"*
- Proximity and access to LANL's diverse technical expertise has lead to significant innovations and applications

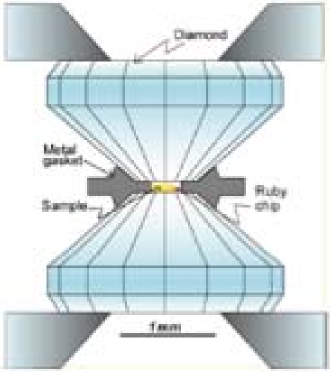
Gas Guns Capability

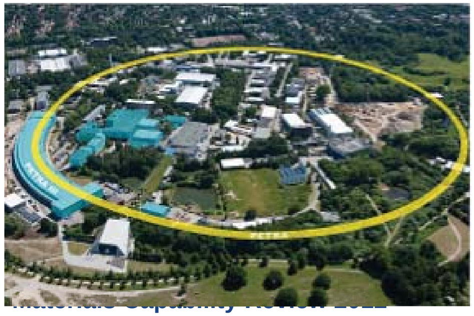
1 to 8 km/s



We utilize local, national, and international high pressure science capabilities for fundamental data for core mission and supporting scientific needs

- **High-Pressure-Preferred-Orientation (HIPPO) @ Lujan Center**
  - *Poster: "High P-T neutron diffraction study of hydrous minerals"*
- **Neutron Refectometry (SPEAR) @ Lujan Center**
  - *Poster: "High P-T (up to 200 MPa) neutron reflectometry of mineral/fluid interfaces"*
- **Diamond Anvil Cell (DAC) and dynamic-DAC (d-DAC)**
- **Collaborators at HP-CAT with CDAC**
  - Membership on their Scientific Advisory Panel
- **Collaborate with HiPSEC at UNLV**
  - Member of their Center Scientific Advisory Committee
- **Collaborations and experiments at NSLS II, DESY, ISIS**
  - *Poster: "Time-resolved measurements of phase transformations using a "pressure-jump" diamond anvil cell and x-ray diffraction at the Extreme Conditions Beamline"*
- **Collaborations on the Z-Machine at Sandia**
  - *Poster: "Isentropic Compression Experiments on Pu using Sandia's Z-Machine (U)"*





We maintain the only HE Crystal Growing Laboratory in the US

Used to characterize sensitivity, mechanical properties and initiation behavior

Goal: Grow large, perfect/almost perfect HE crystals and accurately characterize behavior for constitutive and hot spot initiation models

LANL

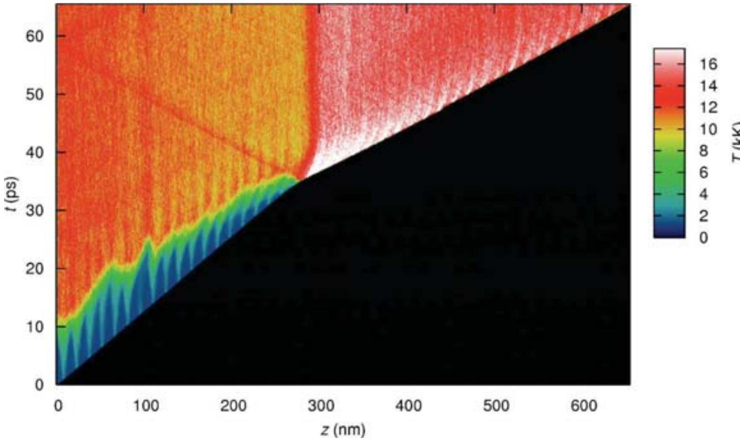
  - Successfully grown gem quality HMX
  - Resonant ultrasound for HMX's 13 elastic constants with MST-8 and B-4
  - Plate impact studies as a function of orientation to evaluate shock initiation sensitivity
- LANL, Navy and WSU:
  - Crystal defects and orientation on initiation

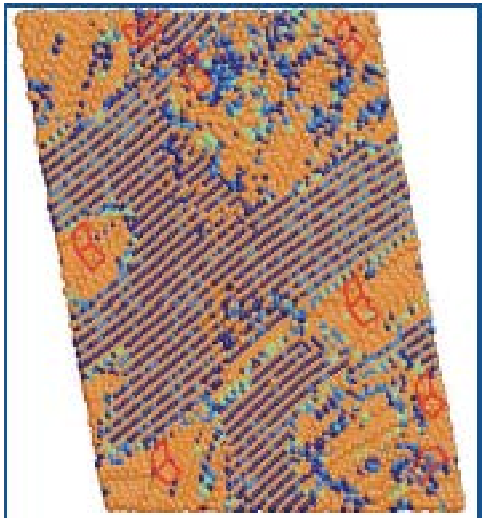
Institute for Shock Physics


▪HMX Crystals

We utilize large-scale molecular dynamic simulations (classical and quantum mechanical) to aid in data interpretation

- **Understanding the effects of void size, density, and arrangement on deflagration and detonation sensitivity**
- **Developing techniques for determining spectral characteristics of reactive mixtures**
  - *Poster: Computing Raman spectra on-the-fly in extended Lagrangian Born-Oppenheimer Molecular Dynamics*
- **Developing multi-scale approaches for the development of methods for modeling microstructure evolution under dynamic loading**
  - *Poster: Modeling Microstructure Evolution for High-Pressure / Strain-Rate Phase Transformations*



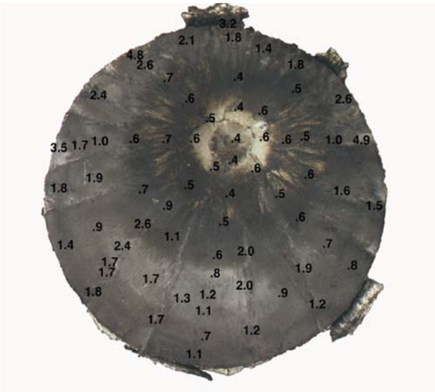


We maintain a full suite of test fire capabilities to meet our national security missions while consolidating and revitalizing our facilities

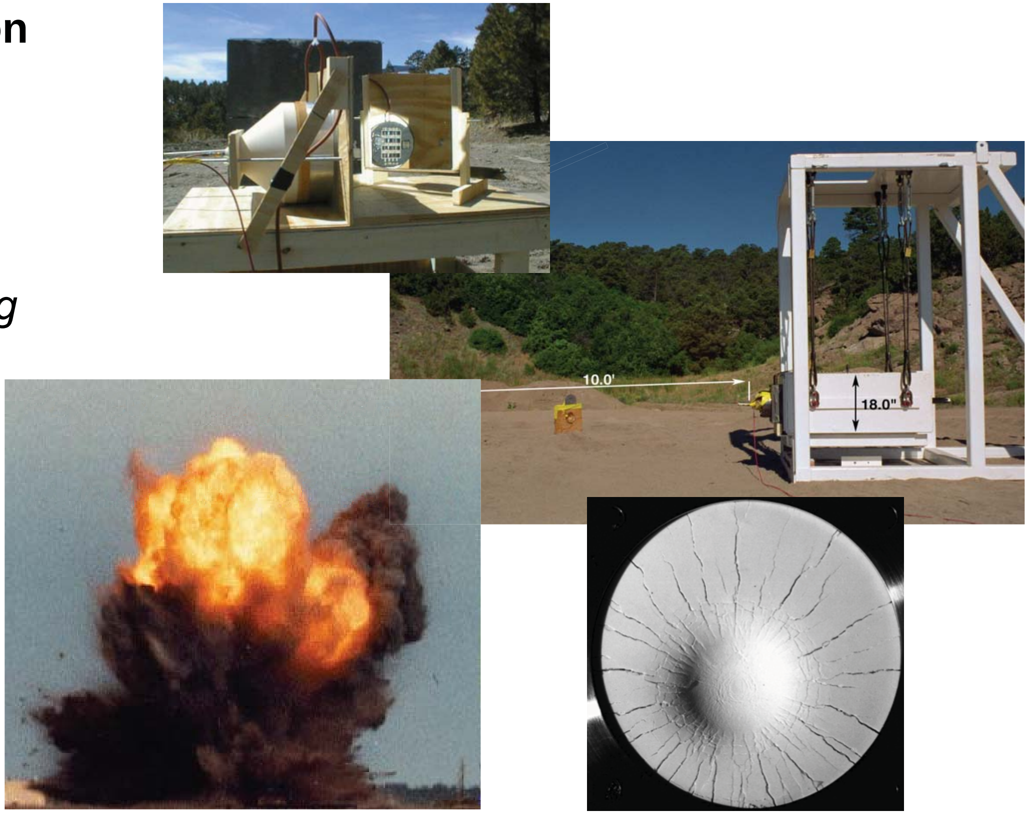
Used for energetics and inerts R&D characterization, performance, safety, and application testing

Small- to large-scale characterization and test capabilities, e.g

- *Multiple Boom boxes*
- *10 lb @ TA-40 Chamber 8*
- *2000 lbs @ TA-39*
- *Eight other firing sites, including pRad at LANSCE and DARHT*



Test DF15-2325



- Damaged CHE PBX 9501 after impact

Our consolidation and revitalization plan's priorities are based on mission need and an evaluation of a gap analysis

- *Revitalize HE Chemistry – replace aged Laboratory with new EMCF and improve 5 process support buildings' HVAC systems (Line Item)*

- Consolidate EOS – move guns into new DEOS Building (GPP) from Ancho

- Consolidate outdoor firing – from 5 TAs & 13 facilities to four facilities (TA-15 R306, Minie and TA-14-Q-site East and West) (GPPs & Capital Equipment). TA-39-88 remains in ready reserve for HE pulsed power as needed

- Convert / improve outdoor to indoor confined firing spaces – increase from 1 to 3 (Chamber 8, TA-40-Chamber 5 and Chamber 15 as needed) (GPPs & Capital Equip)

- Permanently deactivate (41 facilities, 82K square feet) and retain selected others as "Ready Reserve"

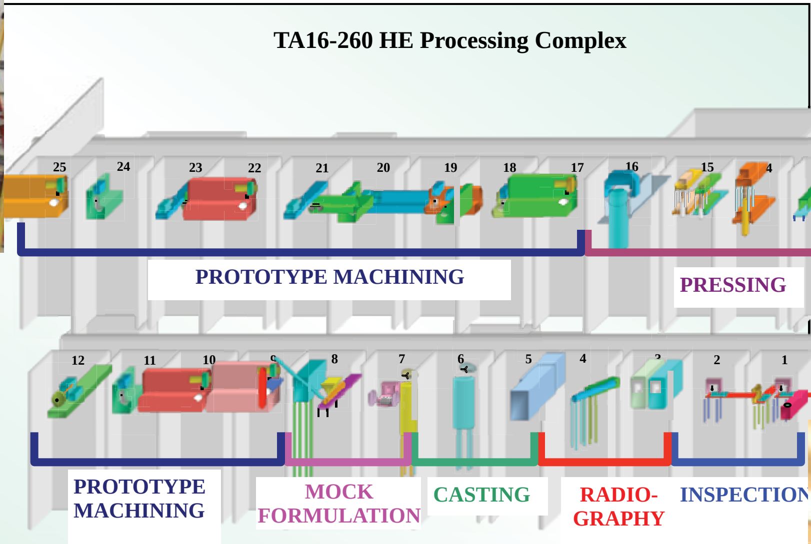
Infrastructure Workshop/Planning being conducted jointly with LANL's RTBF Program Office

We maintain a wide range of HE manufacturing tools to better serve our mission with agile and efficient capabilities

Hardinge CNC Vertical Turning Center

30ksi Isostatic Press – up to 28” diameters

TA16-260 HE Processing Complex



Browne & Sharpe CMM

K&T 5-axis Milling Center

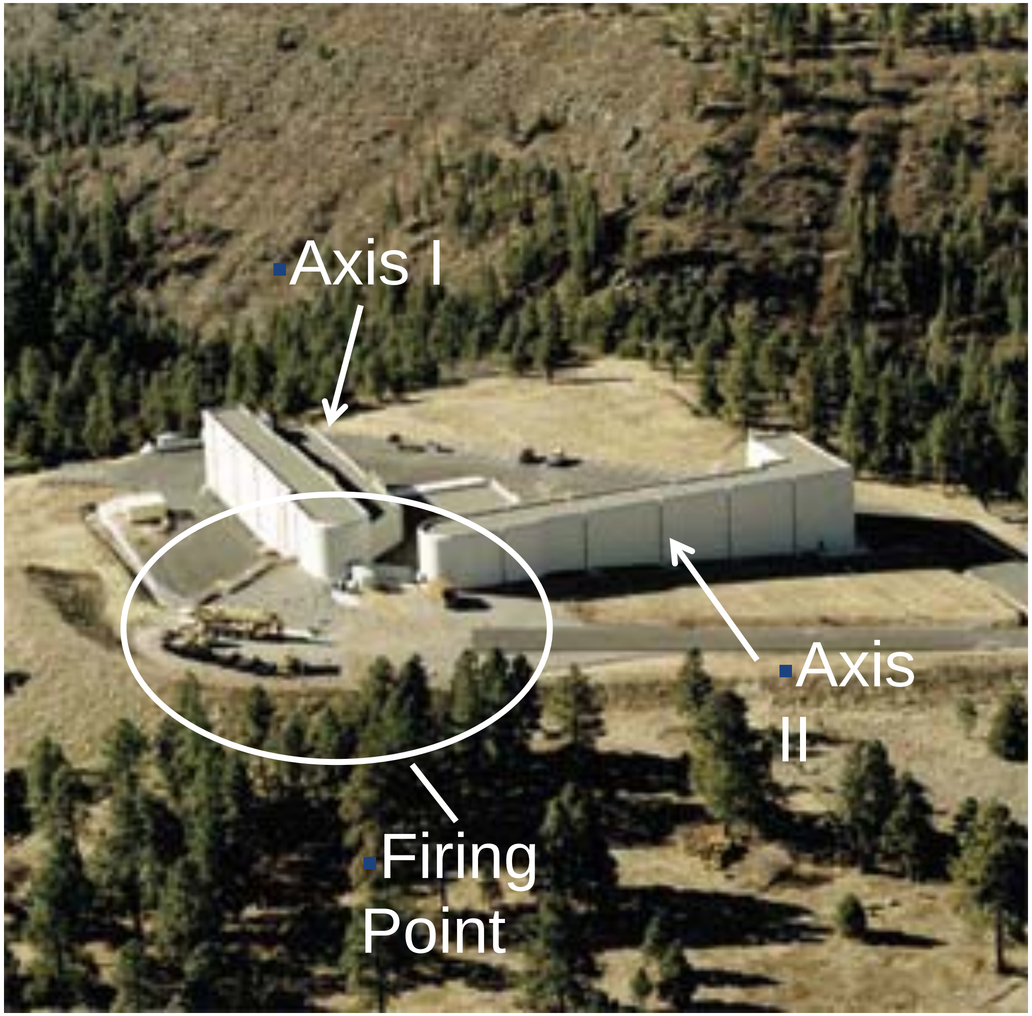
Heald Vertical Lathe – up to 28” diameters

Mock Explosives Formulation

1200-Ton Accudyne Steel Die Press

The ultimate explosively driven high pressure tests are conducted at DARHT (Dual-Axis Radiographic Hydrodynamic Test Facility)

- **Fully commissioned in 2008**
- **First Dual-Axis hydrotest conducted in December, 2009**
- **Ten dual-axis hydrotests to date**
- **Five radiographic images (one with Axis I and four with Axis II)**
  - *Poster: Hydrotest 3648 Executed at The Dual-Axis Radiographic Hydrodynamic Test (DARHT) Facility (U)*

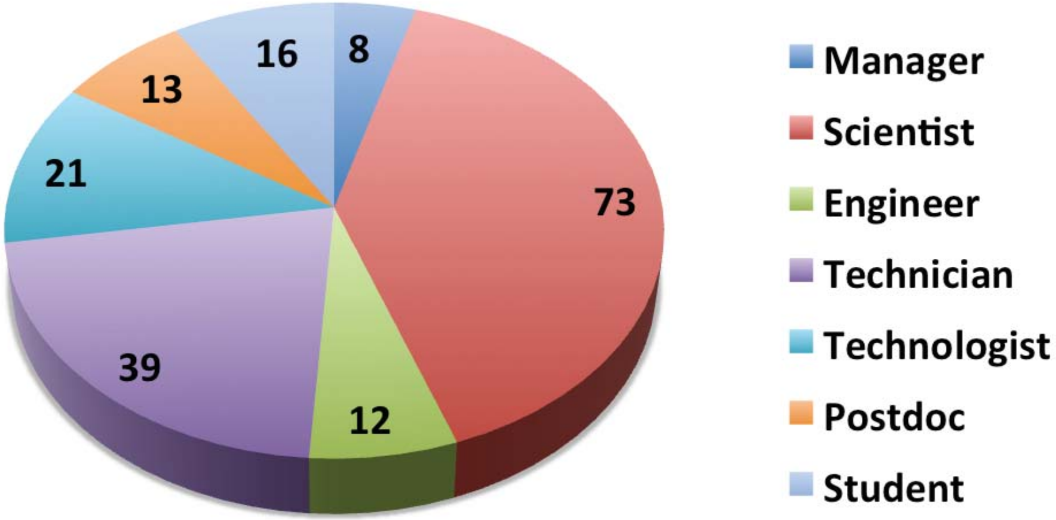


We have developed a future vision for our energetic material capability that includes three critical areas

- **Prediction and Control of Explosives Safety, Initiation, and Performance**
  - First principles understanding of performance (safety and intended use) as a function of molecular tailoring and formulation; prediction and control of engineering performance
  - Focused exploration of interplay between thermal, high pressure, shear, shock and light-driven chemical reaction, leading to control
  - Design and synthesis of new explosive molecules enabling formulations tailored to application
- **"Go-to" Lab for Advanced Detection and Render Safe Technologies**
  - Enhanced techniques for detection (e.g. hyper-spectral; exploitation of energetics)
  - New strategies for detection (systems approach: utilizing data and social knowledge)
  - Maintain and enhance Home Made Explosive (HME) competencies
  - Develop technologies that support mitigation strategies of IEDs and INDs
- **Invent and Utilize Revolutionary Diagnostics**
  - Develop a suite of diagnostic that transcend orders of magnitude in both length scale and spatial resolution to provide exquisite data for direct comparison with high fidelity simulations
  - Ability to probe both chemical and material properties while accessing a range of temperature, pressure, and density conditions
  - Lifecycle probes that provide relevant physical and chemical data without compromising the performance of the article within which they reside

A significant population of Energetic Material and High Pressure Science personnel are required to meet our mission goals

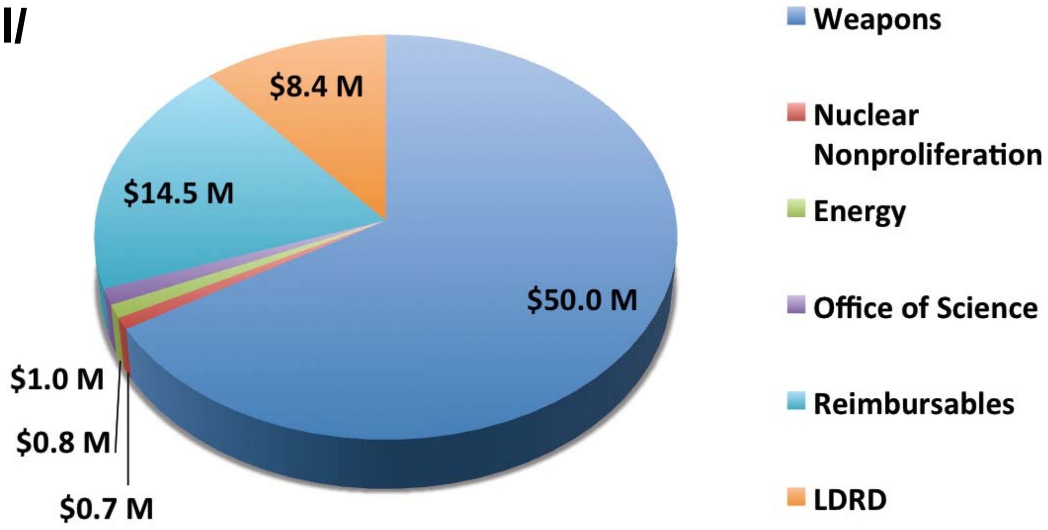
- **WX, EES, T, C, LANSCE**
- **Reasonably sized student and postdoc population**
  - Work tends to be more applied
  - Work occurs in Limited Areas (US citizens - clearance required)
- **Large technician and technologist pool**
- **EM-HP student/postdoc population serves as pipeline for this community**
- **Two E. O. Lawrence Awards in five years (M.H. Hunyh, 2007; D.E. Chavez, 2011)**



"for discovery of new chemical synthetic schemes used to advance development of fundamentally novel, highly energetic, environmentally friendly (high-nitrogen) molecular materials important to national security missions."

The LANL Energetic Material and High Pressure Science portfolio is principly supported by the Weapons Program

- Total funding for materials programs with energetic material/ high pressure component
- Weapons: mixture of Directed Stockpile Work and Science Campaigns
- Reimbursables: Joint Munitions Program (JMP), Work for Others
- LDRD supports fundamental science and serves as seed funding for new capabilities & competencies



DEPARTMENT OF ENERGY UNITED STATES OF AMERICA

U.S. DEPARTMENT OF HOMELAND SECURITY

DEPARTMENT OF THE NAVY ONR Science & Technology

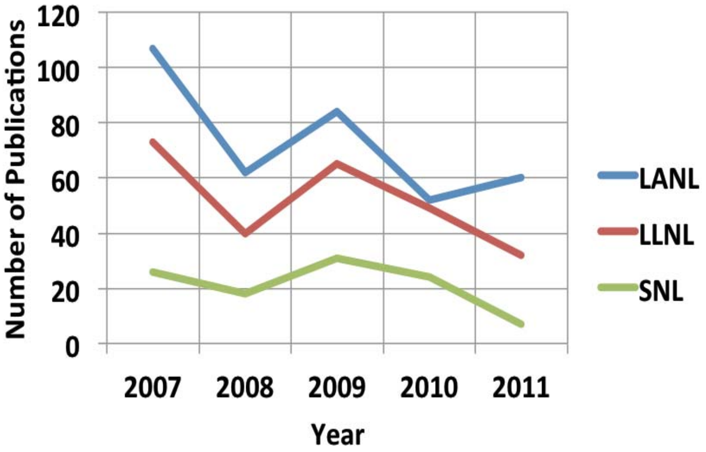
DEFENSE THREAT REDUCTION AGENCY UNITED STATES OF AMERICA

DEPARTMENT OF DEFENSE UNITED STATES OF AMERICA

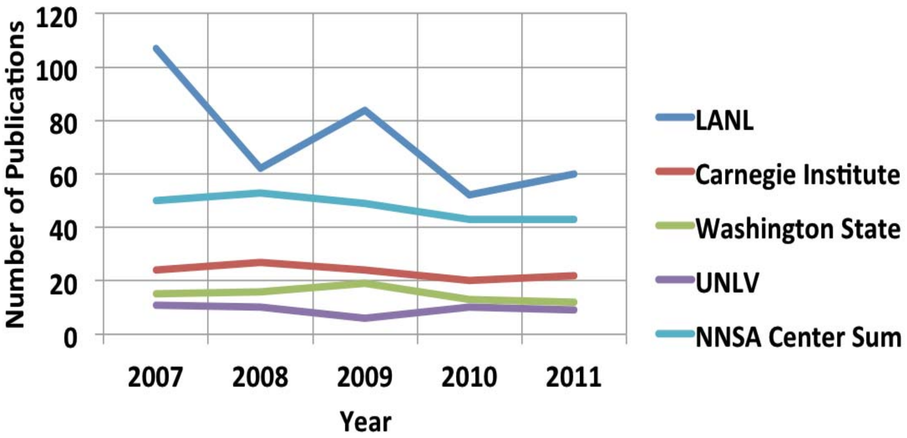
Impact as Measured by Publications: 2007-2011

- **Analysis was conducted for the three NNSA Laboratories and the three NNSA Centers**
  - Los Alamos, Livermore (HP-CAT partner), Sandia (Z-Machine)
  - Carnegie DOE Alliance Center (CDAC), HP-CAT partner
  - High Pressure Science and Engineering Center (HiPSEC),UNLV, HP-CAT partner
  - Shock Physics Institute @ Washington State University

National Lab Comparison



LANL NNSA Center Comparison



- Trend for the National Labs is disconcerting – increased projectization? More classified publications? Less time to write up? Deliverables for Science Campaigns should include peer-reviewed publications.

Unclassified Talk and Posters

- Recent impact experiments probed with Synchrotron X-rays at the Advanced Photon Source," Brian Jensen
- Posters:
  - Homemade Explosives Afghanistan Training at LANL, Virginia Manner
  - Coherent Control Studies for the Initiation and Detection of Explosives, David Moore
  - Modeling Microstructure Evolution for High-Pressure / Strain-Rate Phase Transformations, Frank Addessio
  - Computing Raman spectra on-the-fly in extended Lagrangian Born-Oppenheimer Molecular Dynamics, Josh Coe and Anders Niklasson
  - High P-T neutron diffraction study of hydrous minerals, Monika Hartl
  - Time-resolved measurements of phase transformations using a "pressure-jump" diamond anvil cell and x-ray diffraction at the Extreme Conditions Beamline, Nenad Velisavljevic
  - Thwarting Chemistry in Dynamic Extremes: Multi-shock Compression of High Explosives, Tariq Aslam
  - High P-T Neutron Reflectometry of Solid-Fluid Interfaces, Don Hickmott

Classified Talk and Posters

- Talk: “Applications for fundamental high explosives research for stockpile transformation (U),” Dan Hooks
- Posters:
  - Isentropic Compression Experiments on Plutonium (U), Paulo Rigg
  - EOS Development and Compaction Models for Porous Materials (U), Darcie Dennis-Koller
  - Linking experimental behavior with thermodynamic theory: development of a multi-phase EOS, Frank Cherne
  - Hydrotest 3648 Executed at The Dual-Axis Radiographic Hydrodynamic Test (DARHT) Facility (U), Shirish Chitanvis

Recent Impact Experiments Probed with Synchrotron X-rays at the Advanced Photon Source

B. Jensen (WX-9)

Understanding the dynamic properties of heterogeneous materials and/or processes require experiments capable of examining their time, rate, and spatial dependencies during loading. The development in synchrotron x-ray photon sources (high coherency and flux) and detection and measurement techniques such as phase contrast imaging (PCI) offers unique opportunities for ultrafast, high-resolution measurements to examine dynamic materials response. In the current work, an impact system developed for use at synchrotron sources was used to obtain phase contrast imaging (PCI) data with 3 micron spatial resolution using a single 60-ps width x-ray pulse from the Advanced Photon Source (Sector 32 ID-B). Experiments were performed to examine dynamic loading of materials ranging from foams/powder to study compaction, high strain-rate cylindrical impact to examine material failure, and jet formation in cerium metal to study material strength. Preliminary experiments using dynamic Laue diffraction to examine crystal structure were promising. A description of the impact system along with experimental details from a representative series of experiments will be presented to illustrate the versatility of this new capability.

Recent Impact Experiments Probed with Synchrotron X-rays at the Advanced Photon Source

B.J. Jensen

Shock and Detonation Physics (WX-9), Los Alamos National Laboratory

Presented at *the 2012 Materials Capability Review*

IMPULSE Team

A. Deriy (ANL), K. Fezzaa (ANL), D. Hooks (WX-9), B.J. Jensen (WX-9), K. Kwiatkowski (P-23), S. Luo (P-25),
T. Pierce (WX-9), C. Owens (WX-9), K. Ramos (WX-9), T. Shimada (P-24), and J. Yeager (WX-9)

Collaborators/Contributors:

F. Cherne (WX-9), G. Dimonte (XCP-5), D. Dattelbaum (WX-9), D. Fredenburg (WX-9), R. Saavedra (WX-9)
D. Stahl (WX-9), G. Terrones (XTD-1), B. Glagola (ANL), and R. Valdiviez (W-14)

Outline

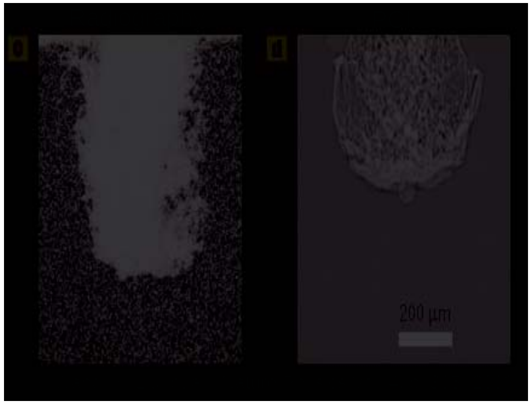
- Motivation
- Development of the IMPact system for ULtrafast Synchrotron Experiments (IMPULSE)
- Experimental results from the Advanced Photon Source (APS)
- Detector Development
- Summary and conclusions

Experiments are needed that provide real-time, in-situ, spatially resolved measurements on relevant timescales

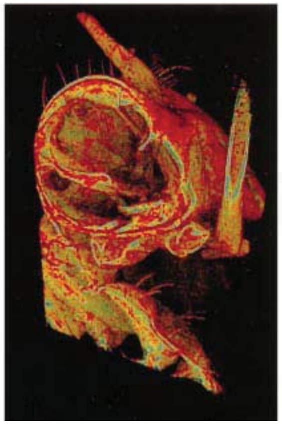
- *Develop a mobile plate impact facility for use at synchrotron sources and to perform PCI and Laue experiments on dynamically compressed materials*
- Diagnostics such as phase contrast imaging (PCI) offer unique opportunities for high-resolution spatially resolved measurements (~2-5 micron spatial resolution; time durations [illegible] μs)
- Impact experiments are difficult for many reasons including
  - Synchronization of impact event with the X-ray beam is challenging
  - Short-lived dynamic states translate to low-photon counts
- Recent detector feasibility tests have shown that it is possible to obtain high-quality images using a small number of X-ray bunches

Examples of Phase-Contrast Imaging

Fuel Injector Flow



3-D Image of a Cricket



Tracheal Respiration in a Beetle

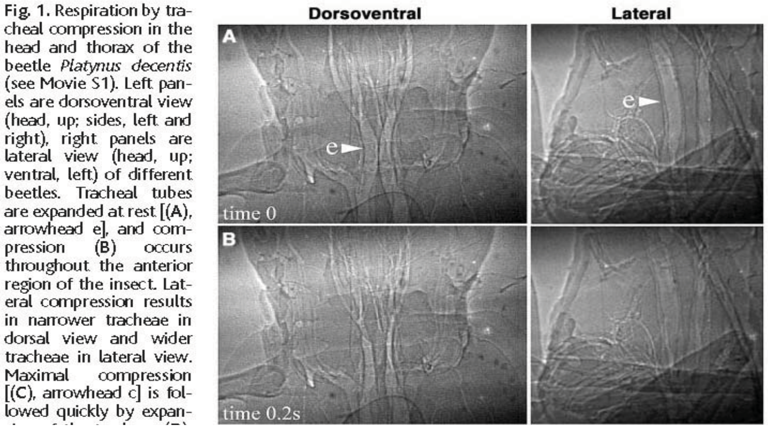
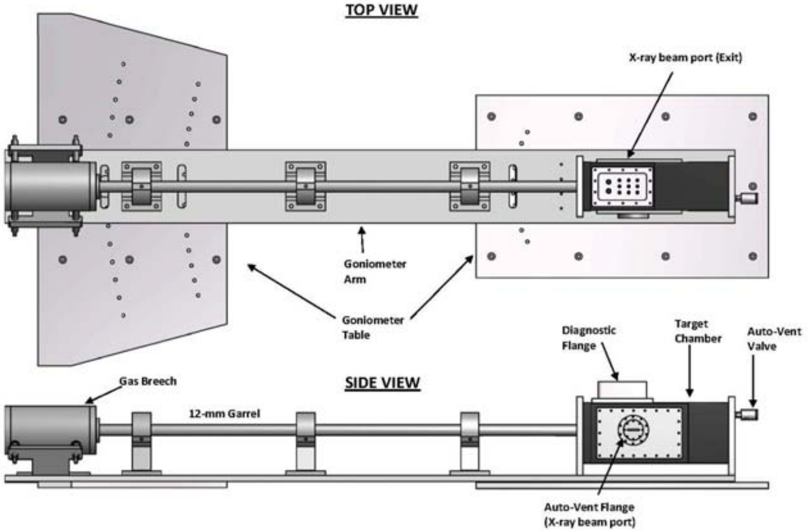


Fig. 1. Respiration by tracheal compression in the head and thorax of the beetle *Platynus decentis* (see Movie S1). Left panels are dorsoventral view (head, up; sides, left and right), right panels are lateral view (head, up; ventral, left) of different beetles. Tracheal tubes are expanded at rest [(A), arrowhead e], and compression (B) occurs throughout the anterior region of the insect. Lateral compression results in narrower tracheae in dorsal view and wider tracheae in lateral view. Maximal compression [(C), arrowhead c] is followed quickly by expan-

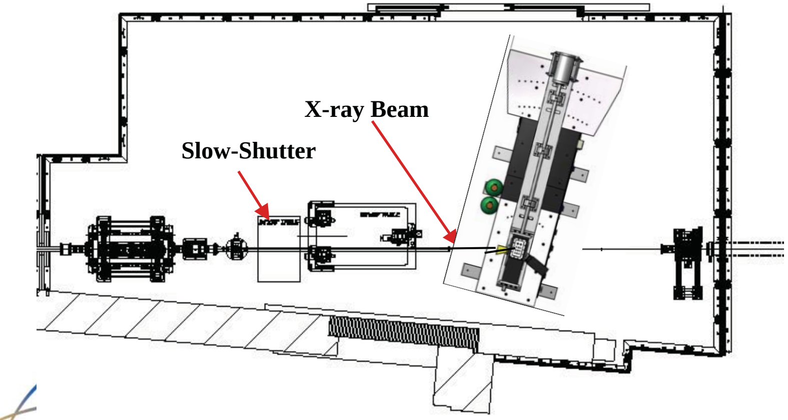
M.W.. Westneat, O. Betz, et al. Science Vol. 299, p. 558 (2003)

A mobile 12-mm Launcher System has been developed for use at APS
IMPULSE = IMPact system for ULtrafast Synchrotron Experiments

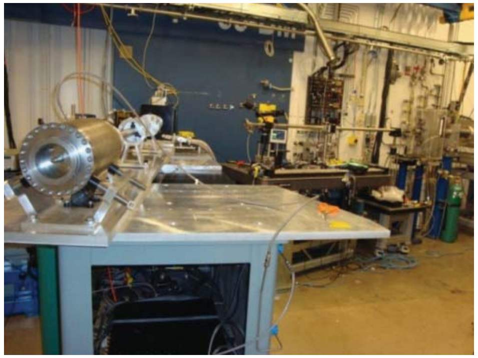
- A 12.6 mm bore mobile light-gas gun was developed to reach velocities up to 1 km/s – Complete engineering analysis performed by W14
- System is mobile to allow for quick insertion and removal; 30 degrees of rotation about the target axis
- Target chamber designed to interface with the synchrotron beam line - x-ray ports to allow x-rays to enter/exit the chamber
- System remotely operated from outside the hutch and includes auto-vent valves to prevent pressure buildup



32ID-B White Beam Hutch



Advanced Photon Source (Argonne, IL)

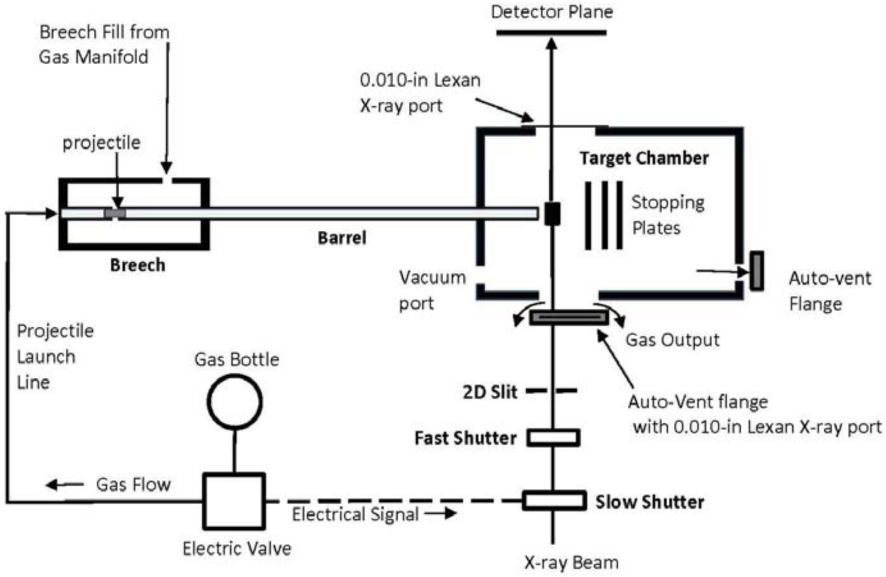


Representative APS experiments and potential applications

Experiments	Potential applications
PCI, steel plunger impact	Ballistics; high strain-rate Taylor impact; cracking; penetration; failure; dynamic friction
PCI, microlattice plastic foam *(w/* D. Dattelbaum *)*	Void nucleation or collapse; compression of low density materials including plastic/metallic foams and gels; low-Z materials; equation of state
PCI, borosillicate glass beads *(w/ Anthony Fredenburg)*	Compression of porous and granular materials; hotspots; powder reactions
PCI, Cerium jets *(w/ F. Cherne, G. Dimonte,* G. Terrones *)*	Jets, ejecta, flow and instability growth: solids, liquids, gases, and likely plasma
Laue diffraction, Fe [100] and Low-Z Materials (Tylenol)	Phase changes; plasticity; concurrent diffraction and PCI measurements.
Modification to existing detectors (large fiber optic taper, multiplexing)	Obtain full Laue diffraction patters Multiplexing allows for multiple images per experiment (PCI)
Static detector test, an existing 3-frame, hybrid Si-CMOS camera	The state of the art; fabrication of a 10-frame, high sensitivity, cameras based on similar technology useful for Science Campaign projects.

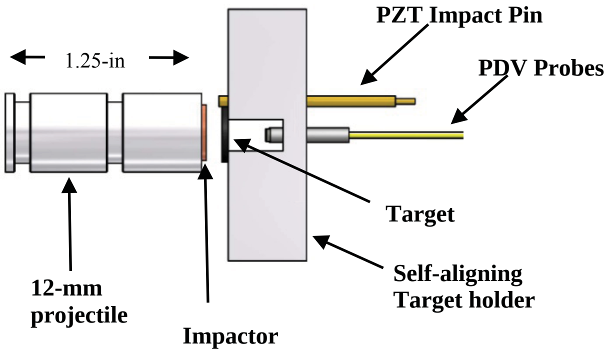
Experimental Configuration (Phase Contrast Imaging)

Experiment Configuration for Phase Contrast Imaging (PCI)

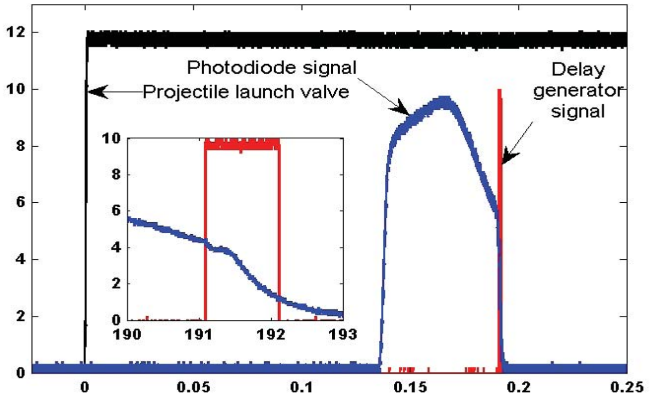


- Beam operated in standard mode with one 60-ps pulse every 153 ns
- Slow shutter synchronized with the projectile launch – opened for 60 ms
- PZT impact pin triggers detector and fast shutter
- Targets designed for quick setup/turn-around resulting in experiments every 1-2 hours

Standard Target Configuration

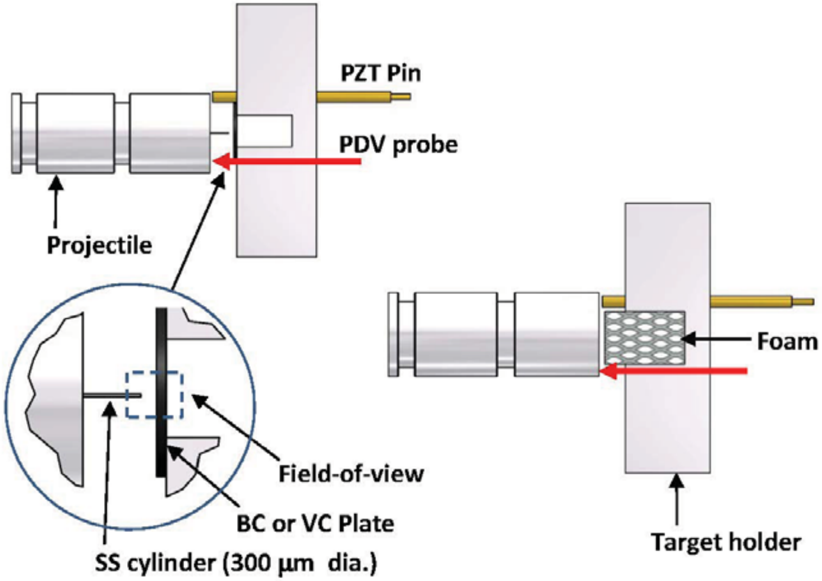


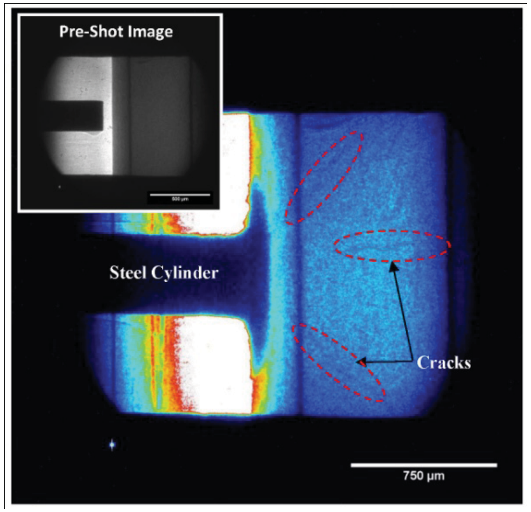
Timing Signals

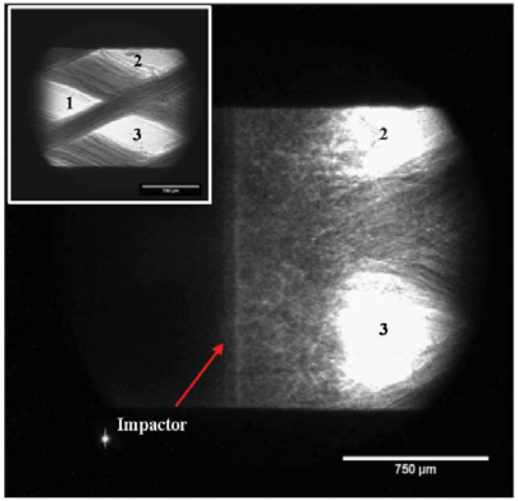


B.J. Jensen, S. Luo, et al, AIP *Advances* **2**, 012170 (2012)

In October 2011, we successfully performed the first dynamic experiments at APS on IMPULSE imaging materials using a single 60-ps X-ray bunch





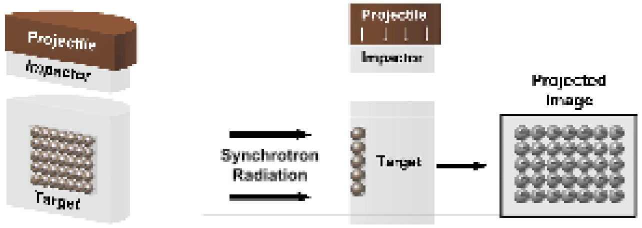


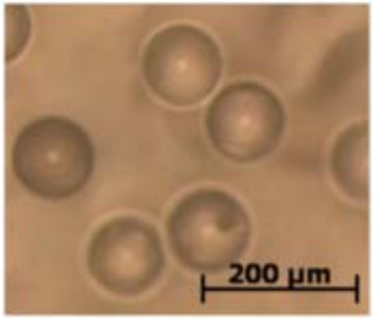
- Applications include: study of material failure, crack nucleation/growth, high strain-rate Taylor impact, void nucleation or collapse; compression of low density materials, etc.

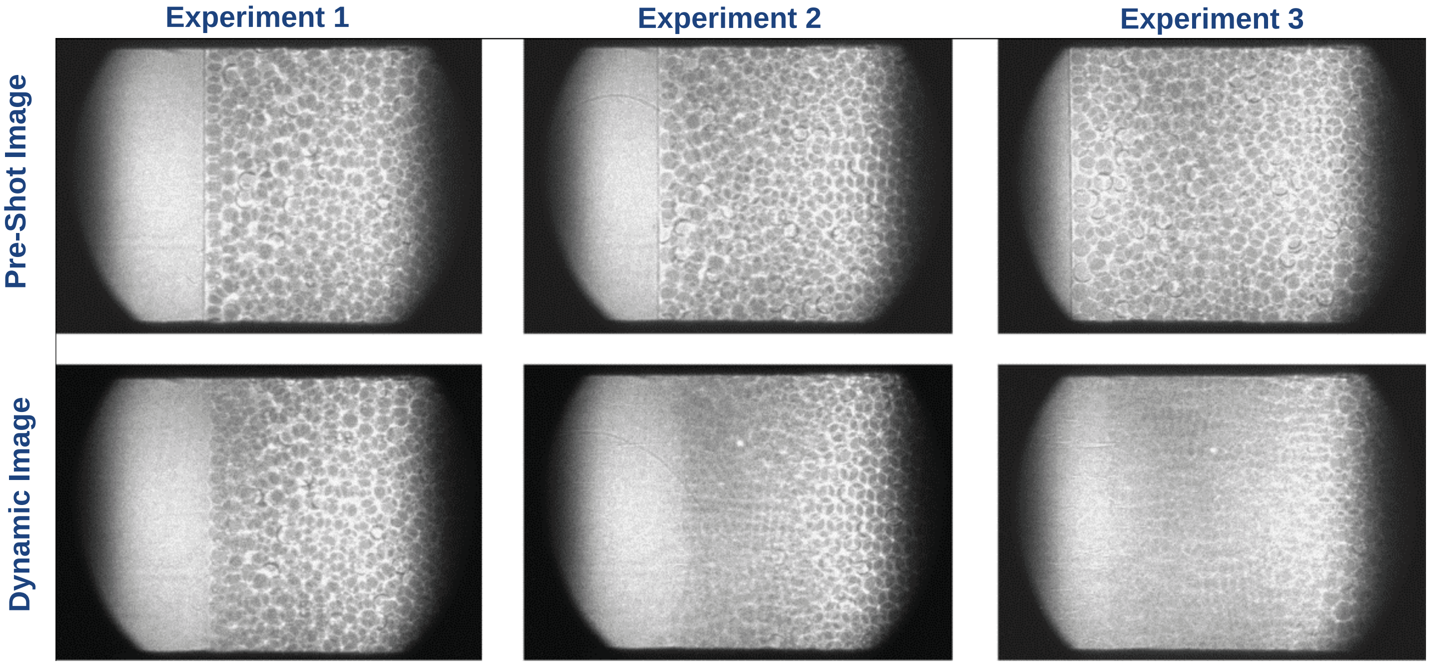
PCI captures progression of dynamic densification through an idealized system on boro-silicate glass spheres for real-time validation of compaction models

As part of a larger effort to build physically based compaction models that incorporate particle-level deformation and fracture behavior for brittle materials, an idealized system of boro-silicate glass spheres is under investigation *(Fredenburg, Agnew Fellowship)*

Spheres are nominally 106 µm ± 6% in diameter







Impact Velocity ~750 m/s
150 ns delay between images

150 ns delay

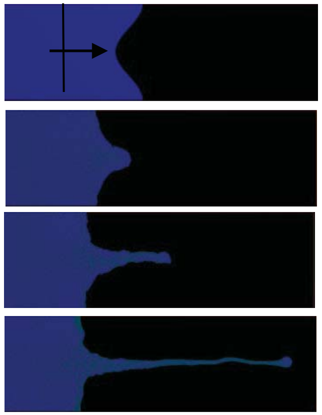
~300 ns delay

UNCLASSIFIED

Cerium RMI-Experiments performed using the IMPULSE system at the Advanced Photon Source to examine multiphase strength using Phase Contrast Imaging (PCI)

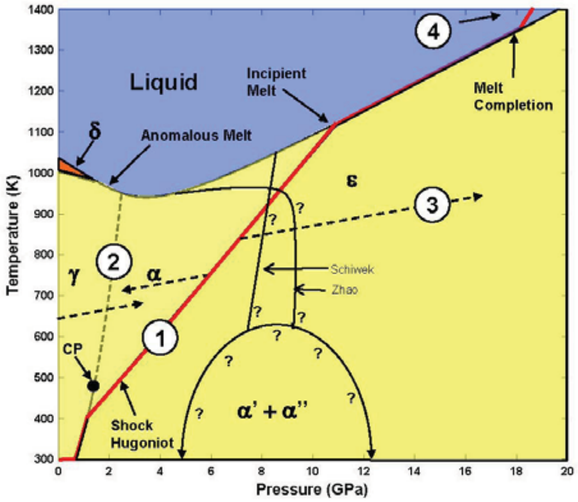
- Richtmyer-Meshkov instabilities used to infer yield stress for cerium
- Data were obtained using PCI to image jets formed during shock loading of cerium.
- Multiple images obtained showing the evolution of the jets with distance.
- Simultaneous velocimetry data also obtained showing saturation free-surface and jet velocities

Fig. 1: MD calculations of jet-formation in Cu for 4 different groove geometries

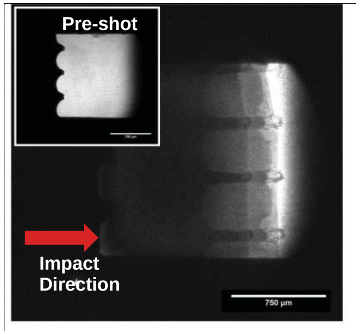


Dimonte, PRL 107 (2011) 264502

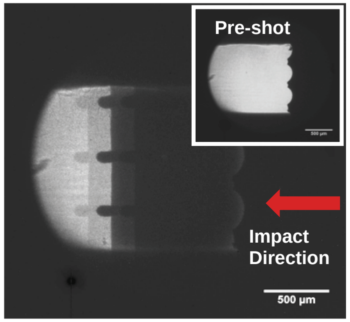
Phase Diagram For Ce (LANL MEOS)



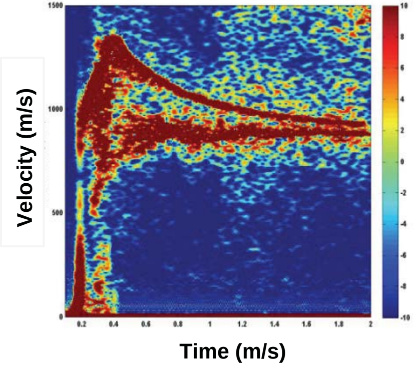
Jet-formation in Ce (Breakup of Jets observed)



Jet-formation in Ce (Saturation observed)



PDV measurements of jet and Free surface velocity



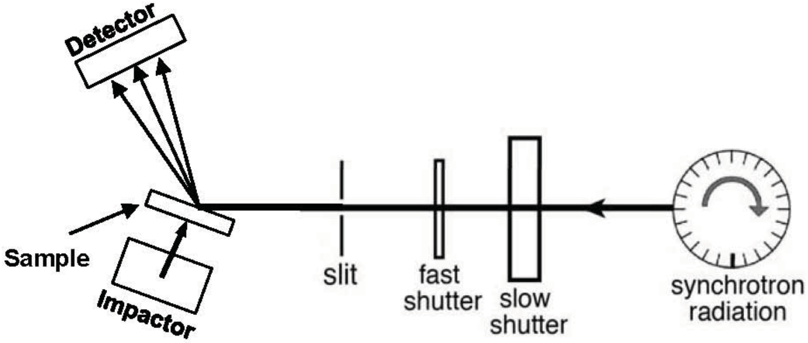
UNCLASSIFIED

Los Alamos NATIONAL LABORATORY EST.1943

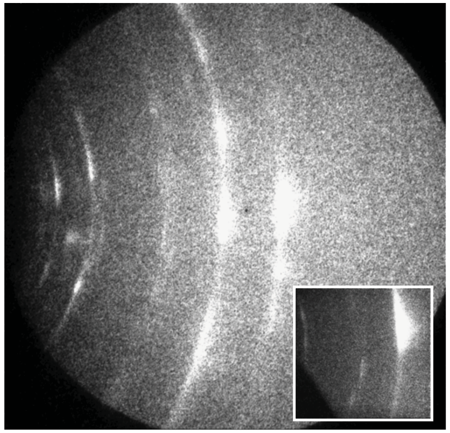
Operated by Los Alamos National Security, LLC for NNSA

Dynamic Laue diffraction to obtain structure measurements on single crystals is promising

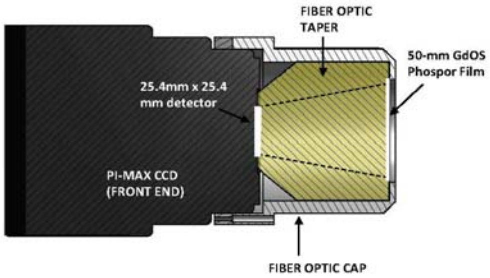
Dynamic Laue Diffraction Experiment Configuration



Diffraction from Cu Using the fiber optic taper

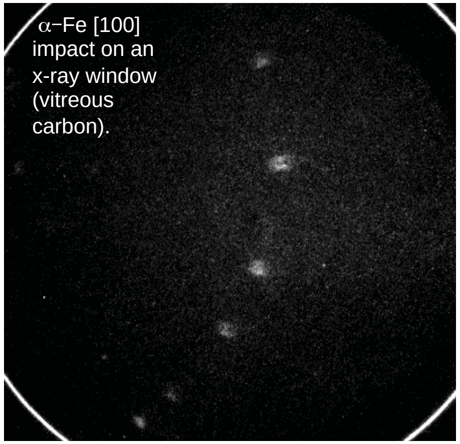


Detector improvements provide a large detection area for Laue diffraction measurements



Fiber Optic Taper

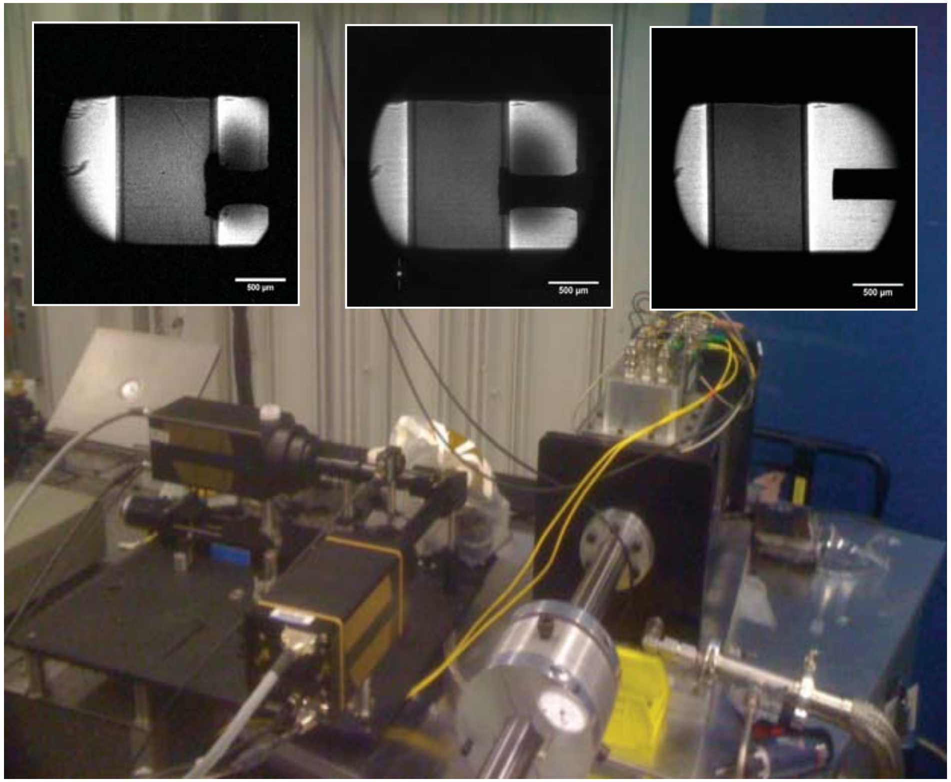
Data from the first dynamic Laue Diffraction experiment



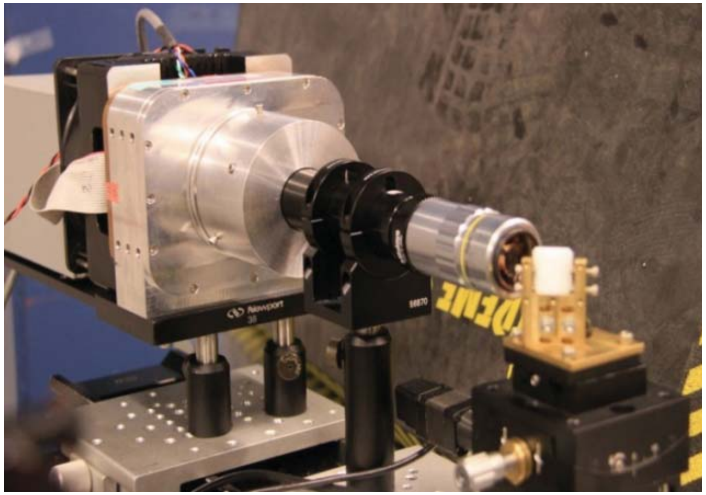
α−Fe [100] impact on an x-ray window (vitreous carbon).

Detector development is key to the continued success at these advanced light sources

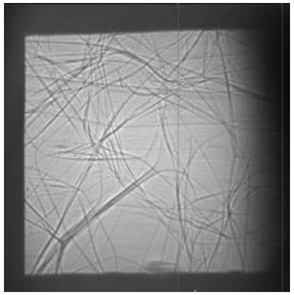
Multiplexed ICCDs to obtain multiple images



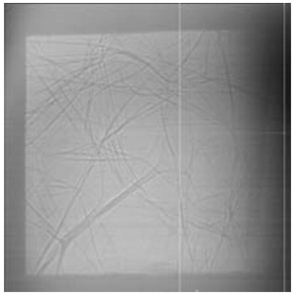
Hybrid Si-CMOS; X-ray, visible (3 frames)



65 pulses, foam



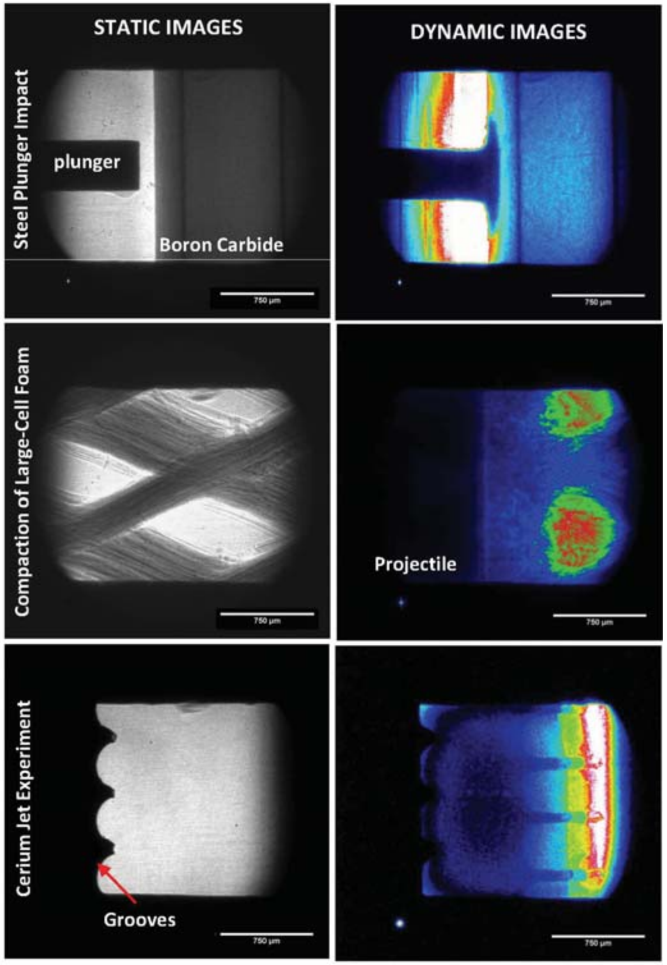
Single pulse, foam



(Field of view is ~1.8x1.8 mm^2; undulator gap 26 mm)

IMPULSE efforts are the first step toward routine dynamic compression experiments at these advanced light sources

- Developed, qualified, and installed a mobile gun system into the experimental hutch (Sector 32 ID-B) at the APS
- Conducted two series of experiments (10/2011 and 2/2012) for a total of 86 experiments
- Obtained the first dynamic PCI data using a single 60-ps X-ray packet synchronized to the event
- Dynamic Laue diffraction obtained for single crystal iron
- Successfully multiplexed ICCDs to obtain two multiple frames
- Work expected to continue in June 2012 with a focus on heterogeneous and/or low-Z materials and Laue diffraction on metals
- Challenges: *Photons, Detectors, Synchronization*
- *This new capability allows us to address many of these challenges – NOW – while doing groundbreaking research*



Questions?

IMPULSE Team

A. Deriy (ANL), K. Fezzaa (ANL), D. Hooks (WX-9), B.J. Jensen (WX-9), K. Kwiatkowski (P-23), S. Luo (P-25), T. Pierce (WX-9), C. Owens (WX-9), K. Ramos (WX-9), T. Shimada (P-24), and J. Yeager (WX-9)

Collaborators/Contributors:

F. Cherne (WX-9), G. Dimonte (XCP-5), D. Dattelbaum (WX-9), D. Fredenburg (WX-9), R. Saavedra (WX-9), D. Stahl (WX-9), G. Terrones (XTD-1), and R. Valdiviez (W-14).

Funding provide by C2 and LANL LDRD. Many thanks to R. Martineau, R. Olsen, C. Barnes, J. Sarrao, D. Robbins, D. Funk, B. Glagola (APS safety), and many others who provided support and encouragement

Homemade Explosives Afghanistan Training at LANL

D. Berning, B. Bluhm, C. Bolme, D. Chavez, L. Davis, J. Golden, M. Greenfield, S. Hanson, S. Kinkead, P. Leonard, B. Lounsbury, V. Manner, S. McGrane, D. Moore, B. Olinger, J. Scharff, B. Tappan, J. Veauthier, S. Wimer

LANL's homemade explosives Afghanistan training course has been designed for DoD and other government agencies, and provides fundamental information on homemade explosives to all four branches of the military service. Unlike many projects at LANL, this course serves an immediate need for troops about to be deployed to theater, and the information provided saves lives in Afghanistan. This is a one-week course developed and taught by PhD scientists at LANL, and is intended to fill a gap in intermediate explosives training in the military. Specifically, information is provided on homemade explosive products and precursors, improvised explosive devices, and situational awareness.

Coherent Control Studies for the Initiation and Detection of Explosives

D. Moore, M. Greenfield, S. McGrane, J. Scharff (WX-9)

Optimal control is utilized to improve both initiation and detection of explosives, whereby time dependent phase shaped electric fields drive the energetic material systems towards a desired state. Phase specific broadband pulses are created and seek to control optical initiation and enhance selective explosive detection. Our control experiments search for optimally shaped ultrafast laser pulses that can be exploited in stand-off technologies for explosives detection (optimal dynamic detection of explosives- ODD-Ex) and mitigation (quantum controlled initiation- QCI). Our results point the way toward several promising paths of opportunity in the field of applied quantum control.

Modeling Microstructure Evolution for High-Pressure/ Strain-Rate Phase Transformations

F. Addessio, C. Bronkhorst, X. Ding, T. Lookman (T-Div); D. Brown, E. Cerreta (MST-8), P. Rigg (WX-9)

Solid-solid phase transformations have an important impact on the properties of materials and the deformation characteristics of engineering structures. Accurate models are required to provide the deformation characteristics for a diverse range of loading scenarios. Predictive models are especially important for extreme conditions where experimental investigations cannot be conducted. To simulate component performance, increased burden is placed on modeling the effects of manufacturing processes on materials and on predicting their design behavior. In the past, uncertainty was mitigated with conservative designs. The macro-mechanical response of materials has its basis in the microstructure of the material. That is, deformation processes are dictated by mechanisms at the subgrain scale. The meso-mechanical length scale (of the order of 10 μm) also serves as a bridge between the atomistic and macro-mechanical scales.

The physics of solid-solid phase transformations has been addressed at many length and time scales. Currently, macro-mechanical models are based on equilibrium phase diagrams in pressure-temperature space. In general, macro-mechanical models do not address issues related to meta-stability, hysteresis, retained high-pressure phases, and the effects of shear on the transformation process. A model is being developed for the large deformation of single crystals under the conditions of high pressure and high strain-rates. The coupled effects of phase transformations, plastic slip and deformation twinning as well as damage are being considered. The model in not intended to resolve individual transformation interfaces. Instead, volume fractions of the constituents within a representative volume of material are modeled. A thermodynamically consistent framework is used to provide the basis for the model. Molecular dynamics simulations also are providing insight into the effects of shear as well as defining material properties. This effort is coupled to small-scale experimental investigations. Plate impact experiments have pursued the effects of peak pressure and temperature on the transformation process and meta-stability of Zr. Recently, experiments were conducted at peak pressures of 8.0 GPa and 10.5 GPa. Results indicate a sluggish transformation process at lower peak pressures. Furthermore, whereas ~35% retained high-pressure phase was observed in past experiments, ~63% and ~82% retained high-pressure phase were observed for the two recent experiments. Diffraction and microscopy investigations are included in the experimental investigation. In addition to determining the amount of retained phase, material texture, shear effects, transformation kinetics, and transformation pathways are being considered.

High P-T Neutron Diffraction Study of Hydrous Minerals

H. Xu (EES-14); D.D. Hickmott (EES-DO); Y. Zhao, J. Zhang, S.C. Vogel, L.L. Daemen, M.A. Hartl (LANSCE-LC)

Significant amounts of water are carried into the mantle at subduction zones via hydrous minerals in oceanic crust. Thus studying the stability of hydrous minerals at high P-T conditions is important in determining the state/fate of water in the Earth's interior and its effects on mantle rheology and melting. As neutron scattering is particularly sensitive to hydrogen, *in situ* high P-T neutron diffraction is a powerful technique for such studies. Using the high P-T toroidal anvil apparatus coupled with time-of-flight neutron diffraction at LANSCE, we have investigated the structures and stability of several hydrous minerals, especially layered hydroxides such as brucite and nickel hydroxide. Rietveld analysis of the data allowed determination of unit-cell parameters, atomic positions and atomic displacement parameters at various P-T conditions. The thermal expansion coefficients, bulk moduli and dehydroxylation P-T conditions of these compounds have also been determined. These studies thus provide important constraints on the physical properties of hydrous minerals, which can be used in global models of the deep-Earth water cycle.

Computing Raman Spectra on-the-fly in Extended Lagrangian Born-Oppenheimer Molecular Dynamics

A.M.N. Niklasson, J. Coe, M. Cawkwell (T-1)

Based on self-consistent density functional tight-binding theory [1] and extended Lagrangian Born-Oppenheimer molecular dynamics [2] we have developed a method for computing the Raman spectra from the polarizability auto-correlation function, which is calculated in real time on-the-fly in a molecular dynamics simulations. To calculate the polarizability tensor we self-consistently solve the density functional response equations using density matrix perturbation theory [3]. In analogy to extended Lagrangian Born-

Oppenheimer molecular dynamics we include the density response as auxiliary variables that are propagated through geometric integration algorithms. This unique approach provides stable, energy conserving and computationally very efficient simulations that are well adapted for linear scaling complexity and multi-core implementations.

[1] M. Elstner et al., Phys. Rev. B, vol 58, 7260 (1998); E. Sanville et al. in Proceeding of the 14th International Detonation Symposium (Office of Naval Research, Alrington VA, ONR-351-10-185, 2010), pp 91-101.
[2] A.M.N. Niklasson, Phys. Rev. Lett., vol. 100, 123004 (20080, P. Steneteg et al. Phys. Rev. B, vol. 82, 075110 (2010).
[3] A.M.N. Niklasson and M. Challacombe, Phys. Rev. Lett., vol. 92, 193001 (2004).

Time-resolved Measurements of Phase Transformations using a “Pressure-jump” Diamond Anvil Cell (DAC) and X-ray Diffraction (XRD)

N. Velisavljevic, D. Dattelbaum (WX-9); H. P. Liermann (DESY, Germany), and S. Sinogeikin (APS, ANL)

Advances in synchrotron radiation facilities, including increases in x-ray brightness and emergence of faster detectors, has allowed for an opportunity to push the state-of-the-art with diamond anvil cell (DAC) techniques. DACs coupled with either piezoelectric drivers [1] or gas membranes offer enhanced control of pressure increases and opportunities for accessing new strain rate regimes, and when combined with the brightest x-ray sources can provide time-resolved structural phase information behavior of materials over wide pressures and strain rates. Using an automatic pressure controller coupled to a gas membrane driven DAC, we were able to generate a rapid pressure-jump, and sustain continuous pressure increase from ambient up to 50 GPa. Using DESY and APS synchrotron facilities, x-ray diffraction (XRD) data were collected simultaneously and continuously at 0.1 to 0.2 s/spectra, revealing new insight into the structural evolution of zirconium metal in the pressure range up to 50 GPa and at strain rates greater than 10^{-2} s^{-1}.

Our experiments provide new insights into behavior of materials at high pressures and demonstrate the feasibility of achieving intermediate stain rates, which bridge the gap between traditional low strain rate ($<10^{-3}$ s^{-1}) DAC and large volume press static high pressure and high strain rate ($>10^{5}$ s^{-1}) compression shock techniques.

1. W. J. Evans, C-S. Yoo, G. W. Lee, H. Cynn, M. J. Lipp, and K. Visbeck, Rev. Sci. Inst. **78**, 073904 (2007).

Thwarting Chemistry in Dynamic Extremes: Multi-Shock Compression of High Explosives

T. Aslam, R. Gustavsen, N. Sanchez, B. Bartram (WX-9); R. Menikoff (T-1)

A long standing debate among high explosive modelers regarding both the equation of state (EOS) of shocked reactants and the mechanisms to detonation has recently been addressed by a series of 2 stage gas gun experiments. These experiments were designed and fielded to shock-deaden PBX 9502 (1st shock ~5-9GPa), and subsequently re-shock to very high pressures - without inciting reaction within the high explosive. This allowed both "debates" to be addressed; the reactants EOS was measured to greater than 50 GPa, and it also showed quantitatively that very little (if any) reaction takes place due solely to high pressures.

High P-T Neutron Reflectometry of Solid-Fluid Interfaces

D.D. Hickmott (EES-DO); A. Lerner (EES-14); P. Wang, J. Majewski, M. Taylor (LANSCE-LC); J.K. Baldwin (MPA-CINT); R.K. Grubbs, (Sandia National Laboratories)

We have designed and built a unique high-pressure (P), high-temperature (T) cell for neutron reflectometry of solid/fluid interfaces at Ps up to 200 MPa and Ts up to 200^{o}C. Fluid/solid interactions at interfaces are important in a range of energy and environmental applications including: geologic carbon sequestration, enhanced geothermal systems, corrosion in reactor environments, and utilization of deep oil and gas resources. The neutron reflectometry cell is constructed of anodized aluminum (5 in. diameter), can be used with both aqueous and gas-saturated fluids, and contains powder-wells for equilibration of solids with fluids. Neutron reflectometry is a sensitive technique for studying angstrom-scale processes at interfaces; it has great potential for high P applications due to the ability of neutrons to penetrate high-P cells.

Initial, proof-of-concept experiments have focused on studies of calcite/fluid interface interactions, which are important for geologic carbon sequestration, and on corrosion applications. Atomic layer chemical-vapor deposition calcite/deuterated water interfaces reveal hydrophilic interactions, with elevated density water within a few angstroms of the interface at ambient P-T. High P (~ 100 MPa) high T (150^{o}C) deuterated water/aluminum corrosion experiments show the progression of aluminum oxidation over 5 hours duration.

Overview: Materials Science Research and Development for the Nuclear Weapons Program – On the Path to Prediction and Control (U)

D.F. Teter (MST-DO)

This talk will present a brief overview of materials research and development for the nuclear weapons programs. The Predictive Capability Framework outlines multi-year milestones for development of predictive models for nuclear weapons performance. These models require improved fundamental understanding of the connection between material microstructure, properties and performance. Recent experimental data is challenging existing models causing us to revisit the fidelity of physics captured in the models. Several examples will be shown illustrating the progress made to improve our understanding of material properties and how they relate to performance. Predictive modeling guiding our manufacturing processes will be shown with a couple of examples.

Applications for Fundamental High Explosives Research for Stockpile Transformation (U)

D. Hooks (WX-9)

Since its inception during the Manhattan project, Los Alamos National Laboratory has been a world-class leader in energetic materials research, development and applications. Today, our National Security Energetics (NSE) capability enables a dynamic, flexible response to address multiple evolving mission needs. As the Stockpile Stewardship Program mission has evolved, the NSE capability has provided a crucial foundation for advancing predictive capability, identifying and resolving issues, and developing strategic energetic materials for the future. Recent advances that demonstrate the link of fundamental science to stockpile transformation in the future will be described in some detail.

A Co-Design Approach to Plutonium Casting Development (U)

D.R. Korzekwa (MST-16); R.M. Aikin, Jr. (MST-6)

The successful induction casting of plutonium is a challenge which requires technical expertise in areas including physical metallurgy, surface and corrosion chemistry, materials science, electromagnetic engineering and a host of other technologies all which must be applied in concert. Here at LANL, we are employing a combined experimental and computational approach to design molds and develop process parameters needed to produce desired temperature profiles and improved castings. Computer simulations are performed using the commercial code FLOW-3D and the LANL ASC computer code TRUCHAS to reproduce the entire casting process starting with electromagnetic or radiative heating of the mold and metal and continuing through pouring with coupled fluid flow, heat transfer and non-isothermal solidification. This approach greatly reduces the time required to develop a new casting designs and also increases our understanding of the casting process, leading to a more homogeneous, consistent product and better process control. We will discuss recent casting development results in support of Subcritical Experiments.

Isentropic Compression Experiments on Plutonium (U)

P. Rigg (WX-9); M. Knudson, J.P. Davis (SNLA); C. Greeff (T-1)

Experimental data are needed to develop accurate equations of state for plutonium. Data on the Hugoniot obtained from shock experiments provide EOS data for a very limited region of phase space. The Z-Machine at Sandia National Laboratories Albuquerque (SNLA) can produce well-characterized one-dimensional loading of metal samples to multi-megabar stresses and can provide off-Hugoniot data not accessible using other dynamic loading techniques. To date, we have performed seven experiments on plutonium metal using the Z-Machine. The results of these experiments have provided new insight into the behavior of Pu at elevated stresses and strain-rates.

EOS Development and Compaction Models for Porous Materials (U)

D. Dennis-Koller, R.J. Scharff, P. Rigg, D. Robbins, D.A. Fredenburg (WX-9); J. Wermer B. Nolen (MST-6)

The LANL goal of a physically based predictive capability depends on an understanding of materials in extreme conditions. While 60 years of studies on materials under extreme conditions has focused largely on structural materials, liquids and gases, very little data exists on porous materials. The response of powders and porous materials to high-strain-rate (shock) loading is a complex process influenced by numerous factors that cause dramatic increases in energy; inclusive of the size and shape of particles and voids, material strength, chemistry, initial density, and possibly others yet to be determined. Currently, there is an on-going effort at Los Alamos National Laboratory to understand and quantify these factors, and how they affect the dynamic response. Determination of what additional models are required to capture the physical mechanisms responsible for energy increases is the goal of this work while establishing the correct formulations for the equation of state for materials of programmatic interest.

Hydrotest 3648 (U)

S. Chitanvis (XTD-3)

Hydrotest 3648 provided insight into material behavior in a regime not usually accessible to laboratory experiments.

Linking Experimental Behavior with Thermodynamic Theory: Development of a Multi-phase EOS

F.J. Cherne, B.J. Jensen (WX-9); C.H. Mielke, D.G. Rickel (MPA-CMMS); D.G. Tasker (WX-6); G. Rodriguez (MPA-CINT)

In the interest of predictive science capabilities, a crucial aspect required is a thermodynamic equation of state (EOS) capable of capturing the dynamic properties of a complex multi-phase material. In this study we have developed a thermodynamically consistent multi-phase equation of state (MEOS) capturing the dynamic and static behavior of the complex f-electron metal cerium. Using a large suite of static data and a minimal amount of dynamic data to constrain the equation of state, we have developed a robust EOS, which captures many of the salient features of this unique metal. We show

how this EOS can be used for targeted experimental design as well as for post experimental analysis. The types of dynamic experiments that the MEOS has been applied to are heated and room temperature transmission geometry plate impact experiments, ambient temperature front surface impact experiments, and a heated quasi-isentropic compression experiments performed at the National High Magnetic Field Laboratory (NHMFL). The MEOS predicts many of the dynamic properties around the low pressure (γ-α) phase transition yet there are some additional adjustments to the EOS could be made to liquid and ε-phase (bct).

National High Magnetic Field Laboratory

C. Mielke (MPA-CMMS)

Magnetic fields have become an indispensable tool for science to better understand and manipulate ground states of electronic materials. As magnetic field intensities are increased the quantum nature of these materials become exponentially more likely to be observed and this is but one of the drivers to go further in high magnetic field generation. At the Los Alamos branch of the National High Magnetic Field Laboratory we have recently achieved a new “World Record” for the highest non-destructive magnetic field of 100.8 (+-0.1) tesla. The pulsed magnet systems of the NHMFL- Pulsed Field Facility provide qualified users with unprecedented access to extremes of high magnetic field. The discovery and characterization of new states of matter are tightly coupled to our ability to measure small changes in a material’s response to the well-characterized experimental extremes in high magnetic fields. Challenges in magnetic field generation and research will be presented, detailing the recent success in engineering and the science conducted within the magnets.

National High Magnetic Field Laboratory

Chuck Mielke

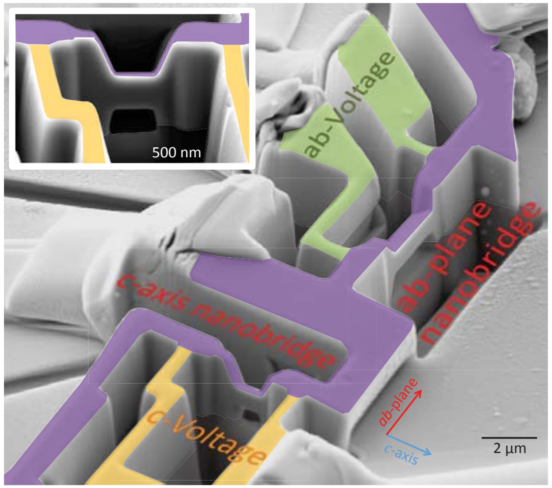
NHMFL-PFF Director

UNCLASSIFIED

Overview

- **The Pulsed Field Facility capabilities.**
  - High Field Science
  - Big Magnets
- **Advanced high field techniques.**
- **Metrics.**
- **Global Perspective & Future.**

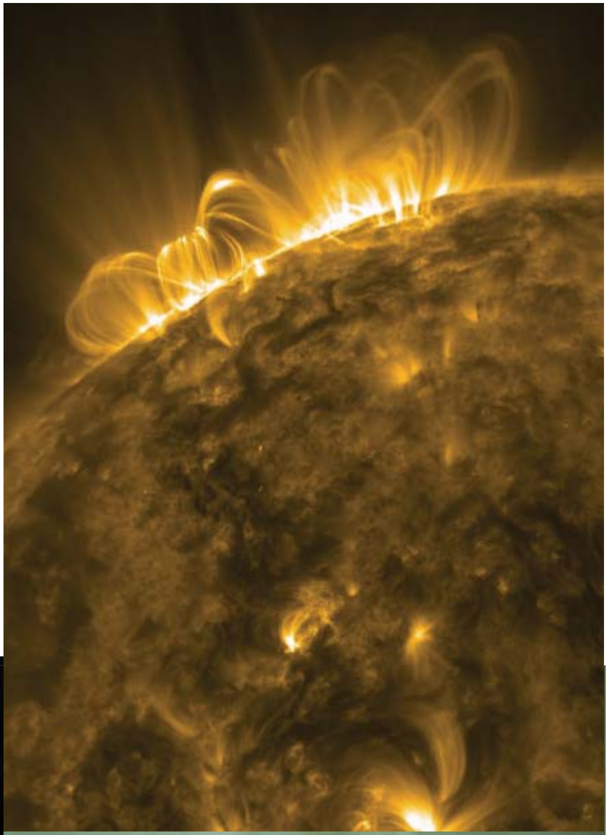
A 170 tesla shot at the NHMFL-PFF.

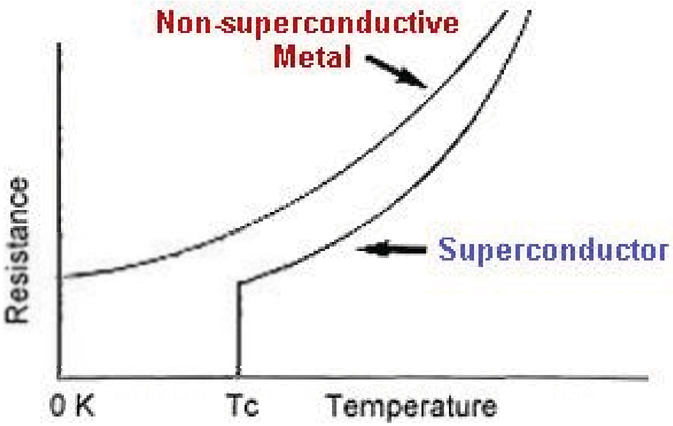


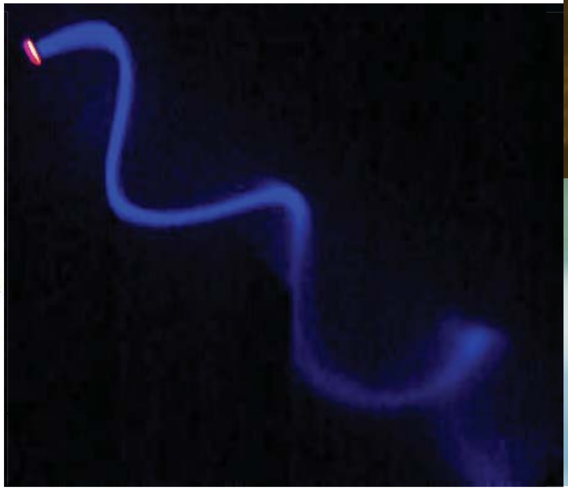
P. Moll et all, Nature Physics, July 2010.

Why High Magnetic Fields?

- **Primarily to study electronic Materials (vis a vis Condensed Matter Physics)**
  - Very predictable, reversible tool,
  - Allows characterizing of electrons in materials (couples to orbital motion of electrons and Zeeman energy)
- **Big Field = Big effect = Precision**







The NHMFL (Three Sites)

Pulsed Field Facility

Los Alamos, NM

DC Field Facility

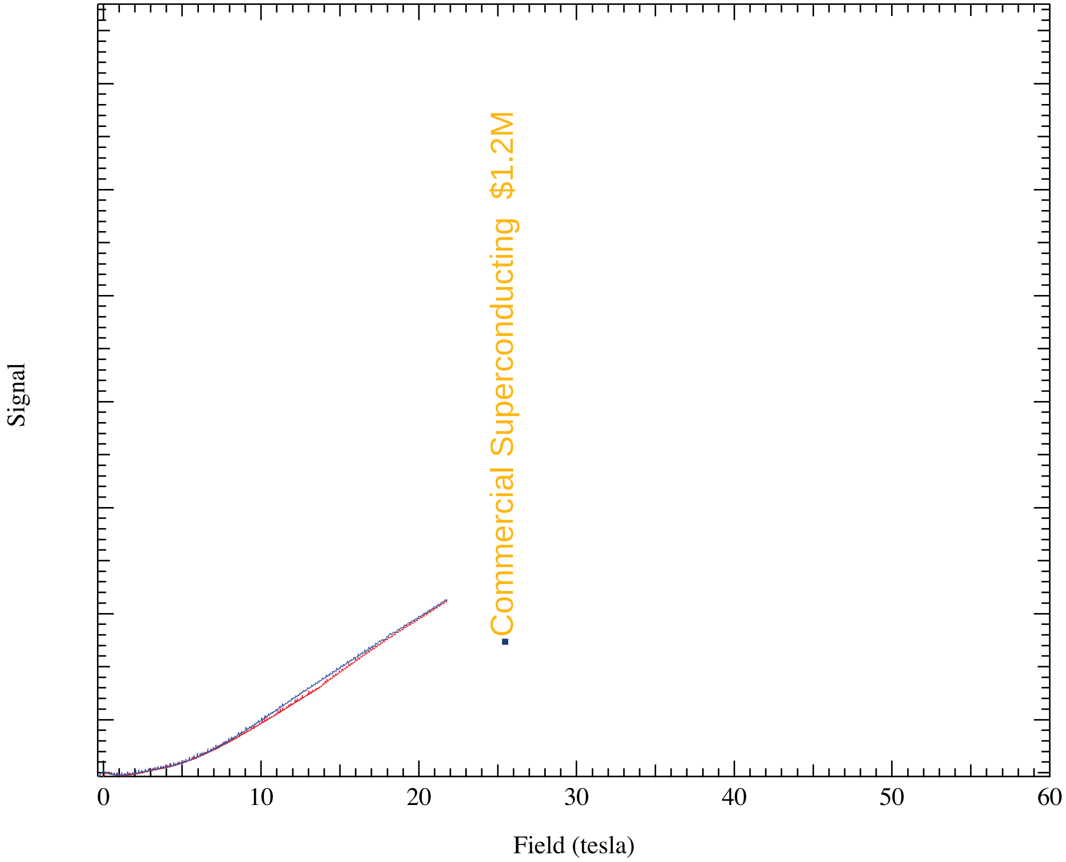
Tallahassee, FL

High B/T Facility

Gainesville, FL

Funded by the NSF at ~$34 M/year

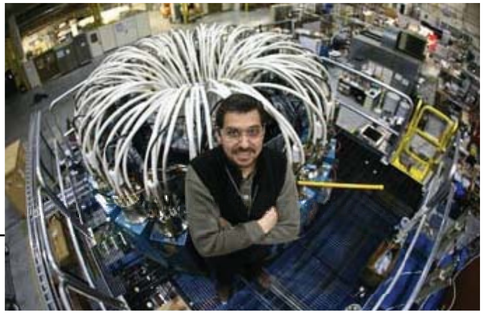
Classic Example: Superconductor



NHMFL-PFF Big Magnets

- **100 tesla Multi-Shot magnet**
  - World record setting magnet
    - Highest non-destructive magnetic field at 100.75 tesla
- **60 tesla Controlled Waveform magnet**
  - Unprecedented high magnetic field capability
    - User specific waveform

- **200+ tesla Single Turn magnet**
  - Only system of its kind capable of measuring actinides safely



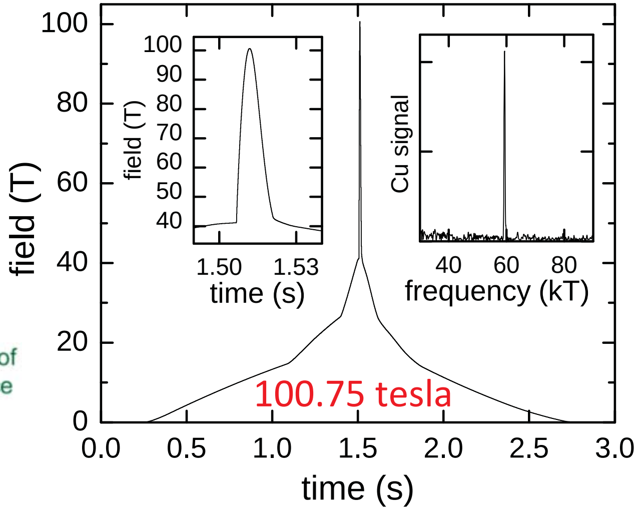
100 tesla Multi-Shot

- **Set world record non-destructive field**

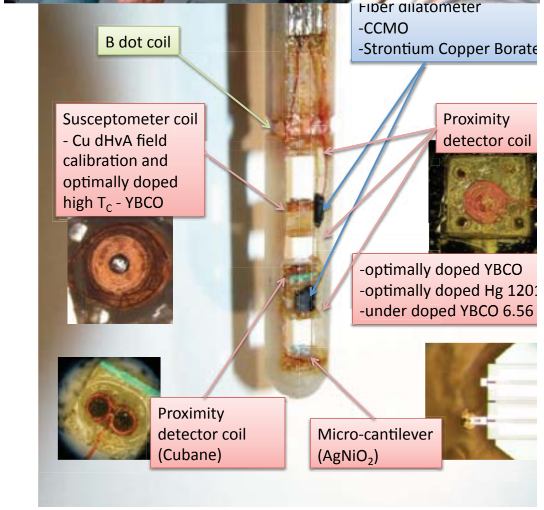
NHMFL breaks the megagauss barrier, reaches 100.75 tesla pulse*

100.75 tesla confirmed via magneto quantum oscillations in poly-crystalline copper. First nondestructive generation of magnetic fields in excess of 100T as a research tool.

This effort represents the culmination of a 15-year project funded by:

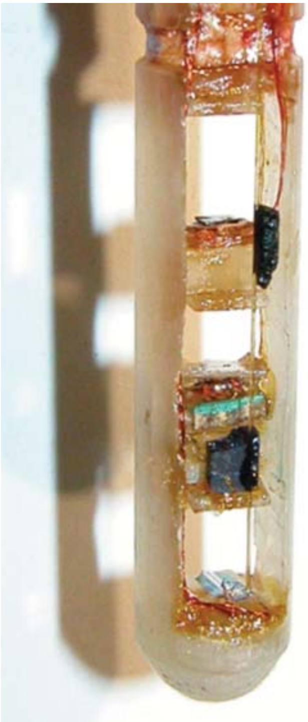


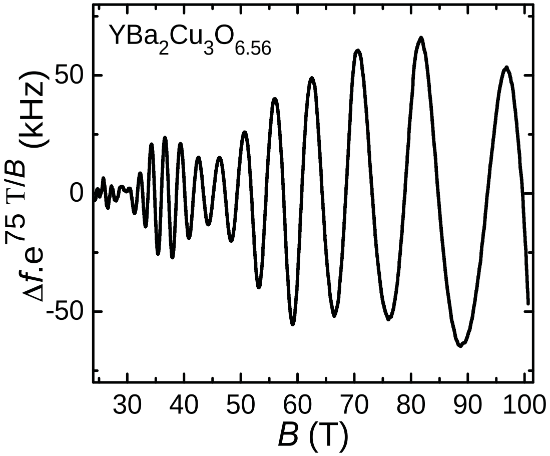
*World Record magnetic field intensity for a Non-Destructive Pulsed Magnet (22 March 2012)

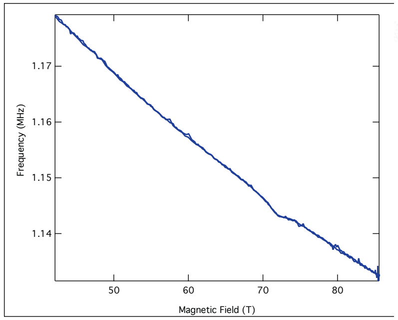


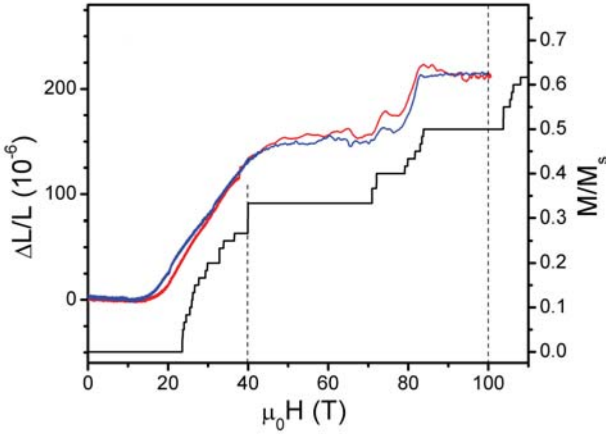
100 T Multiplexed Experiments

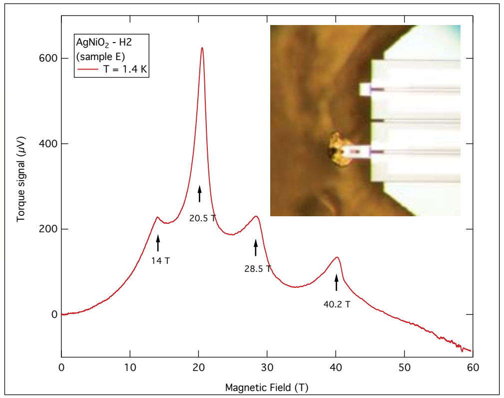
We run 8 simultaneous samples

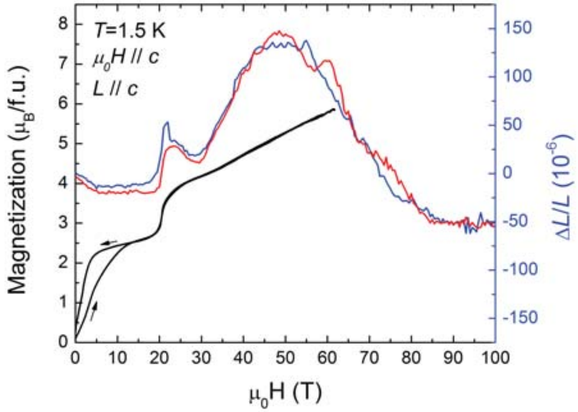




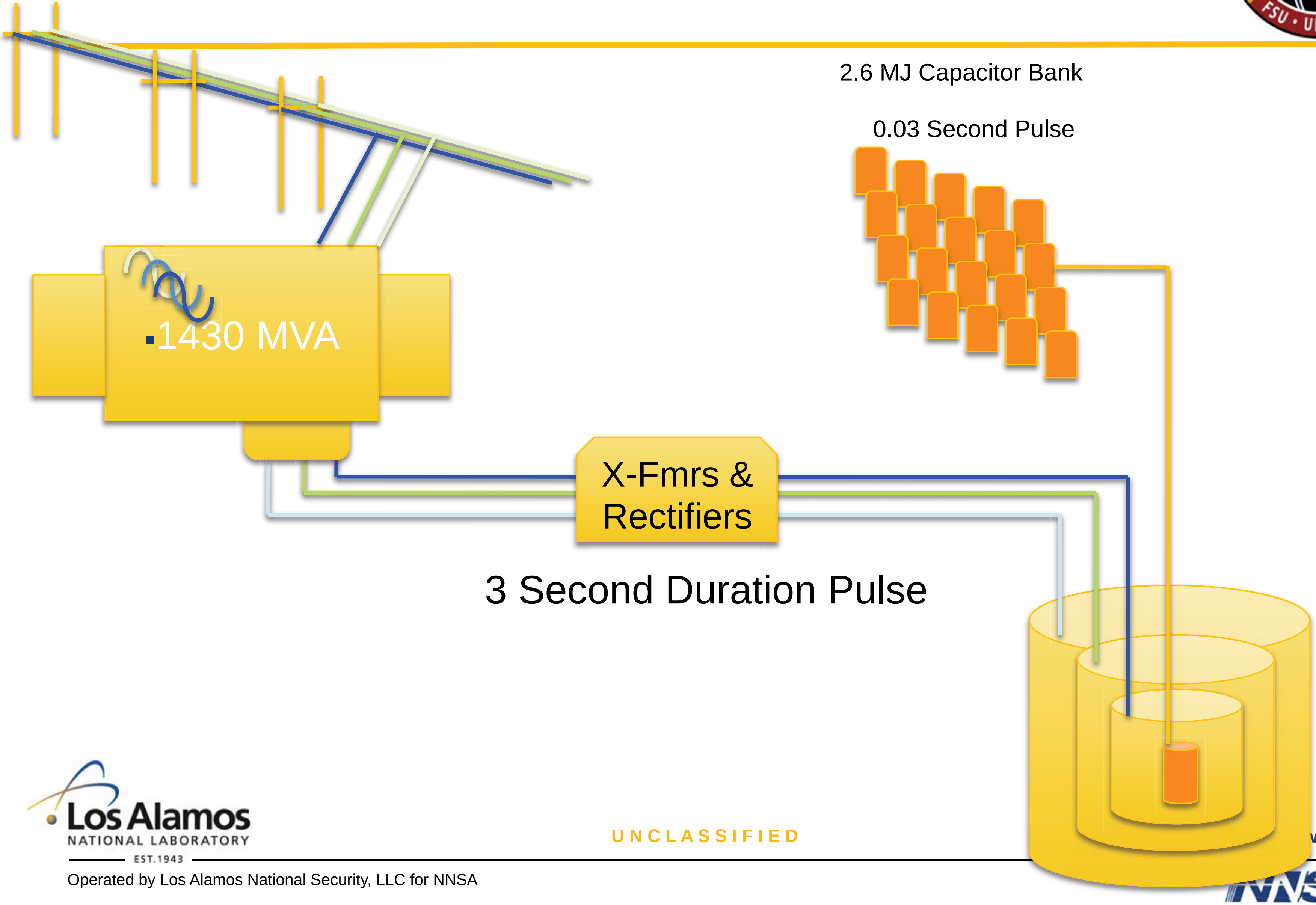








How does it work?



2.6 MJ Capacitor Bank

0.03 Second Pulse

- 1430 MVA

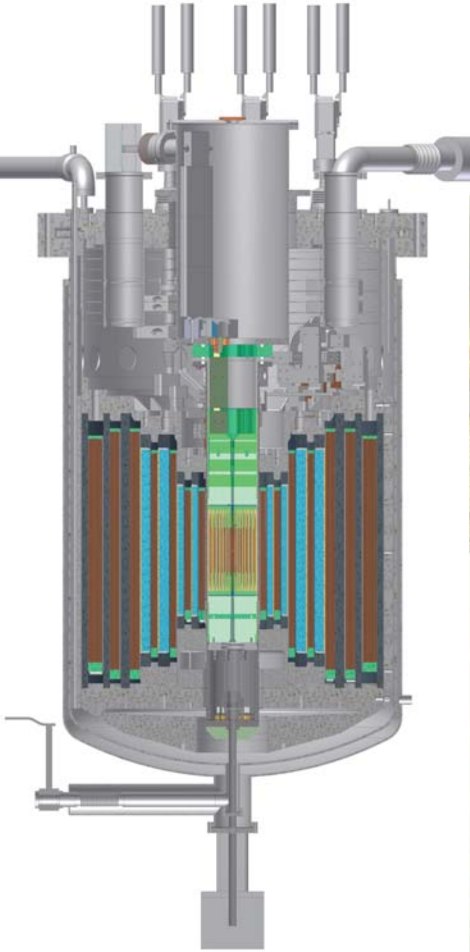
X-Fmrs & Rectifiers

3 Second Duration Pulse

100 tesla Multi-Shot

Extreme fields

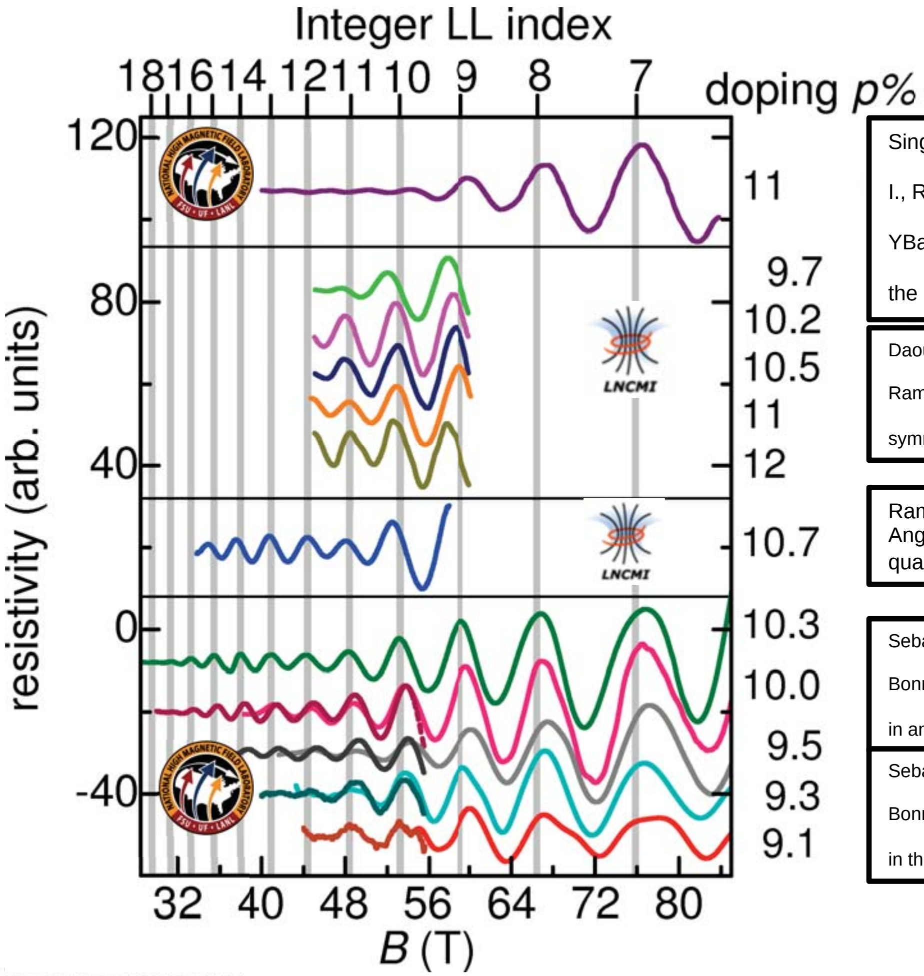
- The 1.43 GW generator is capable of delivering 600 MJ of electrical energy safely.



Insert magnet assembly

Higher fields reveal important details!

Lack of quantum oscillation phase change indicates Fermi surface remains constant



Singleton, J., de la Cruz, C., McDonald, R. D., Li, S. L., Altarawneh, M., Goddard, P., Franke, I., Rickel, D., Mielke, C. H., Yao, X., Dai, P. C. 2010 Magnetic quantum oscillations in YBa2Cu3O6.61 and YBa2Cu3O6.69 in Fields of up to 85 T: Patching the hole in the roof of the superconducting dome Phys. Rev. Lett. 104 086403/1 - 086403/4.

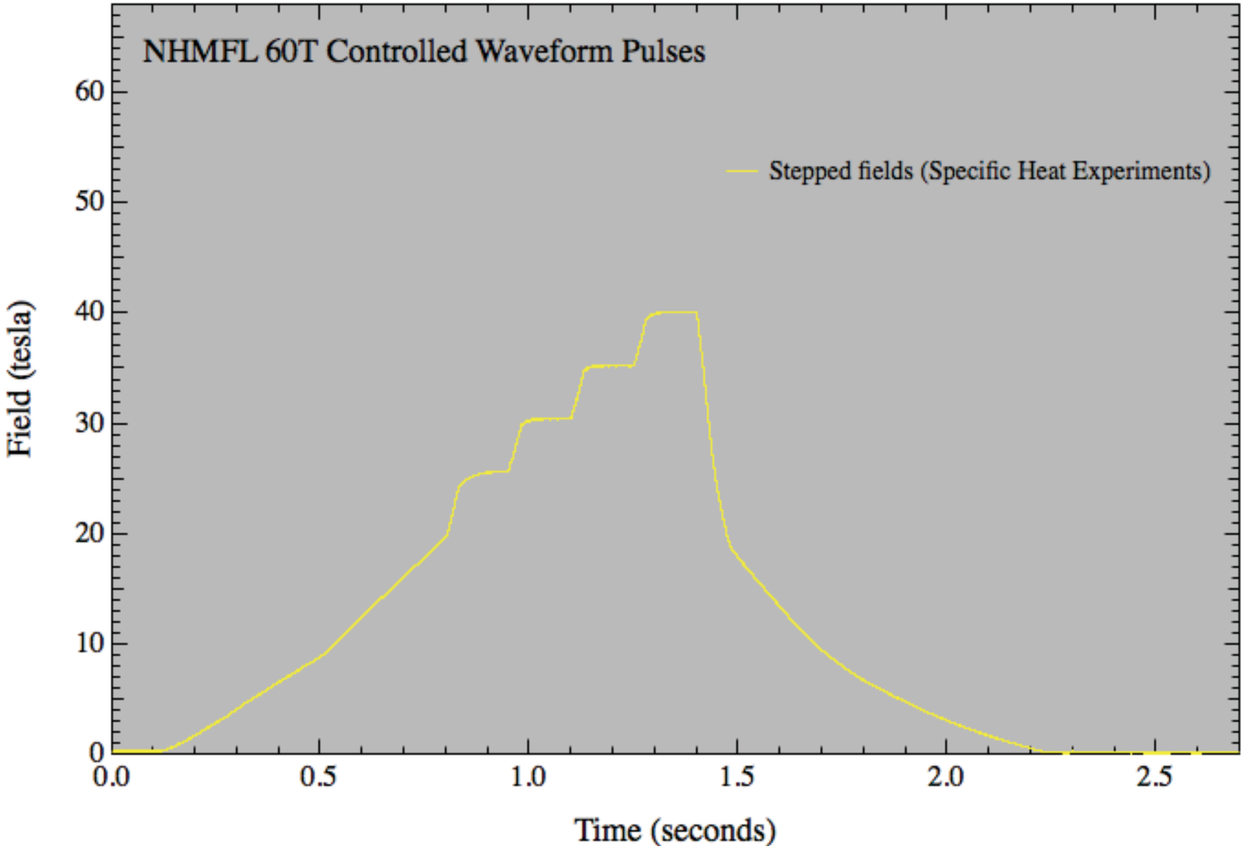
Daou, R., Chang, J., LeBoeuf, D., Cyr-Choiniere, O., Laliberte, F., Doiron-Leyraud, N., Ramshaw, B. J., Liang, R. X., Bonn, D. A., Hardy, W. N., Taillefer, L. 2010 Broken rotational symmetry in the pseudogap phase of a high-Tc superconductor Nature 463 519-522.

Ramshaw, B. J., Vignolle, B., Day, J., Liang, R. X., Hardy, W. N., Proust, C., Bonn, D. A. , (2011) Angle dependence of quantum oscillations in YBa2Cu3O6.59 shows free-spin behavior of quasiparticles ***Nature Phys***. 7 234-238

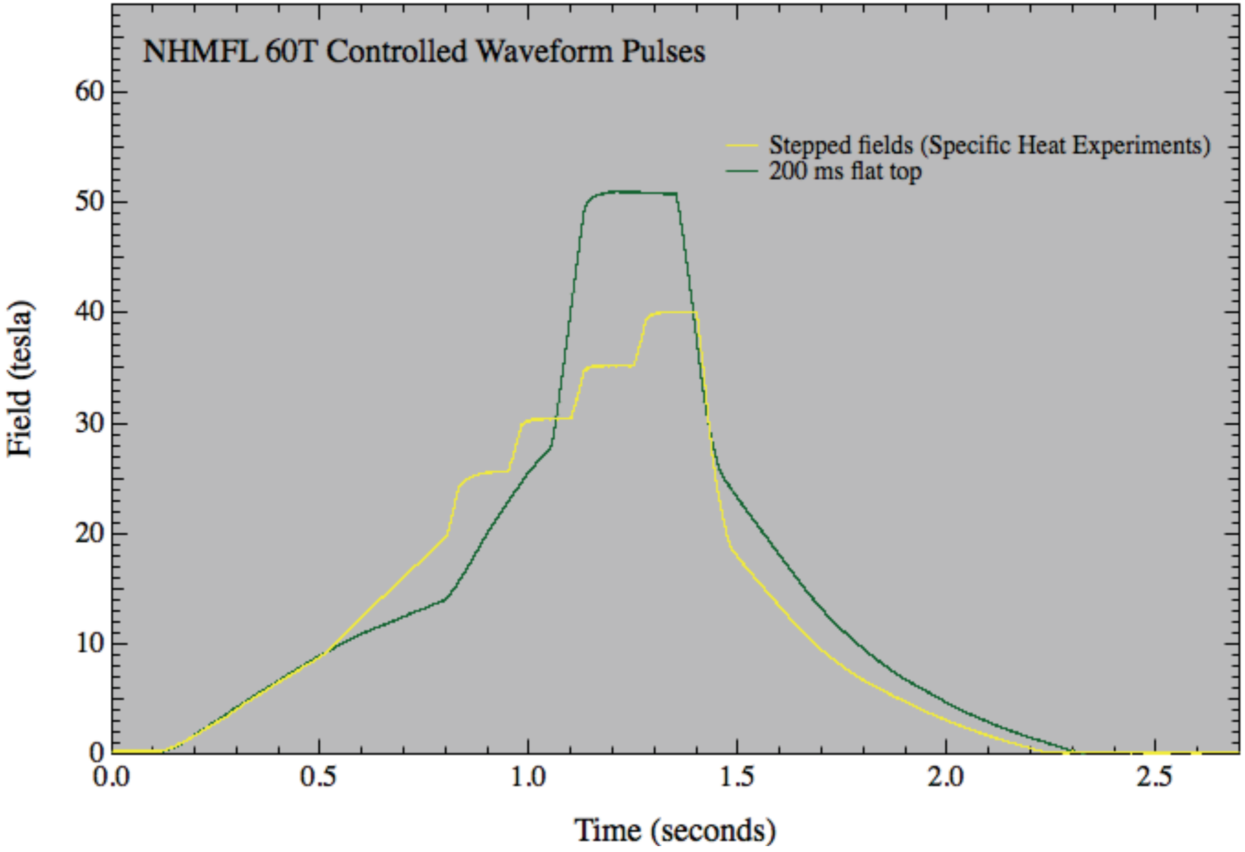
Sebastian, S. E., Harrison, N., Altarawneh, Goddard, P. A., M. M., Mielke, C. H., Liang, R. X., Bonn, D. A., Hardy, W. N. & Lonzarich, G. G. 2010 Compensated electron and hole pockets in an underdoped high-Tc superconductor ***Phys. Rev. B*** 81 214524.

Sebastian, S. E., Harrison, N., Altarawneh, M. M., Balakirev, F. F., Mielke, C. H., Liang, R., Bonn, D. A., Hardy, W. N., & Lonzarich, G. G. 2011 Direct observation of multiple spin zeroes in the underdoped high temperature superconductor YBa2Cu3O6+x arXiv 1103.4178.

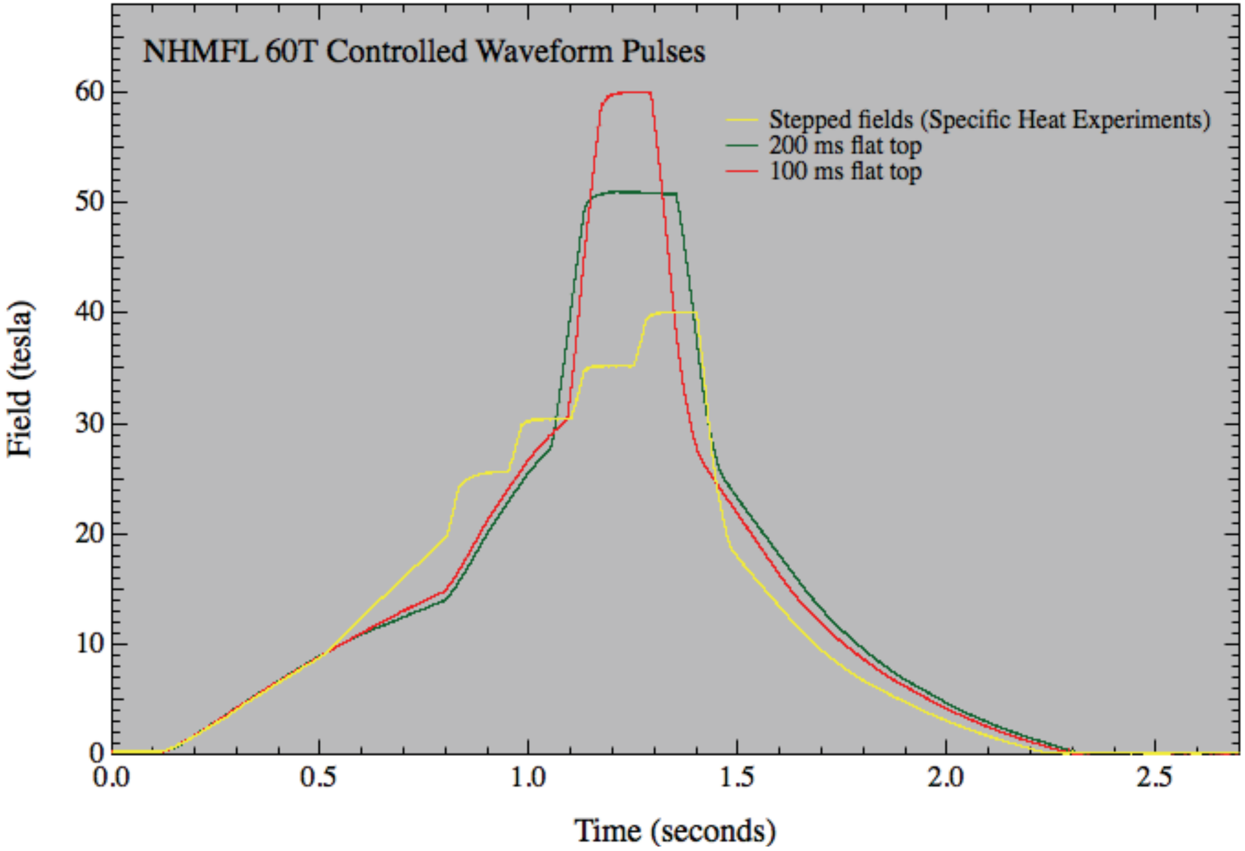
60 tesla controlled waveform magnet



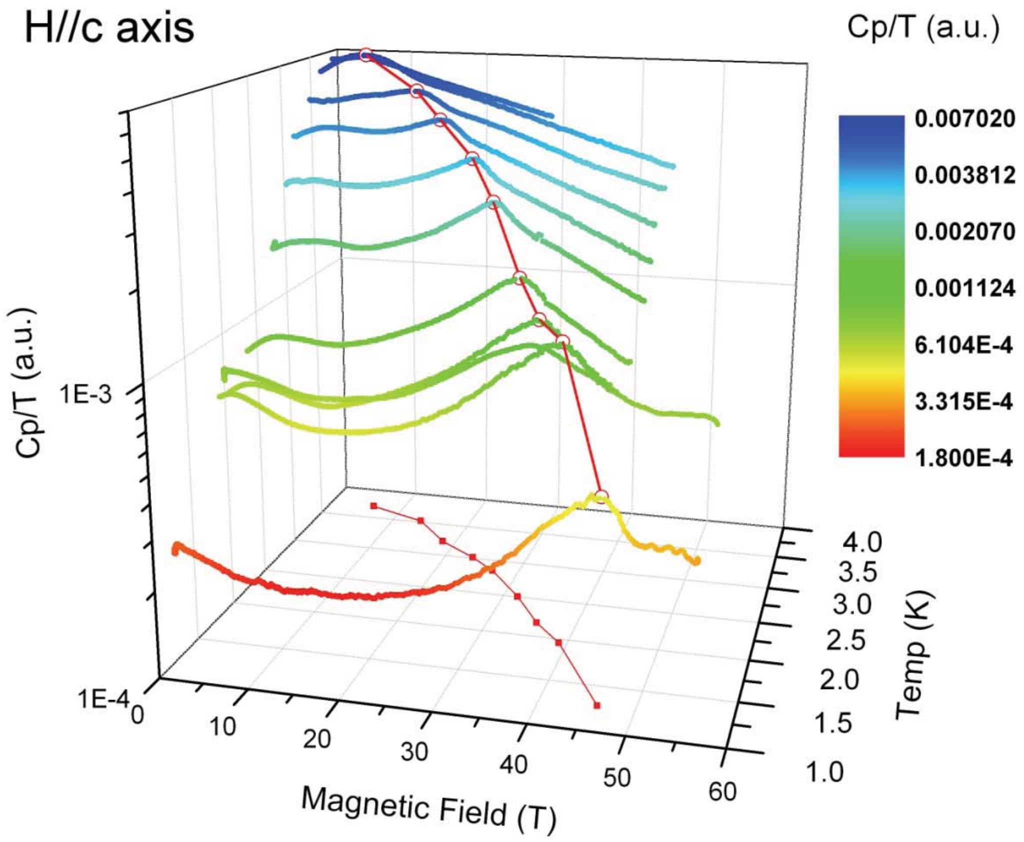
60 tesla controlled waveform magnet



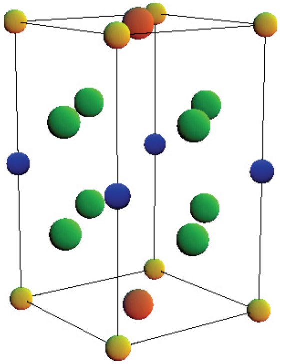
60 tesla controlled waveform magnet

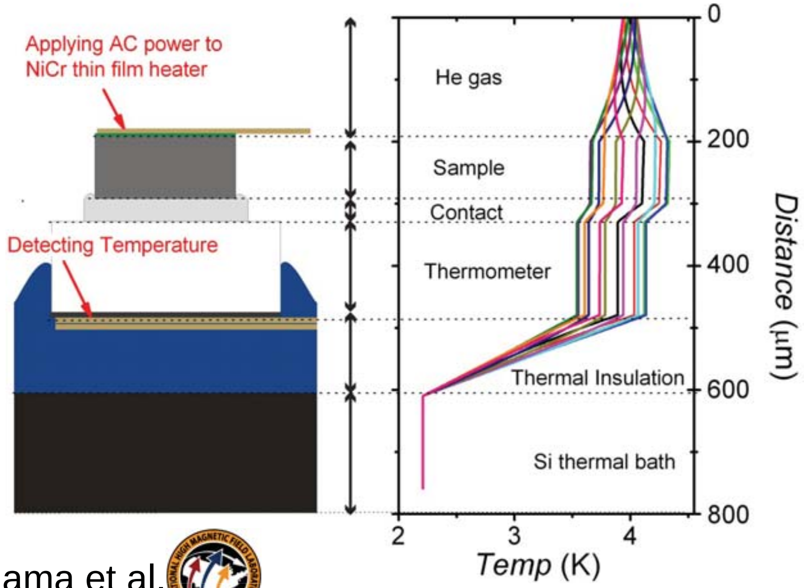


Specific Heat in a pulsed magnet



CeRhIn$_5$

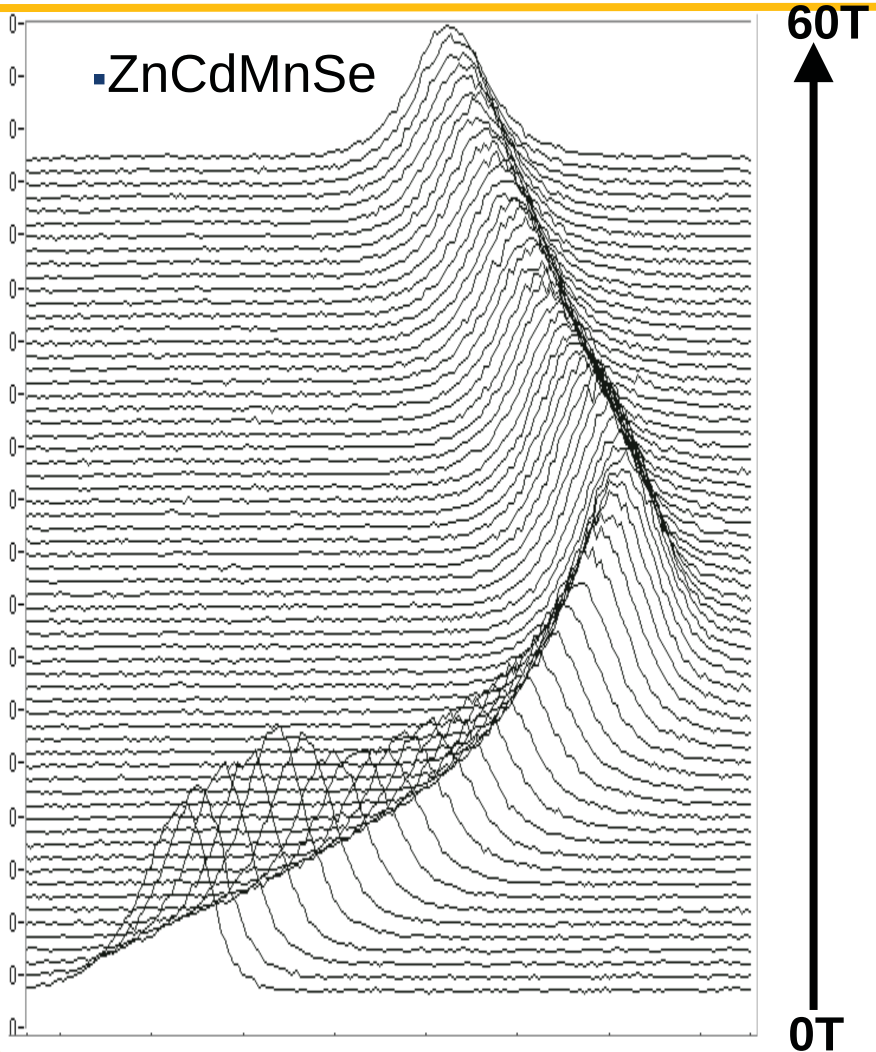




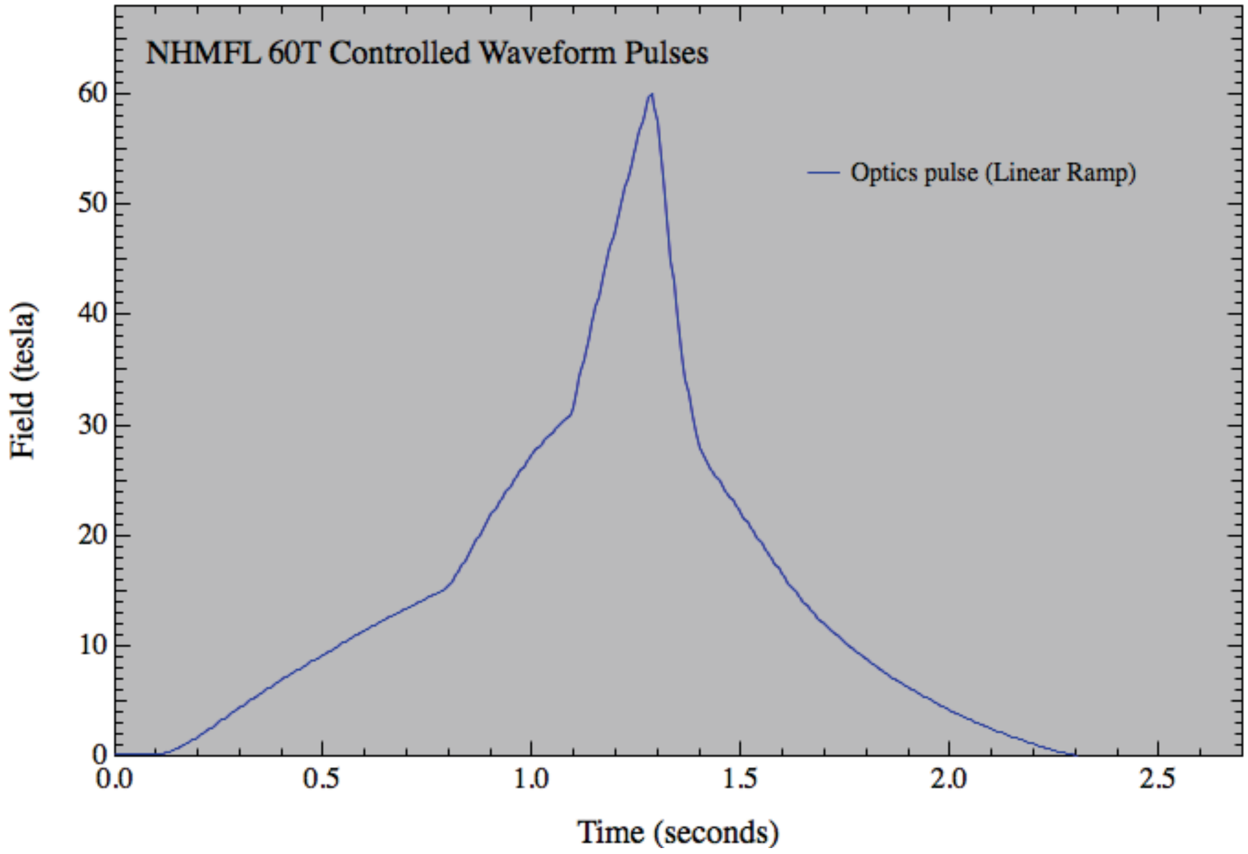
Developed by M. Jaime & Y. Kohama et al.

Optical Spectroscopy (photoluminescence) in High Magnetic Fields

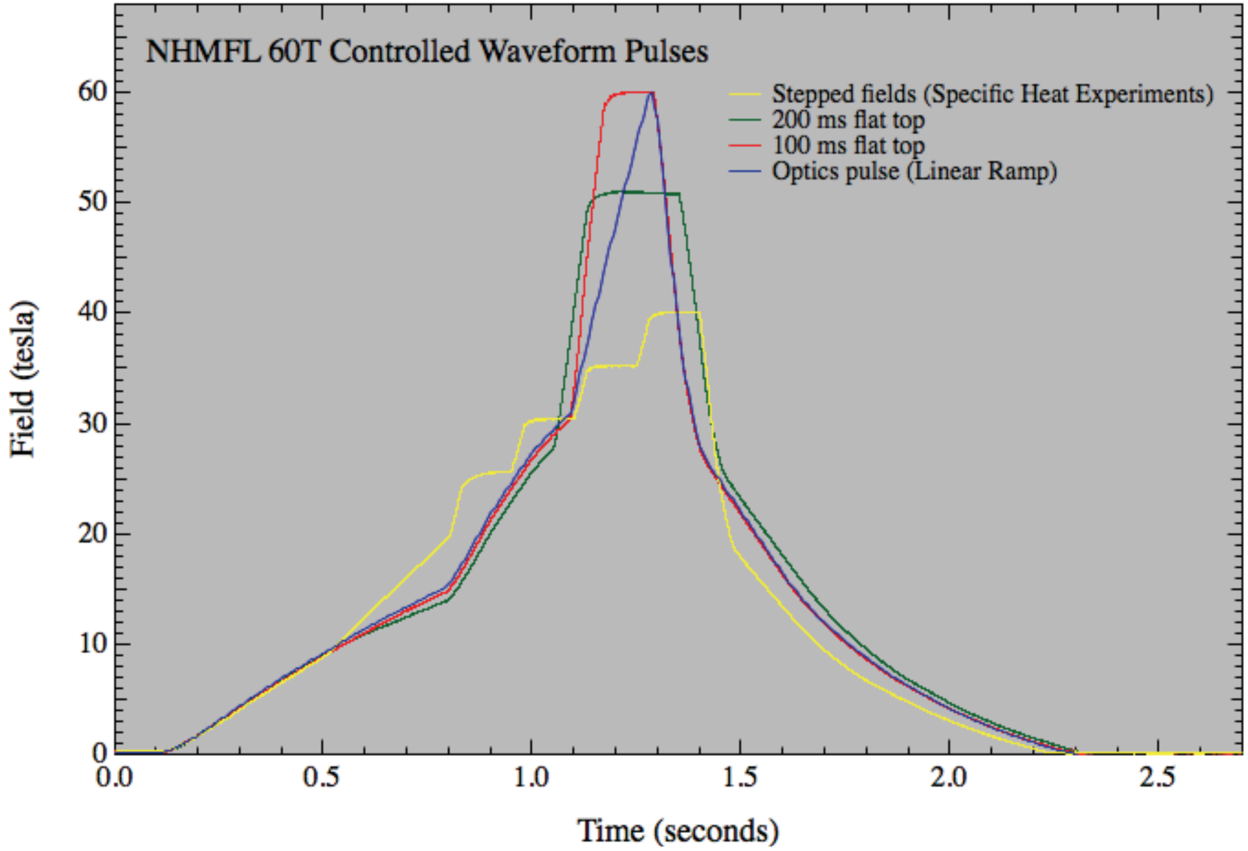
- 60 T Controlled Waveform Magnet



60 tesla controlled waveform magnet



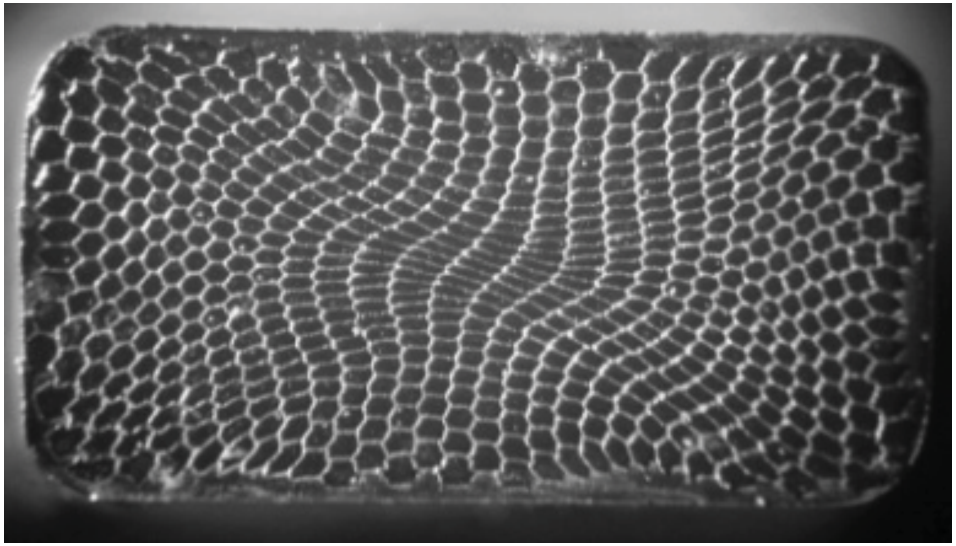
60 tesla controlled waveform magnet



Extreme Fields Demand Advanced Materials

- **Conductor**
  - Need good conductivity
  - Need High Strength

Glidcop AL-60



Bochvar CuNb

Glidcop AL-15

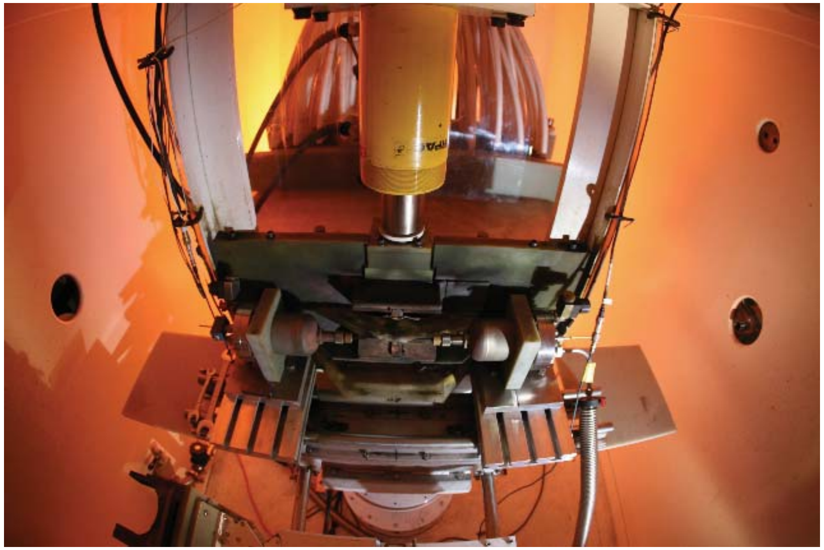
UNCLASSIFIED

See poster by R. Need

Extreme Fields Beyond today's materials

- HEPA Filtered & Sealed

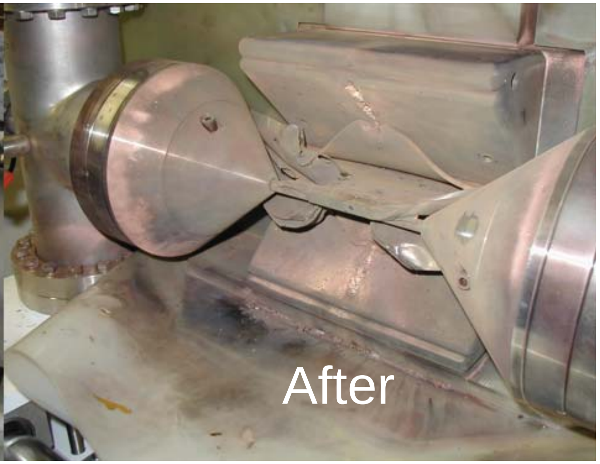
0.26 MJ “Fast” Capacitor Bank



Delicate

Cryostat Tube

Blast is “designed”



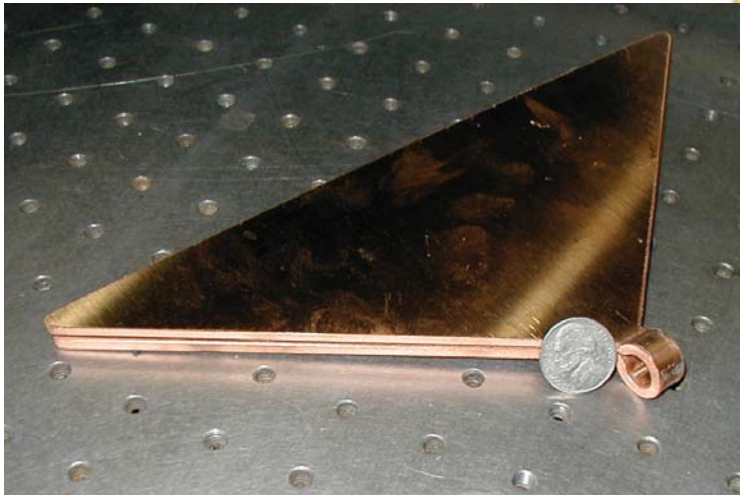
No Damage

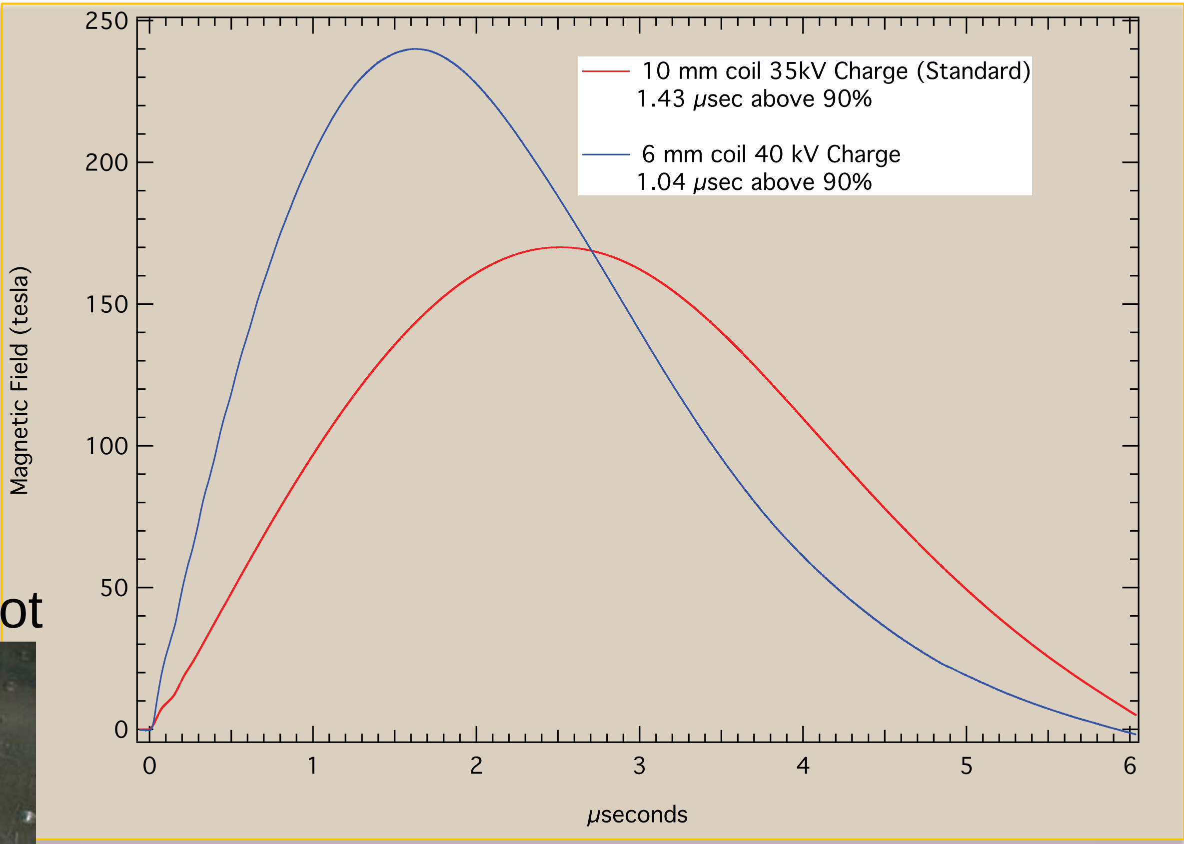
To Plastic Tube

Despite impact craters

Ultra-High Magnetic Field Generation

Still Frame from 240 tesla shot



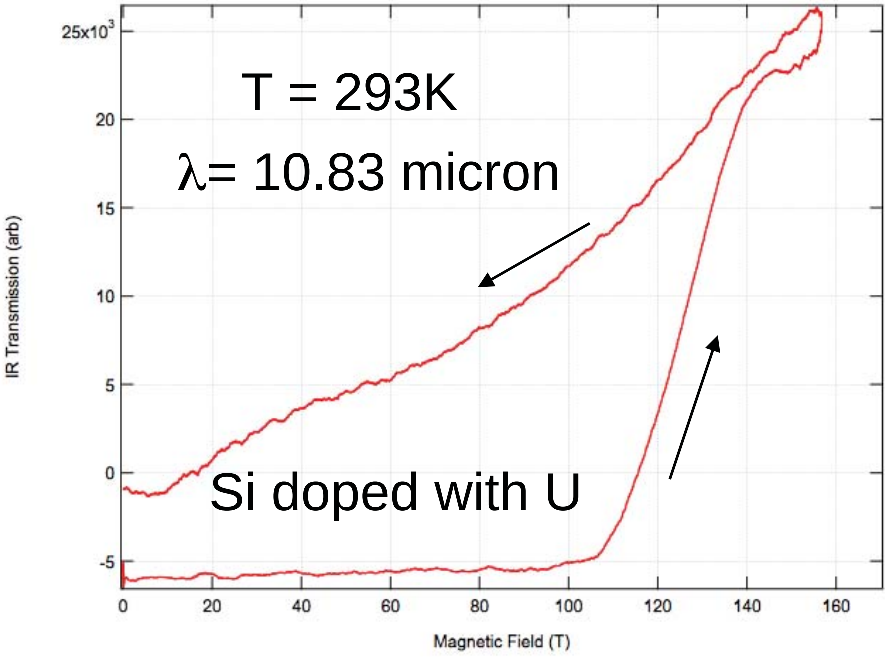


In pulsed magnetic fields we routinely measure:

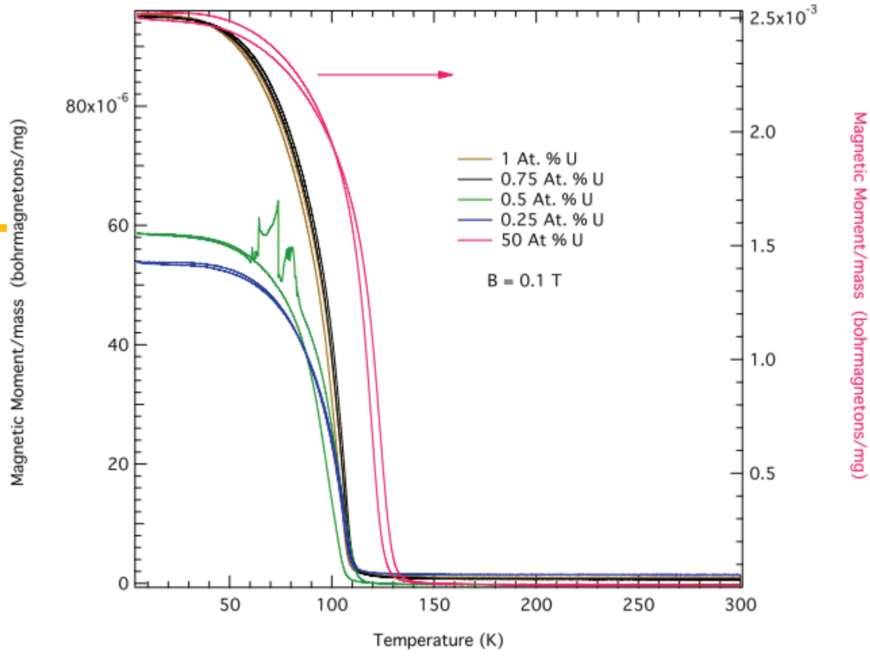
- IR/VIS transmission
- RF conductivity
- Magnetic susceptibility

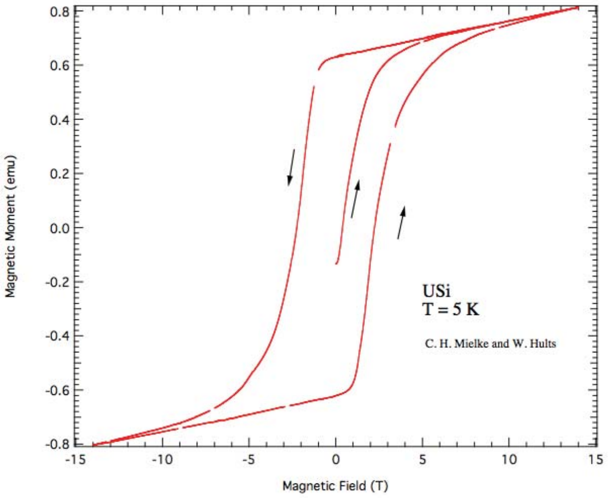
Field induced magnetic state

Can field order in the same way as temperature?

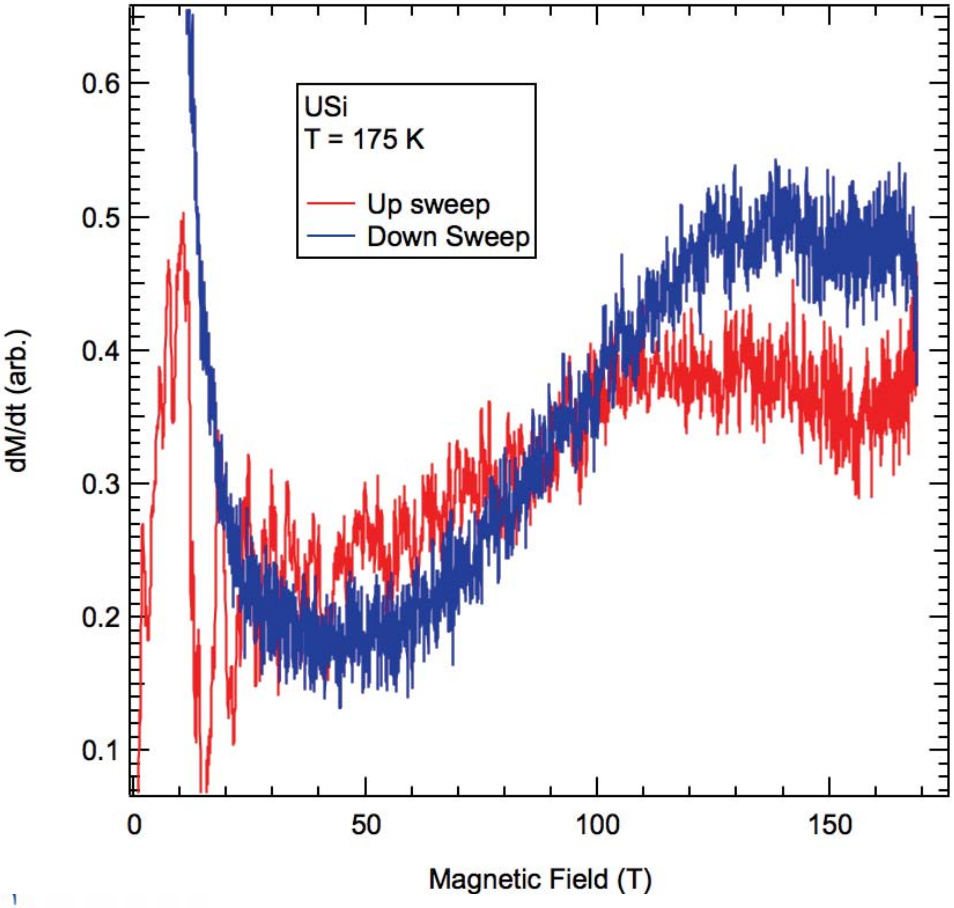


70 micron thick sample ~ 2mm in diameter





Magnetic Susceptibility of USi



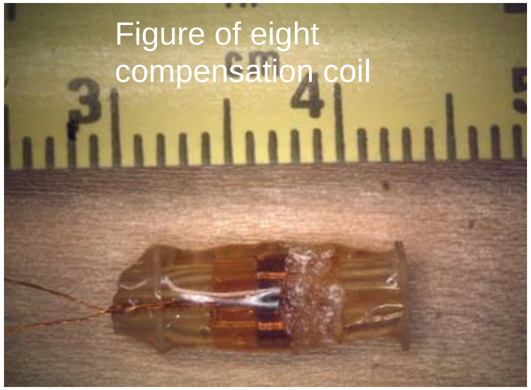
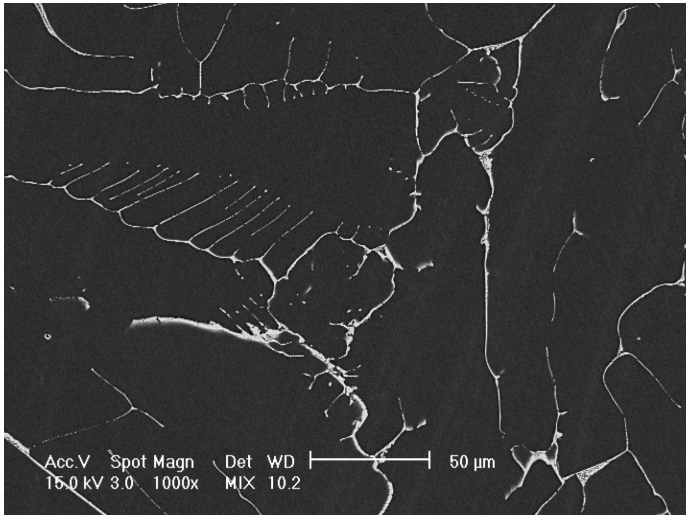
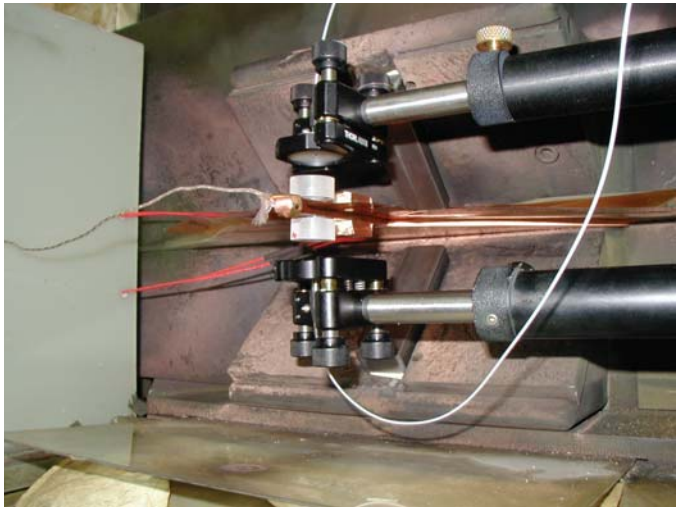
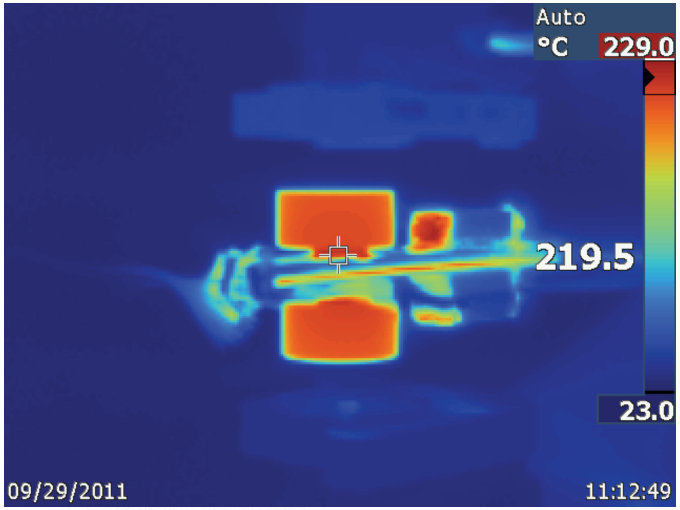


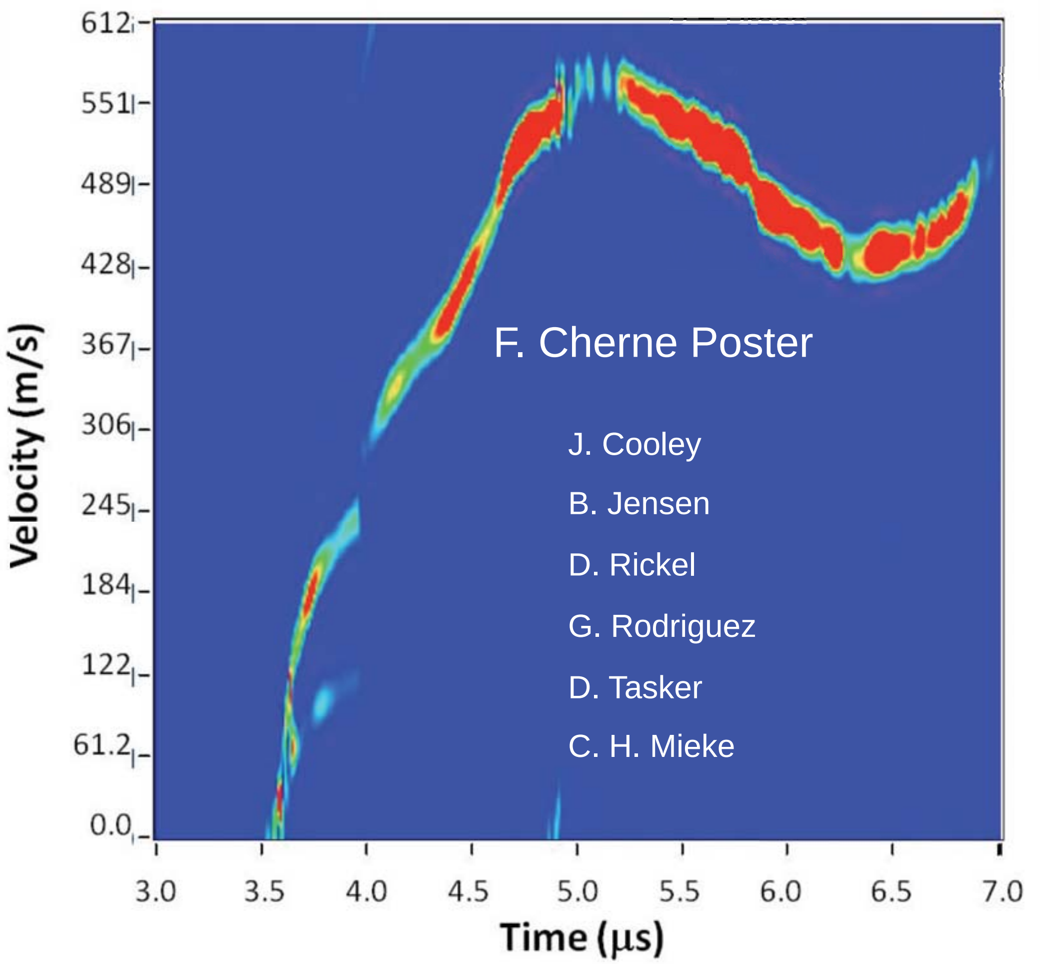
Figure of eight compensation coil



Mag-ICE Setup







F. Cherne Poster

J. Cooley

B. Jensen

D. Rickel

G. Rodriguez

D. Tasker

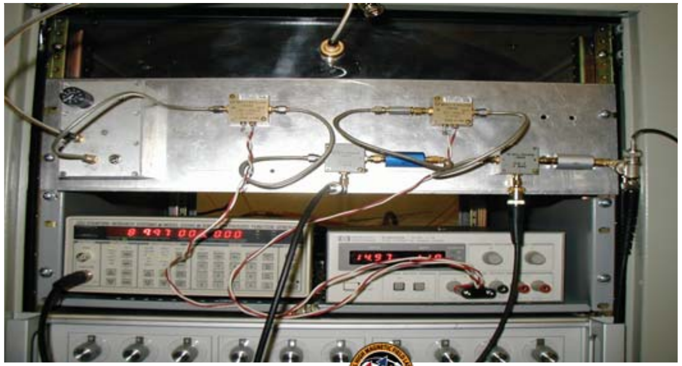
C. H. Mieke

COTS ⟷ Advanced Diagnostics

Unique experimental tools for extreme magnetic fields

rf contactless conductivity

Handheld Metal Detectors



C. H. Mielke et al.

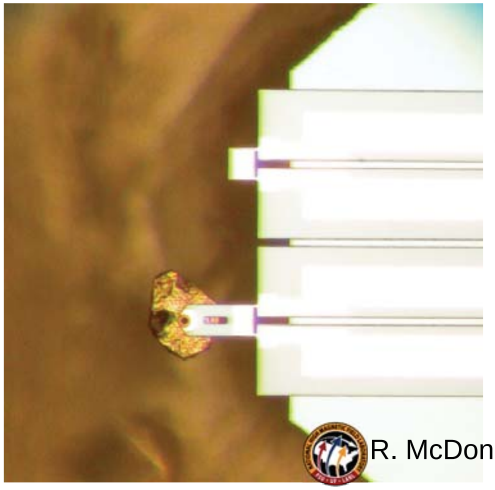
digital lockin

PC based Timing

A. Miglioriet al.

piezzoelectric magnetometry

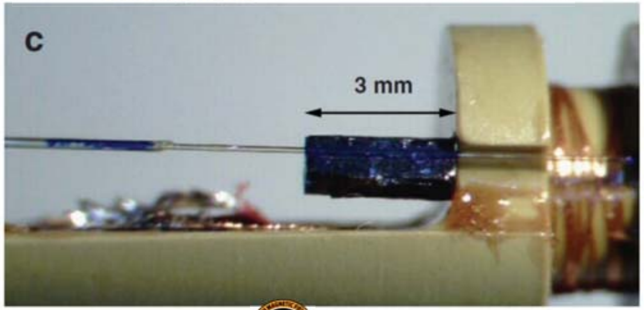
Atomic Force Microscopy



R. McDonald al.

optical strain gauge

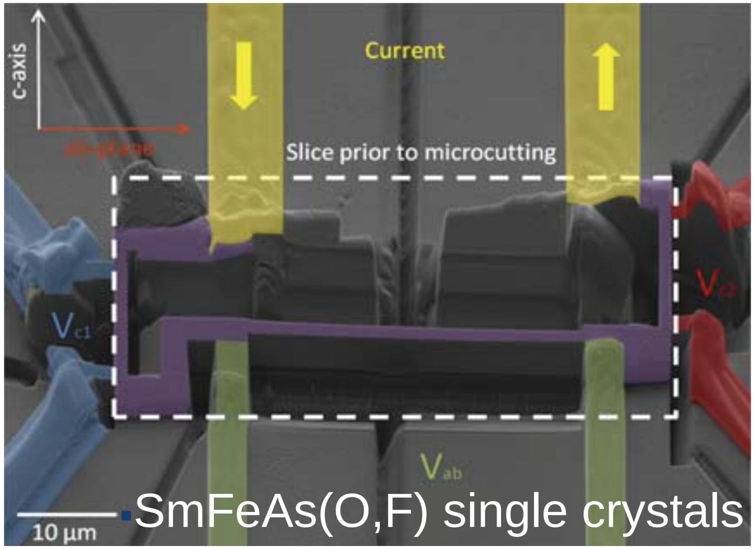
Telecom & Strain Gauges



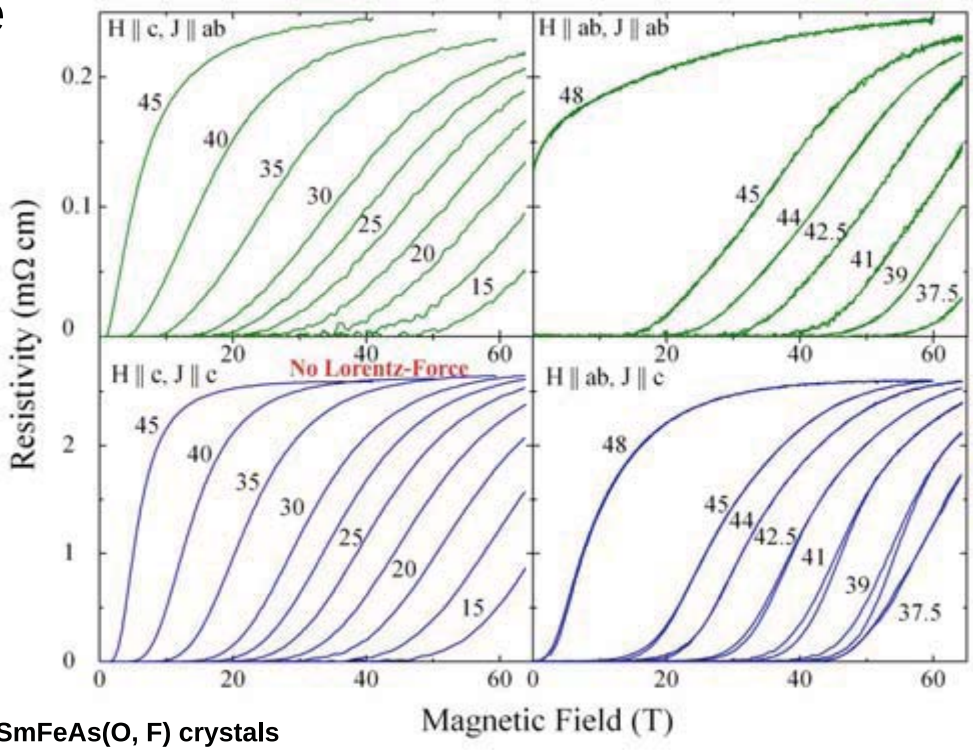
M. Jaime al.

Advanced Techniques
Focused Ion Beam Lithography

- Measurement failed on bulk sample
- Exceptionally clean on FIB sample



- SmFeAs(O,F) single crystals



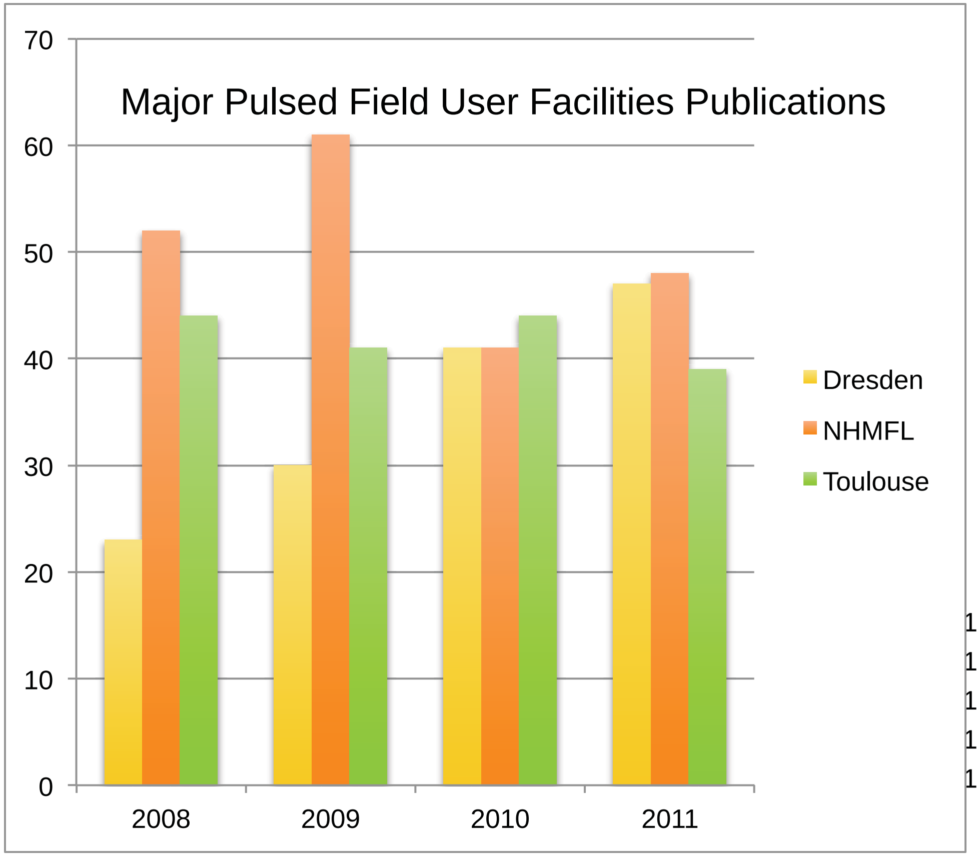
High magnetic-field scales and critical currents in SmFeAs(O, F) crystals

P. J. W. Moll, R. Puzniak, F. Balakirev, K. Rogacki, J. Karpinski, N. D. Zhigadlo, B. Batlogg,

Nature Materials **9, 628–633 (2010)**

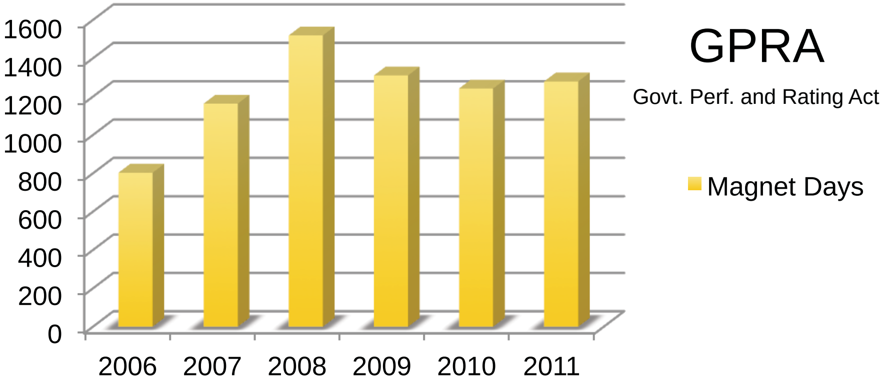
See Poster by F. Balakirev

User Program Metrics



*Wuhan, CN User program goes live 2013

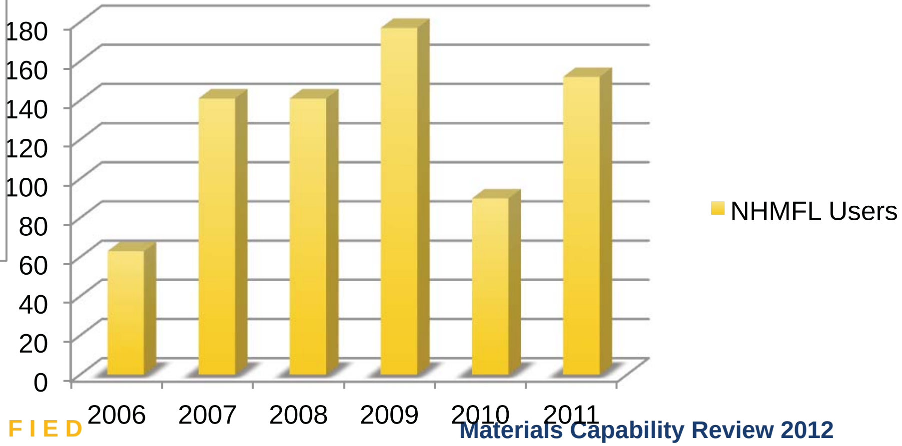
NHMFL-PFF Magnet Days



GPRA

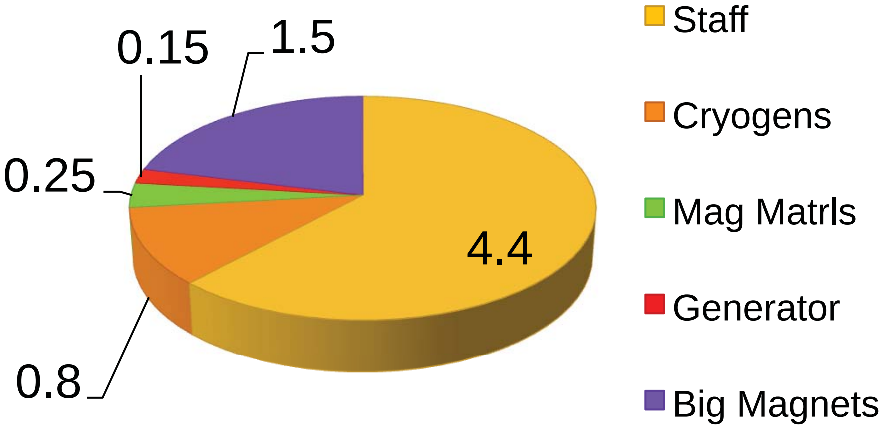
Govt. Perf. and Rating Act

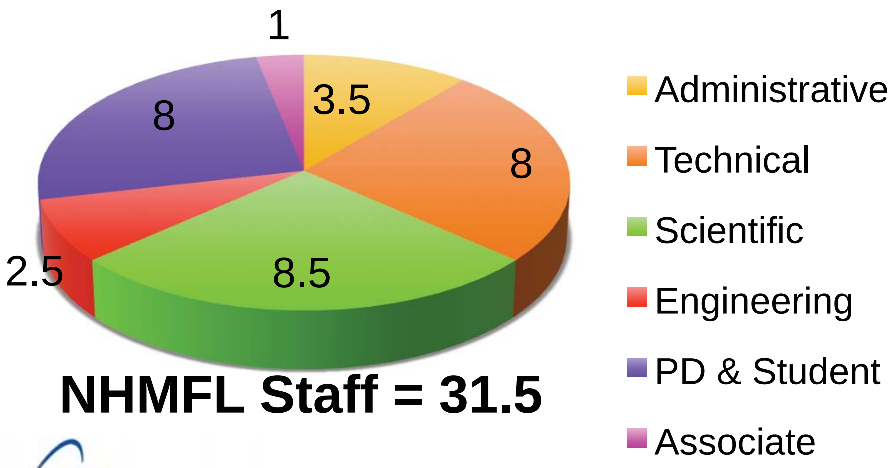
NHMFL-PFF Users



NHMFL Work Force and Users (2011)

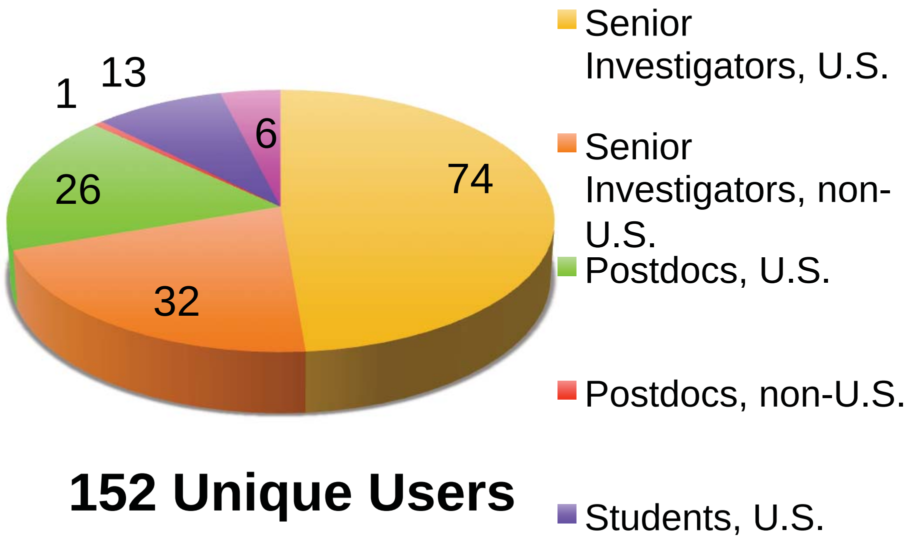
User Prog Budget = $7.1M





NHMFL Staff = 31.5

2011 NHMFL Users



152 Unique Users

In the eyes of the competition

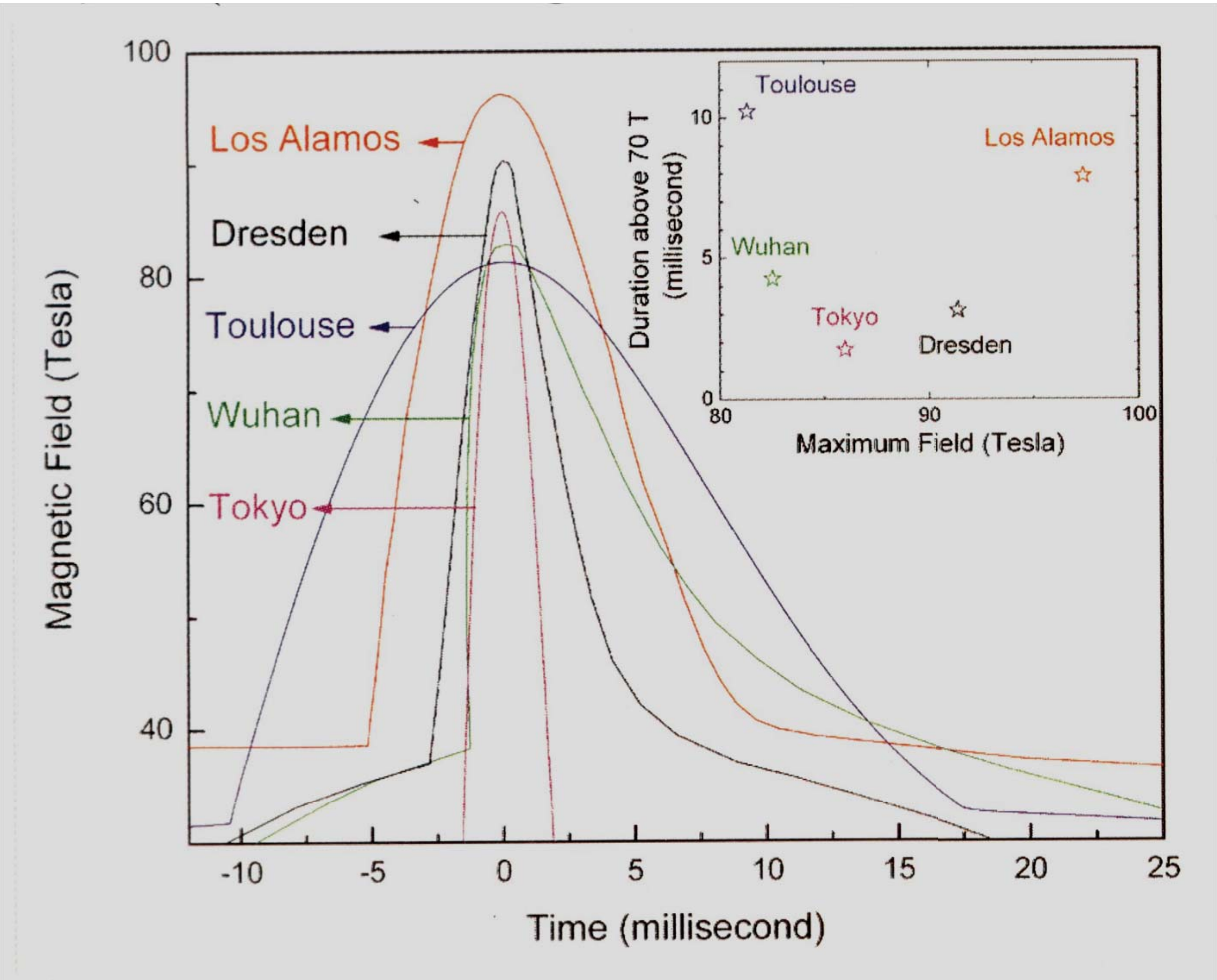
http://www.euromagnet2.eu

EuroMagNEWS
N°12 / October - December 2011

EuroMagNET II - Best wishes for 2012 .... page 2
EuroMagNET II - News from Toulouse and Grenoble .... page 3
EuroMagNET II - Results of the sixth call for access .... page 4
EMFL News .... page 6
Job opportunities .... page 9
High Magnetic Fields in Semiconductor Physics – HMF20 .... page 10
International workshop on Strongly Correlated Electron systems
in high magnetic Fields (SCEF) .... page 11

1st EuroMagNET Summer School - Science in High Magnetic Fields
September 30 - October 07, 2012 - Rügen - Germany

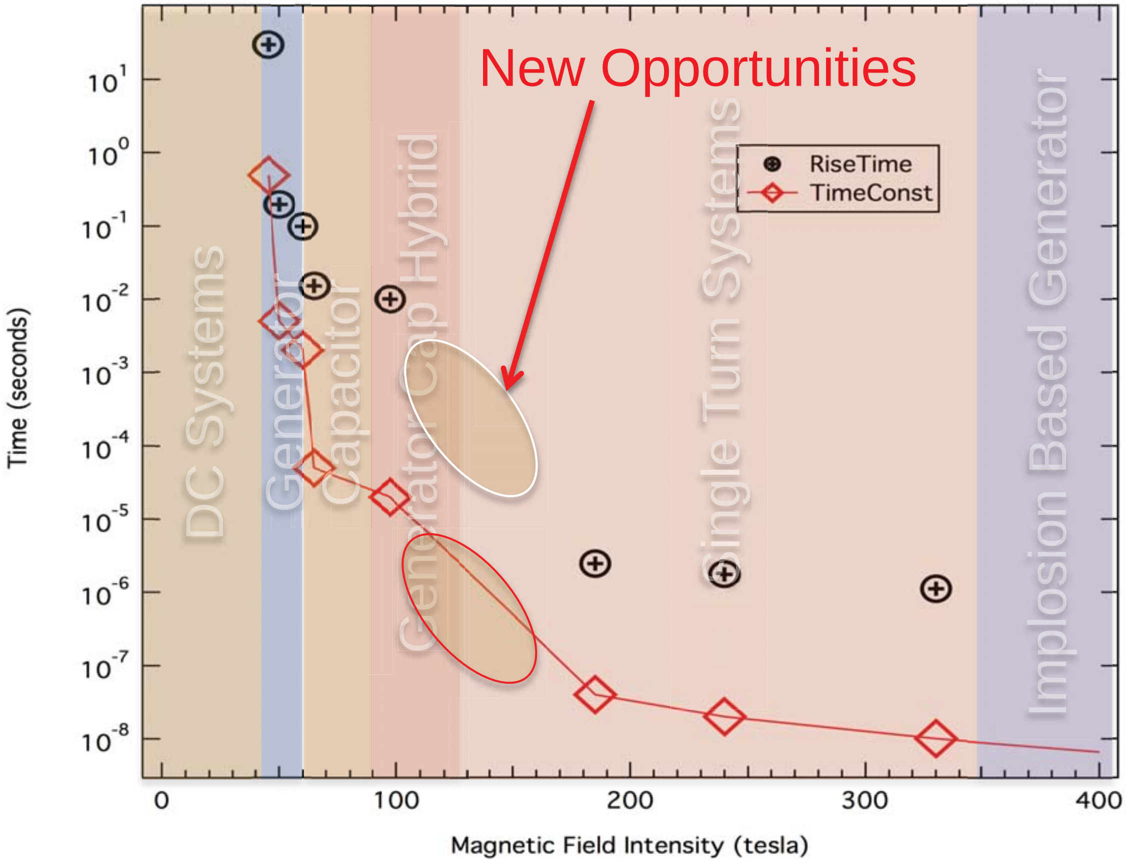
December issue of
EuroMag News



UNCLASSIFIED

Opportunities for Pulsed Fields

Where we go next is strongly coupled to Science needs and techniques



What’s Next?

- **Science needs higher fields**
  - Vis a Vis optimally doped YBCO (still SC at 100.75 T)
  - Light sources and Neutron facilities
    - Huge challenge with repetitively pulsed magnets
- **Precise measurements**
  - FIB technology enables new tougher measurements
    - Meso frontier (see posters by: Cooley and Balakirev and McDonald and Crooker)
- **High Pressure**
  - Clear need from the Cond. Matt. Community for static pressures in High B
  - Have demonstrated piston cell, DAC (goal to have a piston cell at 30 kBar for PF)

Summary

- **NHMFL-PFF capabilities**
  - World leading magnets and techniques at extremes of high magnetic field
  - Developing new inroads to efficiency
  - Well poised to research and discover emerging states of matter
- **Techniques**
  - Developed the leading methods in Pulsed Magnetic Fields today
  - Coupled to discovery science and new realms of extreme conditions
- **Metrics**
  - Well positioned with competition
- **Global Perspective & Future**
  - Growth opportunity in high pressure, FIB

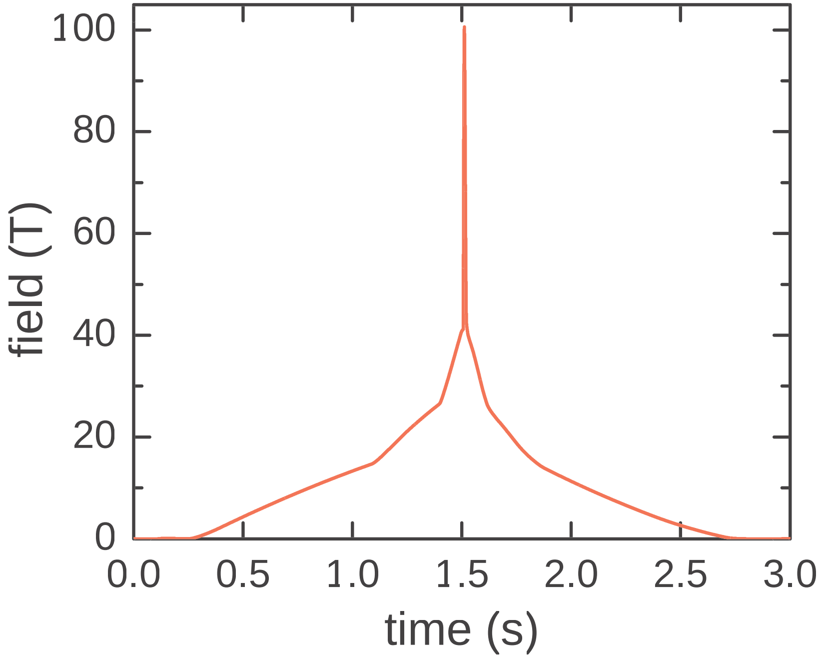
Science in Extremes of High Magnetic Fields

N. Harrison (MPA-CMMS)

Magnetic fields are one of a portfolio of extreme environments for materials research at Los Alamos National Laboratory, as recently demonstrated by the record achievement of a non-destructive 100 tesla magnetic field in conjunction with materials science experiments. Intense magnetic fields enable theoretical predictions to be tested, provide new directions for materials development and can be used to achieve controlled functionality. Here, we will focus on the role of magnetic fields as a tuning parameter in condensed matter physics — in particular (1) the effect of a reduced magnetic length on superconductivity, (2) magnetic fields as an effective "negative pressure" and (3) the realization of emergent phenomena in extreme magnetic fields resulting from commensurability effects.

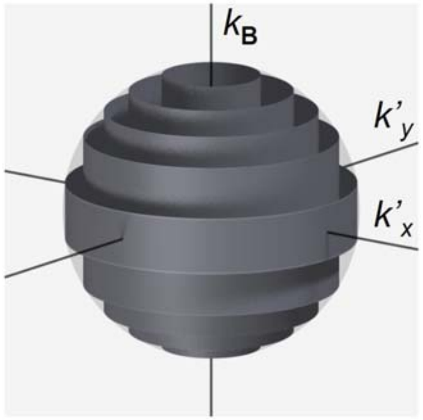
Science in Extremes of High Magnetic Fields

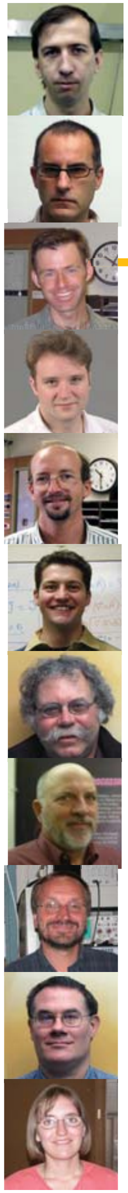
Presented by N. Harrison



Science in extremes of high magnetic fields

- **A key part of the portfolio of extreme environments for materials research at Los Alamos National Laboratory**
  - i.e. intense electromagnetic fields
- **Need to understand how extreme electromagnetic fields interact with matter**
  - Test theoretical predictions & provide new directions for materials development
  - Use magnetic fields to achieve controlled functionality of materials
- **Focus on magnetic fields as a tuning parameter in condensed matter**
  - The effect of reduced magnetic length
  - Magnetic fields as an effective “negative pressure”
  - Emergent phenomena resulting from commensurability





Pulsed Field Science Team

- Fedor Balakirev (Electrical Transport)
- Jon Betts (Resonant Ultrasound/Cryogenics/HoUP)
- Scott Crooker (Optics)
- Neil Harrison (Magnetization)
- Marcelo Jaime (Heat Capacity)
- Ross McDonald (GHz/RF and Torque Magnetometry)
- Albert Migliori (Resonant Ultrasound)
- Dwight Rickel (Pulse Echo Ultrasound)
- John Singleton (Magnetization)
- Chuck Swenson (Pulsed Magnet Design)
- Vivien Zapf (Thermodynamics and Dielectrics)

USER Program (jbbetts@lanl.gov)

Logistics (julietg@lanl.gov)

https://users.magnet.fsu.edu/

Science funding

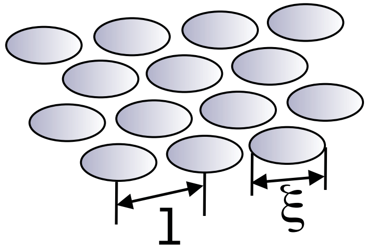
NSF

U.S. DEPARTMENT OF ENERGY | Office of Science

LDRD

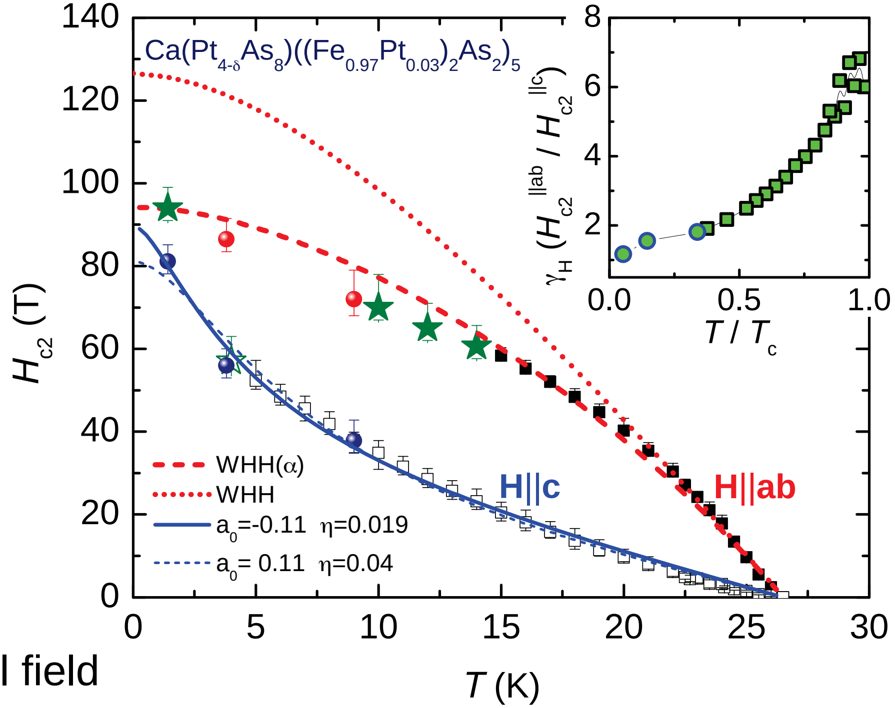
Magnetic length: Suppressing the vortex lattice in high T_c Fe-based pnictides

- **Magnetic length scale falls below superconducting coherence length**
  - Realized below 100 T in new iron-based superconductors



Mun *et al* (Phys. Rev. B. rapid., 2012)

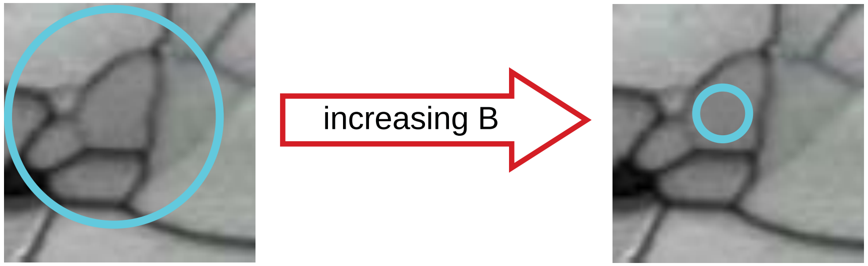
see poster of Balakirev *et al.*

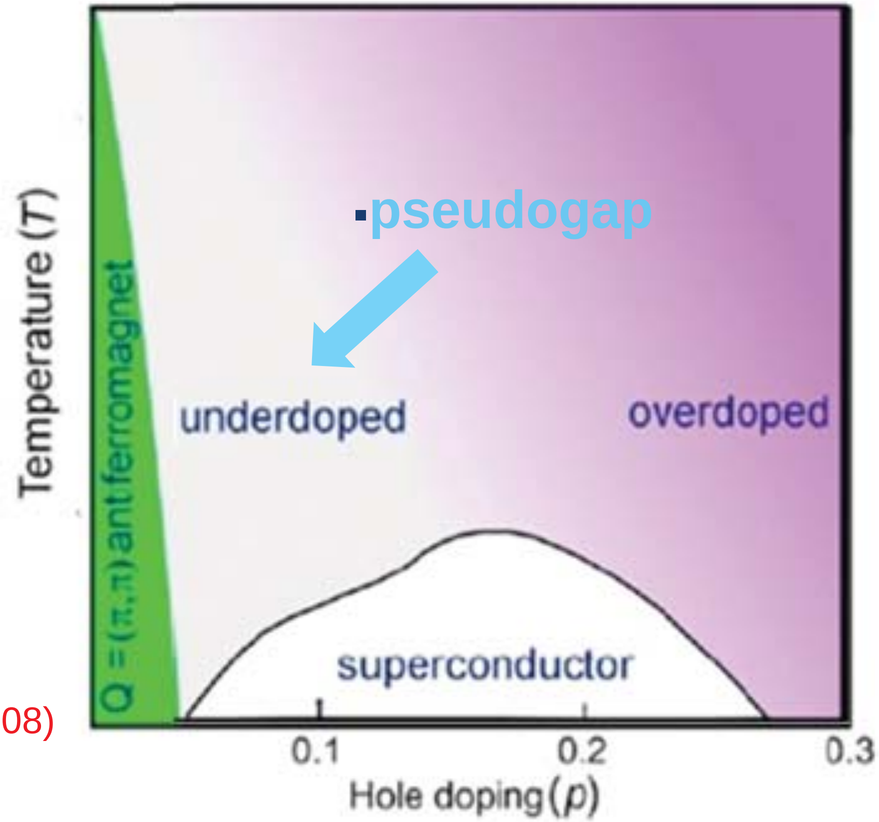


  - Unexpectedly isotropic upper critical field
    - Now established at LANL in several iron-based materials
    - Promising candidates for future high field magnets, superconducting wires

Magnetic length: Collapse of cyclotron radius

- **Landau quantization becomes possible in some disordered materials**
- **Including the high-T_c cuprates**



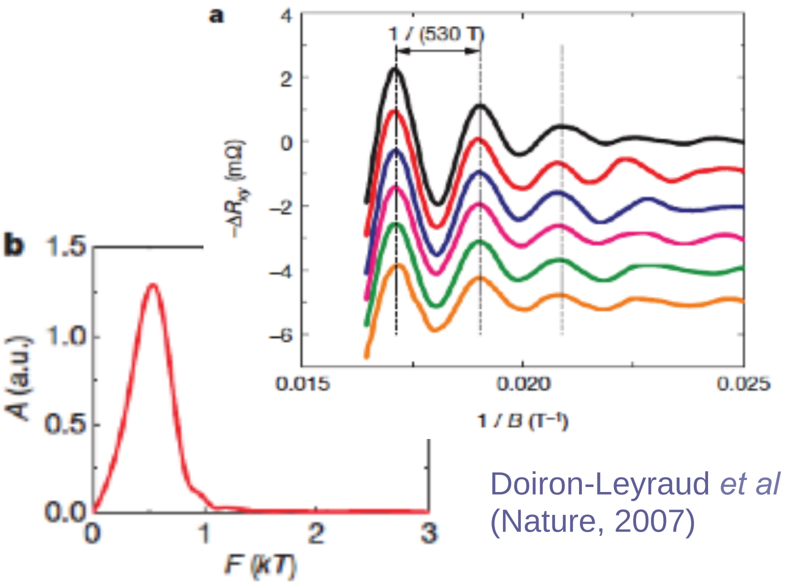


- **Insight into nature of pseudogap**
  - Pursue long-standing questions
    - Is it a broken symmetry?
    - Or a crossover?

Sebastian *et al* (Nature, 2008)

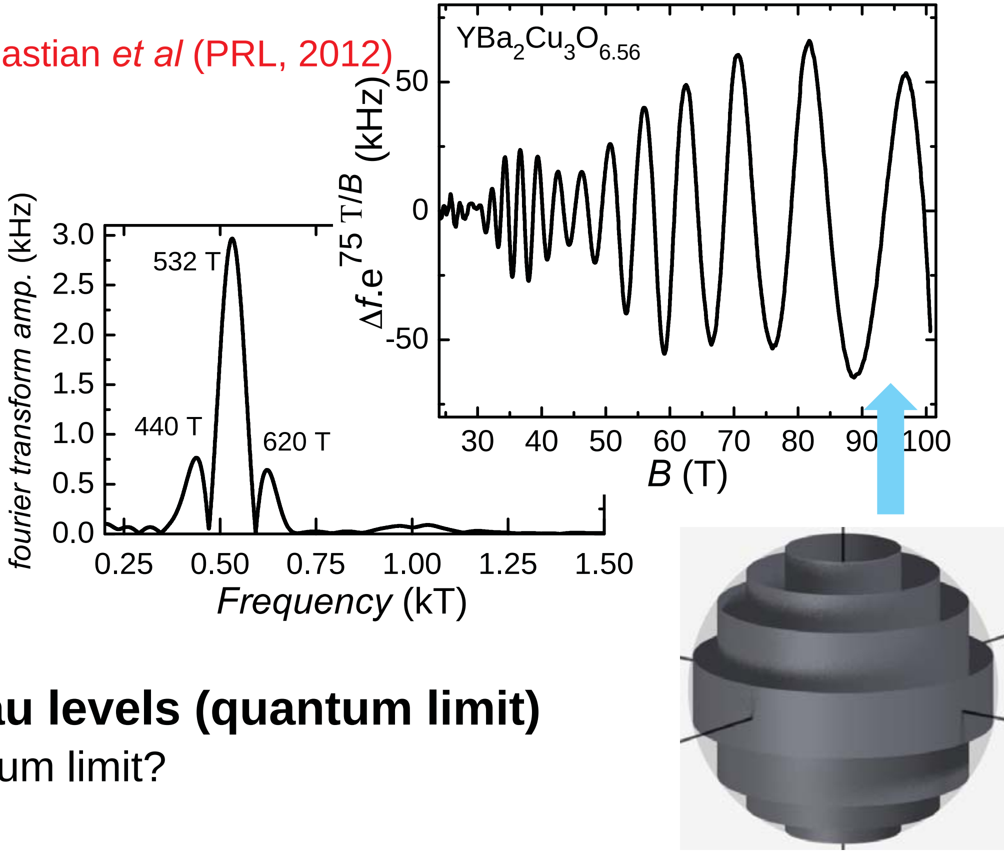
Greatly increase number of observable oscillations since original discovery

- **Unprecedented resolution for mapping Fermi surface**
  - More oscillations = fine structure



Doiron-Leyraud *et al* (Nature, 2007)

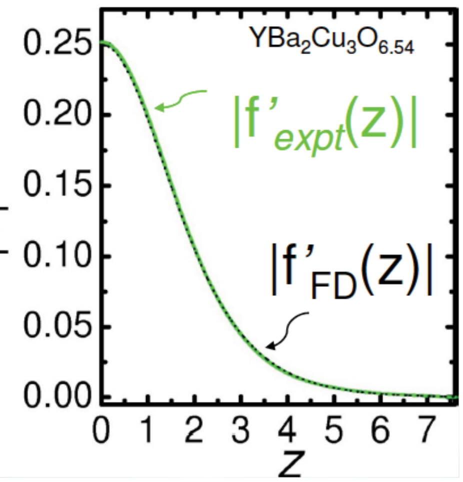
Sebastian *et al* (PRL, 2012)

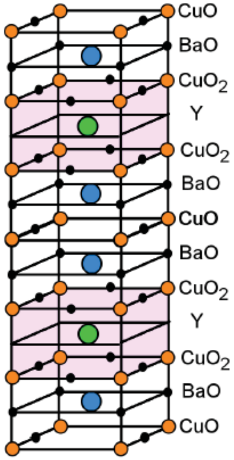


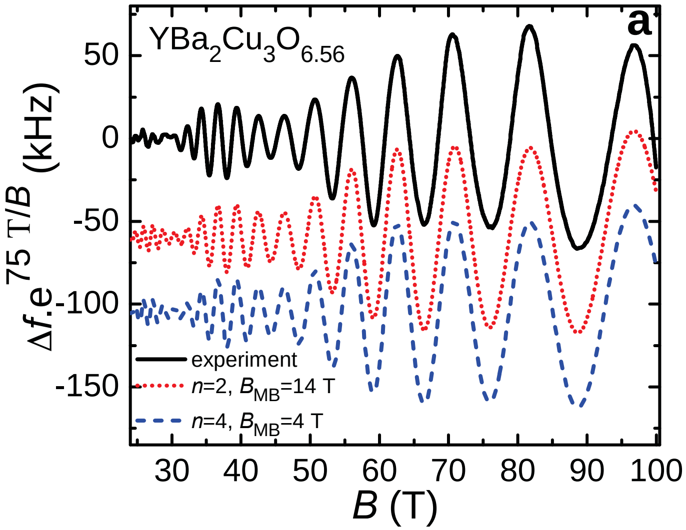
- **Access to few remaining Landau levels (quantum limit)**
  - New physics in the extreme quantum limit?

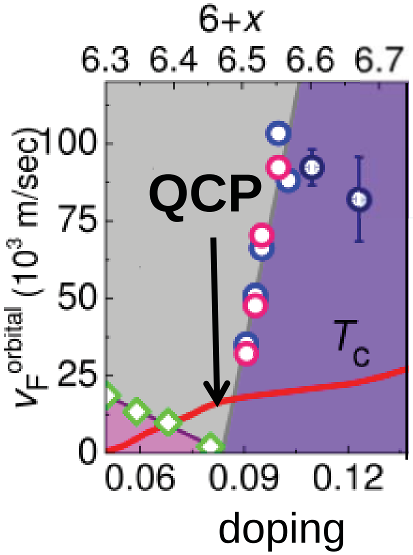
Several things established in pseudogap regime

- **Fermi liquid behavior**
- **Likely quantum critical point at low dopings**
- **Nodal bilayer splitting**
  - Ties in with observations in photoemission







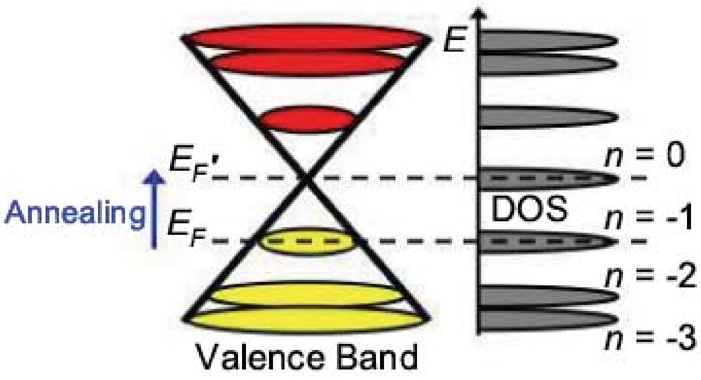


Sebastian *et al* (PRB, 2010; PNAS, 2010; PRL, 2012)

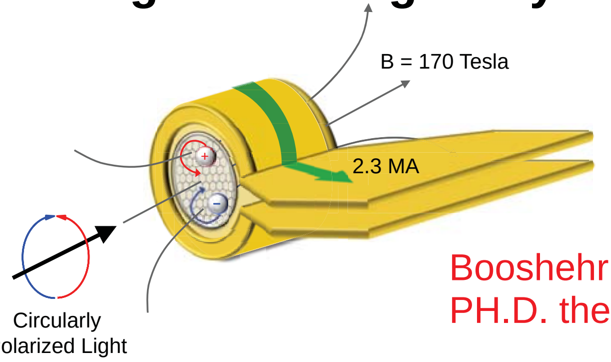
- **Unresolved whether electron or hole pocket?**

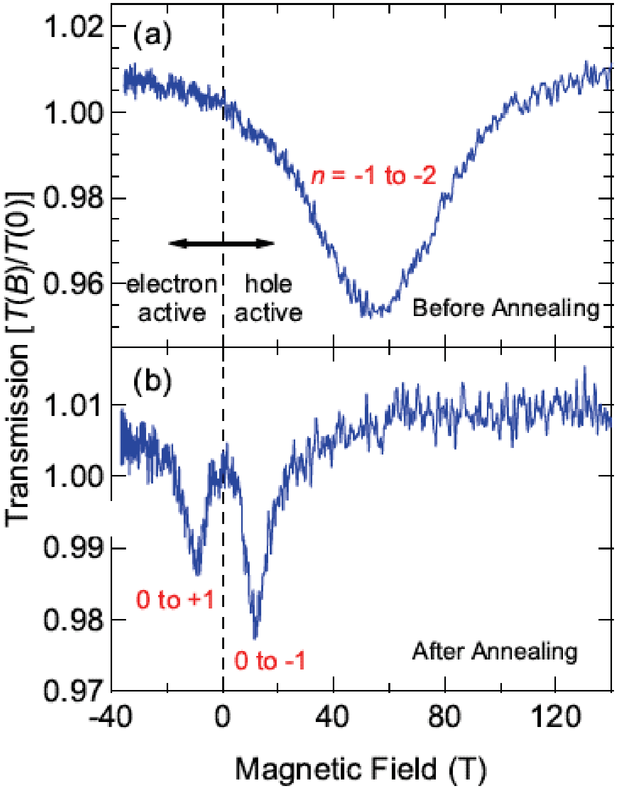
Cyclotron resonance holds the key for determining pocket sign

- **Graphene ideal test case for carrier sign determination**
- **Circularly polarized light can determine sign of Landau transitions**



- **Use single turn magnet system**

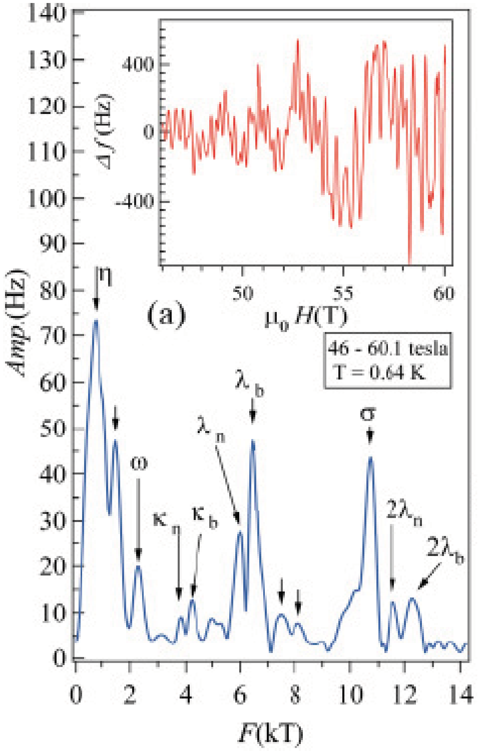


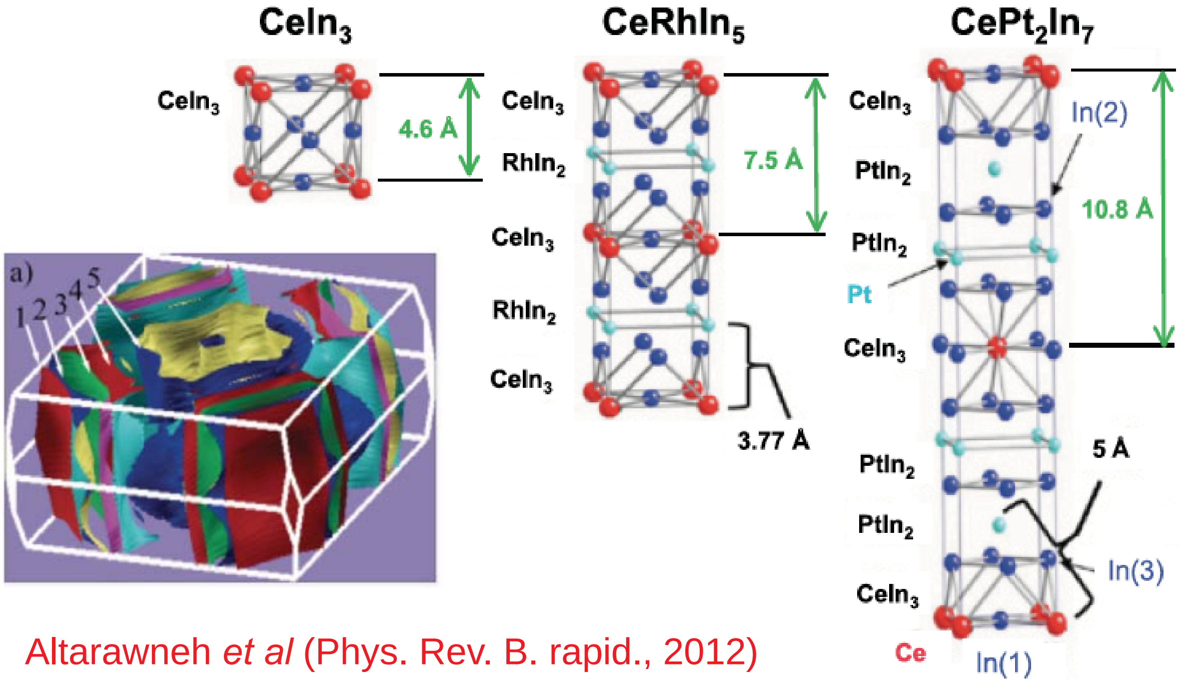


Booshehri *et al* (PRB, 2012);
PH.D. thesis (Rice Univ.)

Field as "negative pressure:" Zeeman energy in heavy fermions

- **Decouple antiferromagnetism and Kondo energy in strong fields**
  - Uncover highly two-dimensional Fermi surface of $CePt_2In_7$



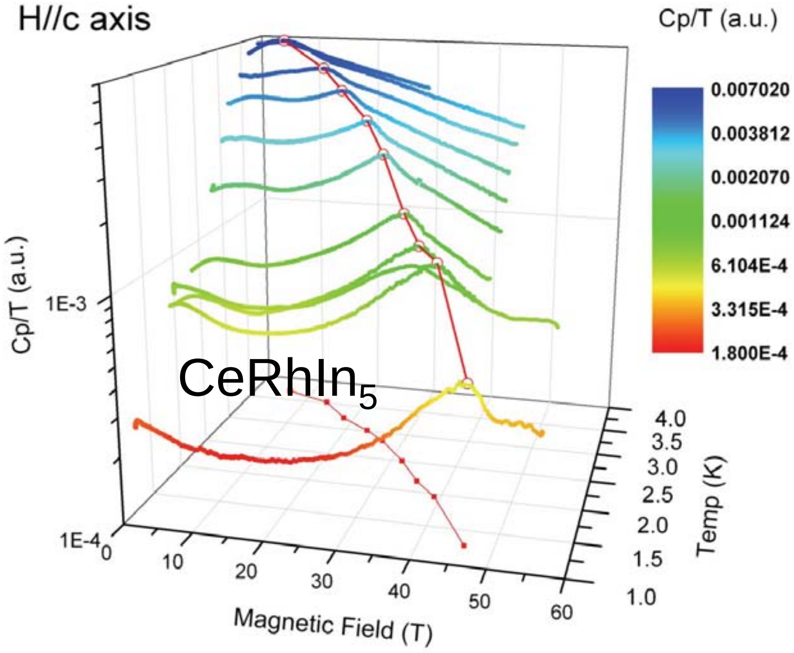


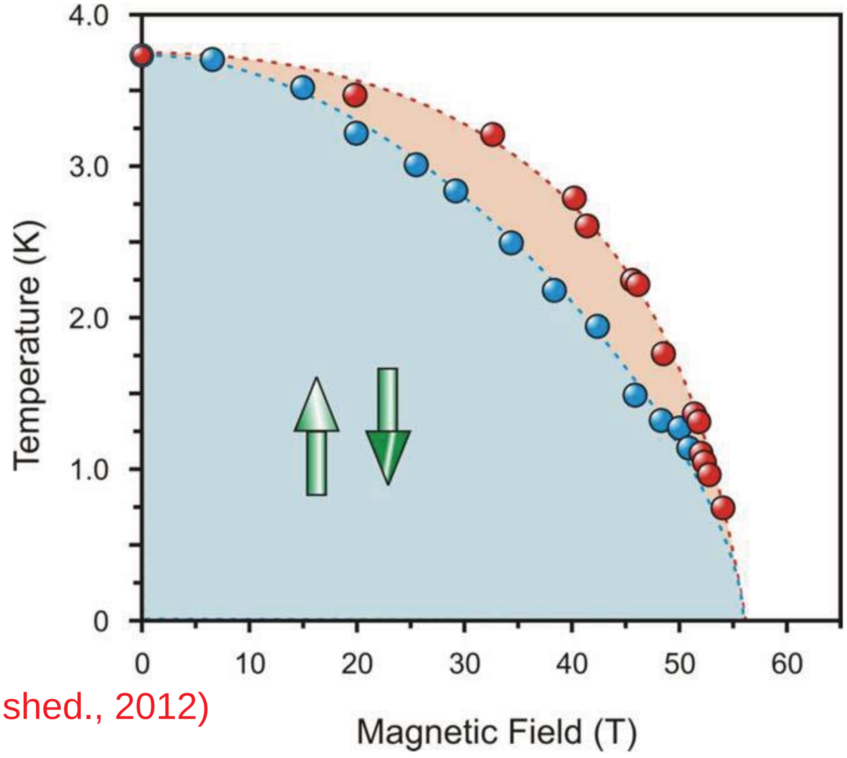
Altarawneh *et al* (Phys. Rev. B. rapid., 2012)

- **Ideal 2D analog of pressured-tuned superconductors**
  - Address relevance of dimensional factors in mechanism of superconductivity

Suppression of antiferromagnetism directly measured

- **Heat capacity in pulsed magnetic fields: e.g. $CeRhIn_5$**
  - Enables thermodynamic experiments in the highest available fields





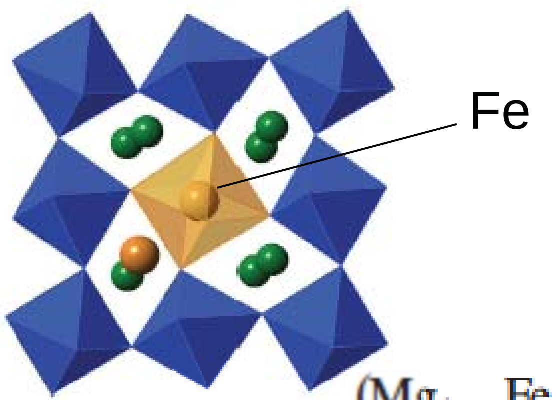
Kohama *et al* (unpublished., 2012)

- **Field enables in-situ tuning of quantum phase transition**

see poster of Jaime *et al.*

Negative pressure: Reverse "volume collapsed" low spin states in Fe, Co perovskites

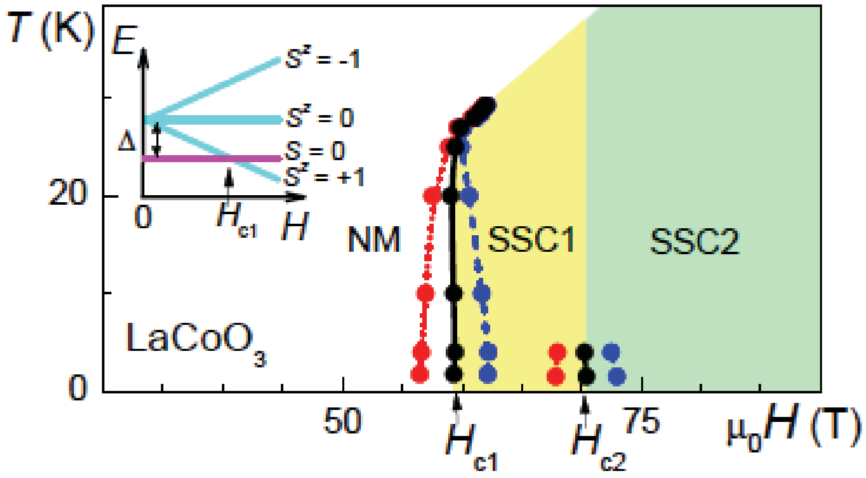
- **Deep within Earth's crust Fe believed to transition from *s* = 5/2 to 1/2**
  - Volume collapse transition between 40 and 70 GPa (~ 10^6 atmospheres)
    - Involves gap between t_{2g} and e_g orbital levels
    - Relevant to propagation of earthquakes



$(Mg_{1-x}Fe_x)(Si_{1-x}Fe_x)O_3$

Hsu *et al* (Phys. Rev. Lett. 2011)

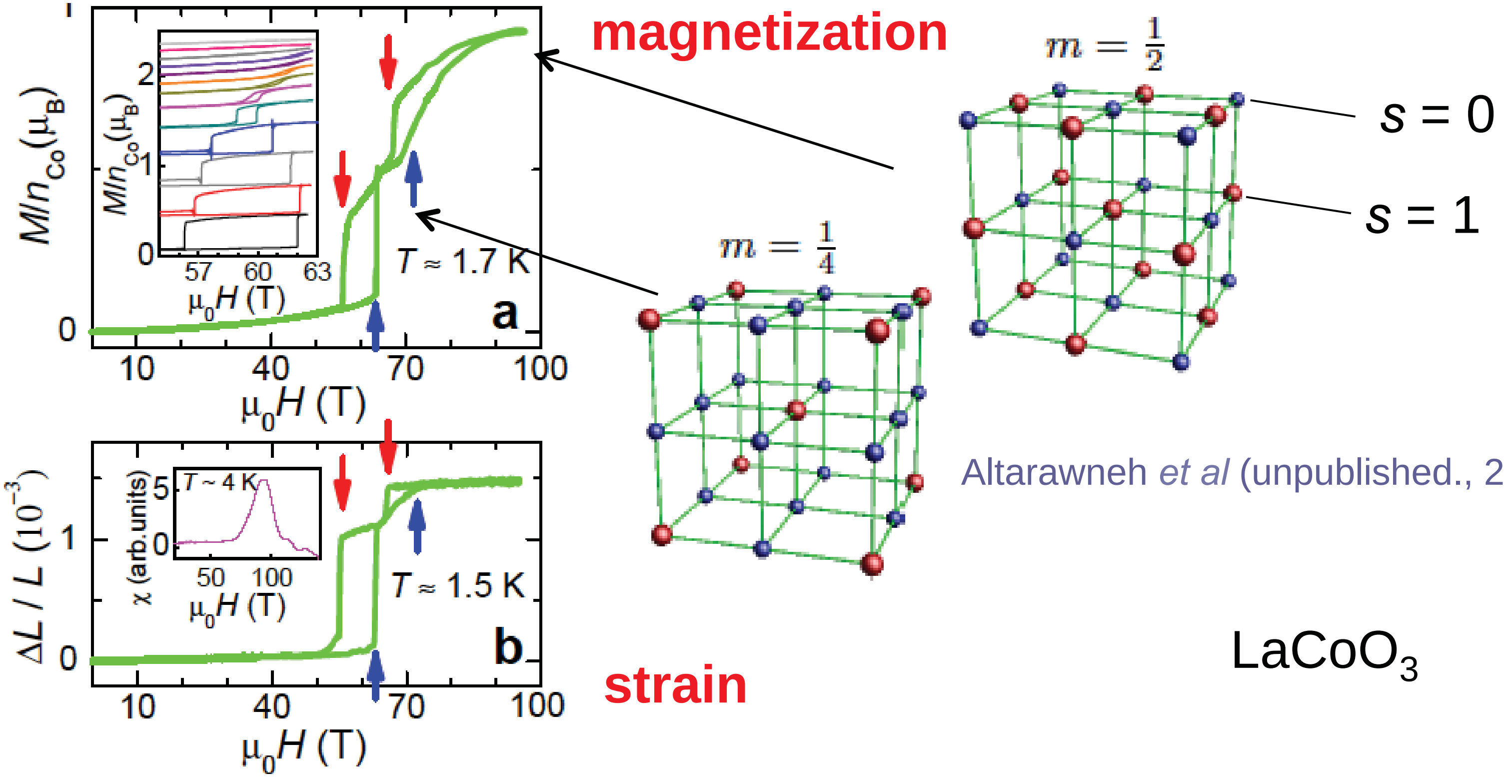
Altarawneh *et al* (unpublished., 2012)



- **In $LaCoO_3$, Co exists in "pre-collapsed" *s* = 0 state at ambient pressure**
  - Detune with a magnetic field

Diffusionless structural phase transitions in extreme magnetic fields

- **Spin state crystallization involving *s* = 0 and larger *s* = 1 sites**



magnetization

$s = 0$

$s = 1$

Altarawneh *et al* (unpublished., 2012)

$LaCoO_3$

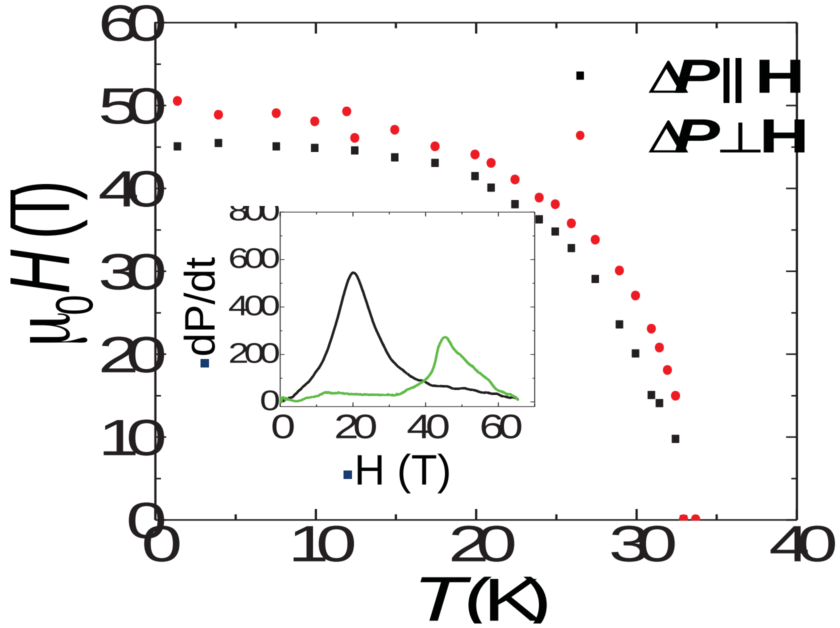
strain

- **Unusually strong orbital / lattice coupling in an insulator**
  - Opportunity for new kind of controlled functionality

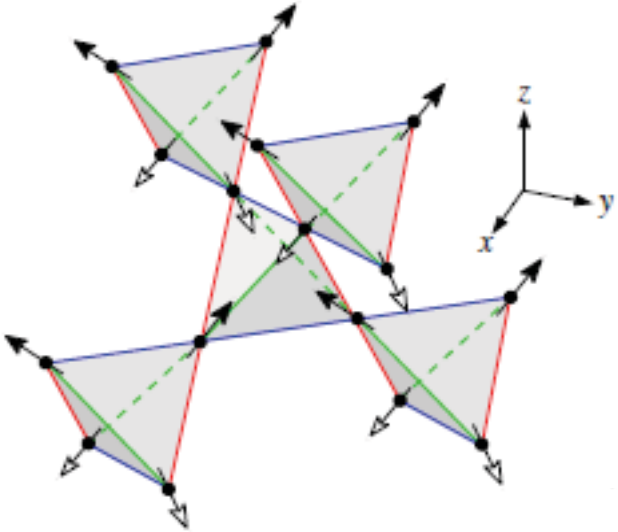
Electric polarization provides a tool for probing broken inversion symmetry

- **Multiferroics have broken inversion symmetry due to complex magnetic structure**
  - Electric polarization

CdV_2O_4



B = 0

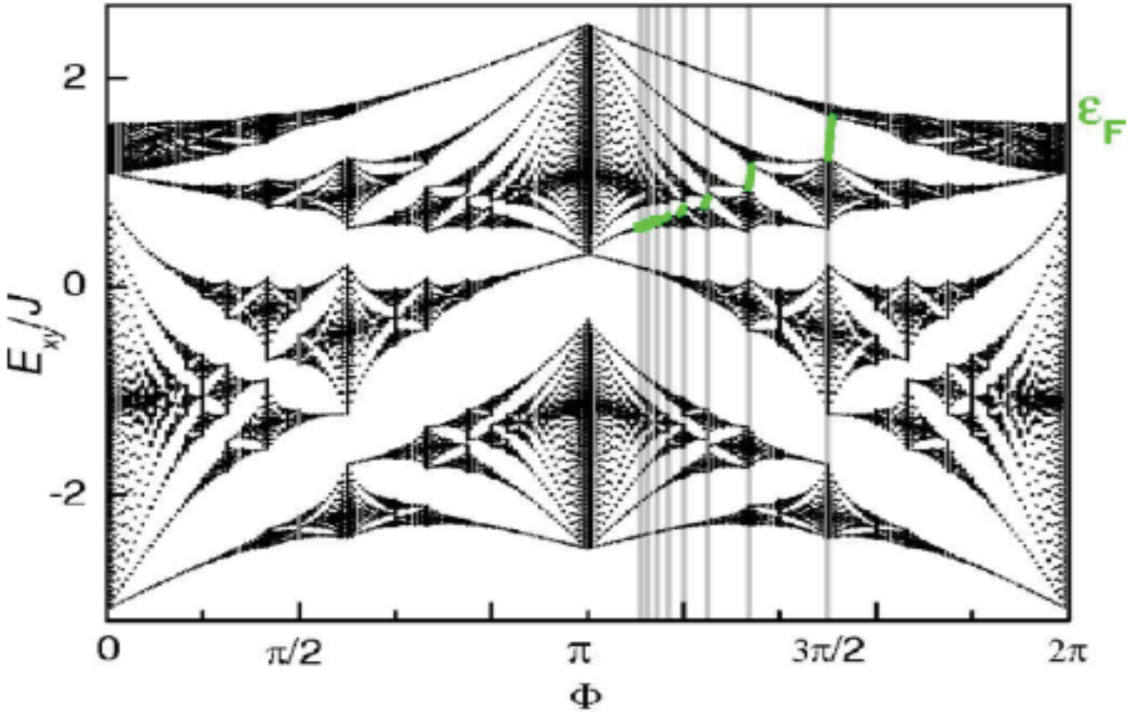


Mun *et al* (unpublished., 2012)

- **Polarization appears to be quenched at high magnetic fields**
  - Restoration of inversion symmetry upon alignment of moments

Emergent phenomena involving commensurability effects

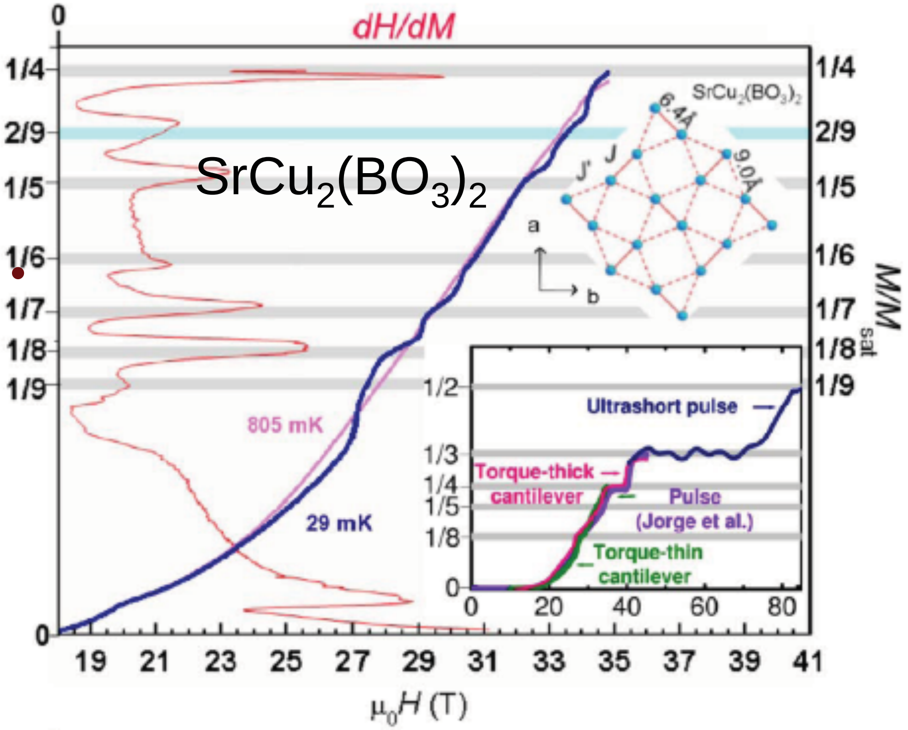
- **Field / lattice commensurability anticipated in 10,000 + tesla**
  - Fractalization of Landau level spectrum



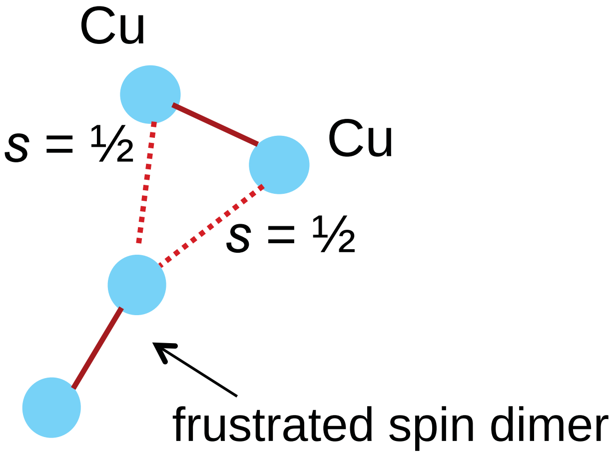
- **Similar commensurabilities accessible in laboratory-accessible fields**

Spin/lattice commensurability in frustrated magnets

- **Shastry-Sutherland lattice quintessential frustrated spin dimer system**
- **Frustration gives way to fractional magnetization states**
  - Higher fractions associated with increased density of flipped Cu spins



$SrCu_2(BO_3)_2$



Cu

$s = ½$

Cu

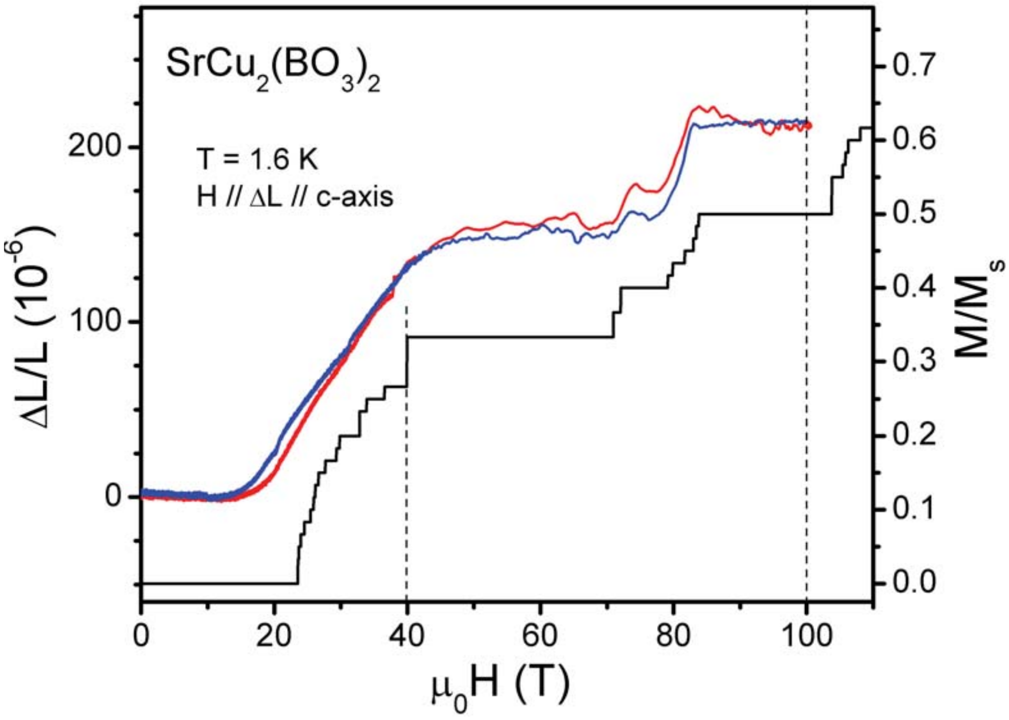
$s = ½$

frustrated spin dimer

Sebastian *et al* PNAS (2009)

New breakthrough in fields of 100 tesla: ½ plateaux

- **Both magnetization and strain consistent with each other and theory**
- **Simplicity of high field states (i.e. smaller superstructure) facilitates robust comparison with theoretical models**
  - Extensive collaboration with T-4
  - Key milestone in understanding geometrical frustration

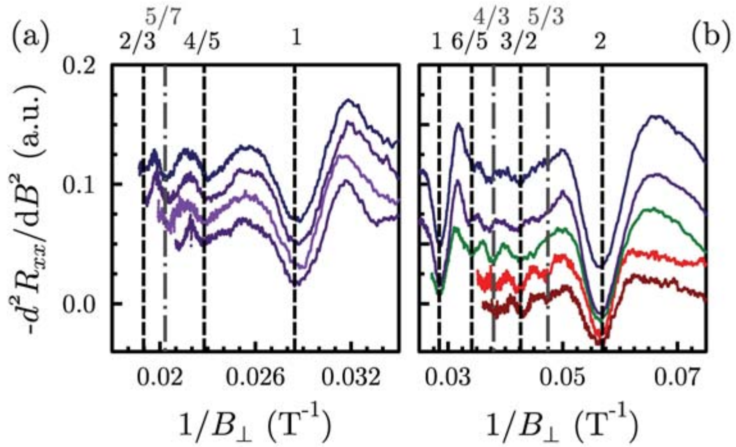


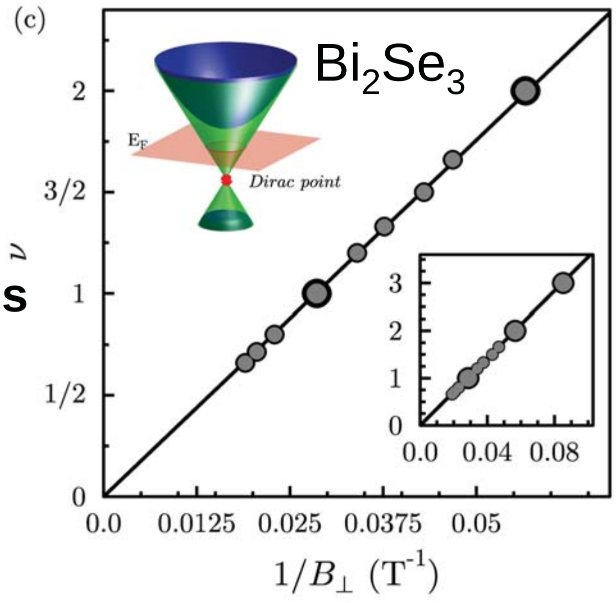
Jaime *et al* (unpublished., 2012)

see poster of Jaime *et al.*

Field/particle density commensurability in topological insulators

- **Quantized surface Dirac-states protected by spin-orbit coupling**
- **Subject to quantum limit at ~ 60 + tesla**
- **Additional structure suggests fractional states**
  - Reminiscent of fractional quantum Hall states?





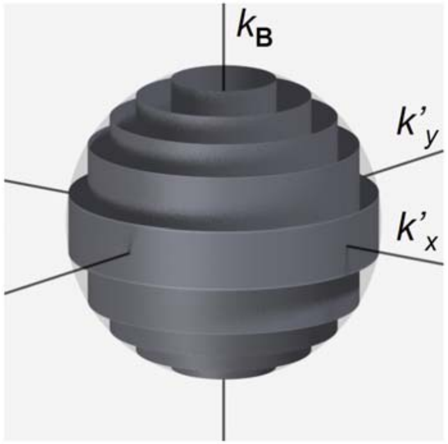
Analytis *et al* Nature Phys. (2012)

see poster of McDonald *et al.*

Summary

- **Extreme magnetic fields as a tuning parameter**
  - Collapse of magnetic length crucial tool for understanding high *T*c superconductors
  - Field can also behave as "negative pressure" in condensed matter
  - Field-tuned emergent phenomena involving commensurability effects

- **Link to materials research and development strategy at Los Alamos**
  - Test theoretical predictions in most extreme conditions
  - Identify new directions for materials development
  - Uncover new forms of controlled functionality involving electromagnetic fields



Designing High Strength, High Conductivity Wire for Pulsed Electromagnets

R.F. Need, C.A. Swenson (MPA-CMMS); D.J. Alexander, J.C. Cooley (MST-6); E. Lavernia, University of California, Davis

It is not power generation or delivery that currently prevents nondestructive electromagnets from reaching extreme magnetic fields. In fact, the limiting factor is the availability of conducting materials strong enough to withstand the immense forces generated during a magnet pulse.

Accordingly, the National High Magnetic Field Laboratory (NHMFL) has devoted considerable time and resources to improving existing conducting materials and developing new ones. There are currently three projects at the NHMFL focused on this goal: 1) To improve the strength of the alumina dispersion-strengthened (ADS) copper alloys by grain refinement; 2) To evaluate the potential of Cu-Cr in situ composites as a replacement for ADS copper alloys as the outsert conducting material; and 3) To demonstrate the fabrication of Cu-Nb preform billets by the inexpensive, spray forming (or Osprey) method.

Dirac Materials in High Magnetic Fields

R.D. McDonald (CMMS-LANL); J.G. Analytis S.C. Riggs, J.-H. Chu, I.R. Fisher (Stanford University);
G. S. Boebinger (NHMFL-FSU)

Topological insulators possess a metallic surface state of massless particles, known as Dirac fermions whose spin is coupled to their momentum. The realization of this in Bi_2Se_3 has sparked considerable interest owing both to the potential for spintronic devices and in the investigation of the fundamental nature of topologically non-trivial quantum matter. However, the conductivity of these compounds tends to be dominated by the bulk of the material owing to chemical imperfection, making the transport properties of the surface nearly impossible to measure. We have systematically reduced the number of bulk carriers in the material Bi_2Se_3 to the point where a magnetic field can collapse them to their lowest Landau level. Beyond this field, known as the three-dimensional (3D) 'quantum limit', the signature of the 2D surface state can be seen. At still higher fields, we reach the 2D quantum limit of the surface Dirac fermions. In this limit we observe an altered phase of the oscillations, which is related to the peculiar nature of the Landau quantization of topological insulators at high field. Furthermore, we observe quantum oscillations corresponding to fractions of the Landau integers, suggesting that correlation effects can be observed in this new state of matter.

Dimensionality Control in Organic Quantum Magnets

J. Singleton (MPA-CMMS); J. Manson (Eastern Washington University); P. Goddard (Oxford University);
P. Sengupta (Nanyang Technological University); J. Schlueter (Argonne National Laboratory);
R. McDonald (MPA-CMMS); I. Franke (Oxford University)

Gaining control of the building blocks of magnetic materials and thereby achieving particular characteristics will make possible the design and growth of bespoke magnetic (nano)devices. The advent of molecular materials, and especially coordination polymers, represents a significant step towards this goal, allowing magnetic centres to be arranged on a variety of crystalline frameworks. In this way, diverse magnetic materials with different effective dimensionalities and/or anisotropies have been synthesized. Magnetization (M) measurements in very high magnetic fields H have a very important role to play in such work. The characteristic shape of the M(H) curve can be modeled to extract the effective dimensionality of the magnet in question;

moreover, the magnetic fields at which features in M(H) occur give accurate values of the various microscopic exchange parameters. The poster will illustrate various “molecular architecture” strategies, including the use of chemical pressure via space-filling counter-ions, isotopic substitution, and judicious alteration of synthesis conditions. These techniques allow the effective dimensionality and size of the exchange interactions to be adjusted almost at will, as evidenced in data from high-magnetic-field experiments.

Photo-induced Magnetization in Copper-doped Semiconductor Nanocrystals

S.A. Crooker (NHMFL; MPA-CMMS), J. Pietryga, S. Brovelli, A. Pandey, V.I. Klimov (C-PCS)

Nanoscale materials have been extensively investigated for applications in memory and data storage applications. Recent advances include the demonstration of memories based on metal nanoparticles, nanoscale phase change materials, molecular switches as well as diluted magnetic semiconductors (DMS). Traditional magnetic storage devices make use of magnetic fields to address individual storage elements. Materials with magnetic properties addressable via alternative (e.g., electrical or optical) means may lead to improved data storage densities and are consequently very desirable.

Here we demonstrate that copper-doped ZnSe/CdSe core/shell nanocrystals exhibit not only the classic signatures of DMS materials (namely, a strong spin-exchange interaction between paramagnetic Cu dopants and the conduction / valence bands of the host lattice), but also exhibit a pronounced and long-lived photo-induced magnetization. Magnetic circular dichroism studies reveal that the magnetic response of these NCs can be increased up to two-fold by illumination with above-gap (UV) light, and can be reset using light with lower photon energy. This enables these materials to retain a magnetic memory for hour-long timescales (in the dark) up to relatively high temperatures of ~80 K.

Nanometer Resolution Magnetostricion in Pulsed Magnetic Fields to 100T

M. Jaime (MPA-CMMS); R. Daou (CRISMAT, Univ. de Caen); S.A. Crooker, F. Weickert (MPA-CMMS)

We report on a new high-resolution optical technique for measuring magnetostriction suitable for use at cryogenic temperatures in pulsed high magnetic fields to 100T. Optical fiber strain gauges based on fiber Bragg gratings are used to measure the strain in small samples. We describe the implementation of a fast measurement system capable of resolving strains in the order of 10^{-7} with a full bandwidth of 47kHz. We demonstrate its use on single crystal samples of the highly frustrated Shastry-Sutherland compound $SrCu_2(BO_3)_2$, the insulating perovskite $LaCoO_3$, the frustrated spin-ladder system $BiCu_2PO_6$ and the multiferroic $Ca_3Co_xMn_{1-x}O_6$, where a rich variety of field-induced phase transitions are evident in the response of the crystallographic lattice.

High-Field Characterization of High Temperature Superconductors

F. F. Balakirev (MPA-CMMS)

High temperature superconductivity in cuprates emerges in the transition region between Mott insulator and a Fermi-liquid-like metal states. Many speculate that HTS results from the proximity of a quantum phase transition (QPT) in the underlying normal state, both from the theoretical and experimental perspective. Extreme high field reveals the Hall number anomaly peak at the exact location of doping that maximizes T_c, suggesting common normal state QPT that underlies the high-temperature superconducting phase. The peak is ascribed to a Fermi surface reconstruction at a QPT that is co-incident with the collapse of the pseudogap state. Newly discovered Fe-As based layered pnictides are comparable to high-T_c cuprates and can reach T_c as high as 56K. Is reduced dimensionality a key ingredient common for all high-T_c? Can we identify isotropic superconductors beneficial for real-world applications? Central to any superconductor capabilities is the ability to sustain supercurrent in the presence of the magnetic field. Shaping samples into nano-bridges via Focused Ion Beam lithography enables critical current measurements in pulsed magnets.

New Multiferroic States in Frustrated Ising Spin Chain Compound

J. W. Kim, E.D. Mun, V.S. Zapf, M. Jaime, S. Crooker, J.D. Thompson, N. Harrison (MPA-CMMS); C.D. Batista (T-4); H.T. Yi, Y.S. Oh, S-W. Cheong (Rutgers)

Multiferroic materials couple magnetic and electric long-range order, and thus hold promise for future applications for novel smart circuitry, sensors, and low-power electronics. Ca_3CoMnO_6 is one of the first multiferroics to show a large ferromagnetic-like magnetization coupled to large net electric polarization. Thus it is important to understand the magnetic structure and magneto-electric coupling mechanism in this material. We have measured magnetization, electric polarization, and magnetostriction in fields up to 100 T. According to previous studies, frustration stabilizes an ↑↑↓↓ spin configuration at zero field, which changes to ↑↑↑↓ and eventually to ↑↑↑↑ at 30 T with applied magnetic field. At each phase slip between regions of up and down spins, an electric polarization results due to lattice distortions. Consequently the magnetization and electric polarization are coupled and sensitive to external magnetic and electric fields. However, our pulsed-field experiments show that there exist at least two more phase transitions and a true magnetic saturation occurs at 85 T. These results clearly indicate that the Co^{2+} spin configuration is high spin (S=3/2) instead of low spin (S=1/2). Furthermore, we find additional steps in all measurements below 10 T which was not observed in DC measurements. We attribute this to metastable states captured with transient field sweeps that exists due to magnetic spin density waves or solitons.

Binary Alloy Solidification at 35 Tesla

J.C. Cooley, S.D. Imhoff (LANL); T.J. Ott (Florida State University); S.J. Tracy (California Institute of Technology); T.J. Tucker (LANL); K.N. Collar (Florida State University), S. Lillard, J.C. Foley, T. Wheeler, J. Balog, A. Duffield (LANL): B. Pullum (Florida State University)

Chandrasekar showed in 1957 that the viscosity of a metallic liquid increases quadratically perpendicular to an applied magnetic field. At tens of tesla, this increase in viscosity can be by orders of magnitude, resulting in very anisotropic diffusion constants. Also, the field can orient paramagnetic crystallites in the liquid. Our work is focused on identifying alloys in which an applied field has an effect on the solidification microstructure, determining its magnitude, and understanding why it occurs. Because the field is an external parameter independent of temperature, composition, and pressure, its ability to effect solidification microstructures has profound implications for the development of engineered microstructures. We report on the solidification microstructures of binary alloys at and near eutectic compositions in 0 and 35 Tesla fields. In Al-Ni and Mg-Sb alloys the microstructures are layered perpendicular to the applied field, while those in the Al-Cu and Ag-Ge systems are parallel.

Overview: Condensed Matter Physics

M.F. Hundley (MPA-CMMS)

Condensed matter physics research at LANL focuses on emergent phenomena with a particular emphasis on correlated electron physics, f-electron systems, actinides and plutonium. This focus is driven by LANL mission needs and the emphasis on emergent phenomena directly couples to the institutional Materials Strategy. In order to realize LANL missions needs our materials R&D vision is transitioning from observing and exploiting the properties of materials to a science-based capability to create materials with properties optimized for specific functionality. The field of condensed matter physics focuses on the underlying mechanisms that are responsible for macroscopic materials behavior. As such, LANL condensed matter physicists contributed to the Materials Strategy by developing the *design principles* that are required in order to realize controlled materials functionality. These activities at LANL involve a close interplay between experiment, theory, and materials synthesis.

In this presentation I will provide a brief overview of current condensed matter physics activities at LANL and outline key scientific questions that define our future research thrusts. The scope of this theme area will be explored by use of demographic and budgetary data, while impact will be quantified by comparing LANL publication data to that of other national labs and research universities. I will also present technical highlights and accomplishments that demonstrate notable condensed matter physics contributions to LANL materials initiatives.

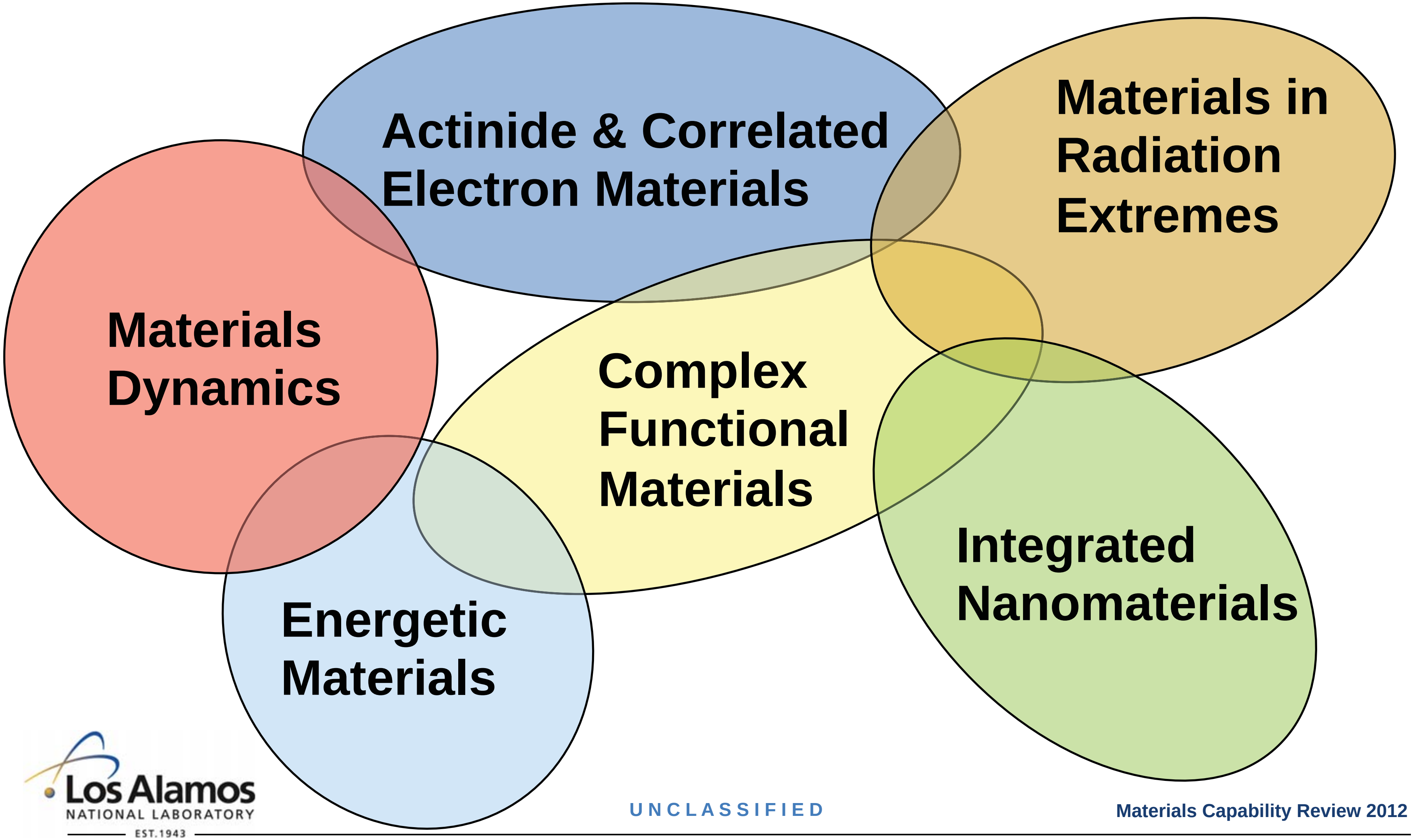
Overview:
Condensed Matter Physics

Michael Hundley

MPA-CMMS Group Leader

(Condensed Matter & Magnet Science)

LANL's Areas of Materials Leadership



Actinide & Correlated Electron Materials

Materials in Radiation Extremes

Materials Dynamics

Complex Functional Materials

Integrated Nanomaterials

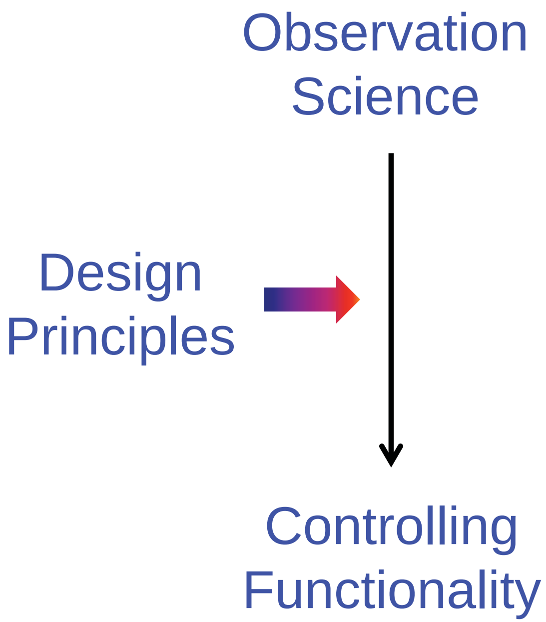
Energetic Materials

LANL Condensed Matter Physics

- **f-electron physics with an emphasis on actinides/plutonium**
- **Correlated electron systems**
  - Unconventional superconductivity
  - Quantum critical phenomena
  - Materials discovery
  - Magnetic frustration as route to functionality (multiferroics)
  - Vortex matter & vortex dynamics
  - Many-body theory & electronic structure calculations
- **Novel spectroscopies & characterization**
  - Angle-resolved photoemission spectroscopy (ARPES) for transuranics
  - Ultrafast spectroscopy
- **Unique facilities**
  - LANSCE, NHMFL, CINT

LANL Materials Strategy

- **LANL materials R&D vision is transitioning from observation-based to control science**
  - Goal is controlled functionality through discovery/ application of fundamental materials properties
  - Crucial for meeting LANL mission needs
- **Underpinning need: Realizing *design principles* towards controlled functionality**
- **Fueled by LDRD investments**
- **Aligned with BES materials grand challenge, Materials Genome & Mesoscale Initiatives, MaRIE**



Observation Science

Design Principles

Controlling Functionality

Condensed Matter Physics Aligned with Materials Strategy Thrust Areas

- **Emergent Phenomena**
  - Correlated electron materials
  - Multifunctional and adaptive materials
  - Materials for energy utilization
- **Defects and Interfaces**
  - Integrated nanomaterials
  - Heterostructures (2D and 3D)
- **Extreme Environments**
  - Inducing new states of matter
  - Extracting information on fundamental properties (NHMFL)
- **Crosscuts: Making, Measuring, and Modeling Materials**
  - ➢ Integration is crucial for success

What' s To Come: Key Science Questions and Future Thrusts

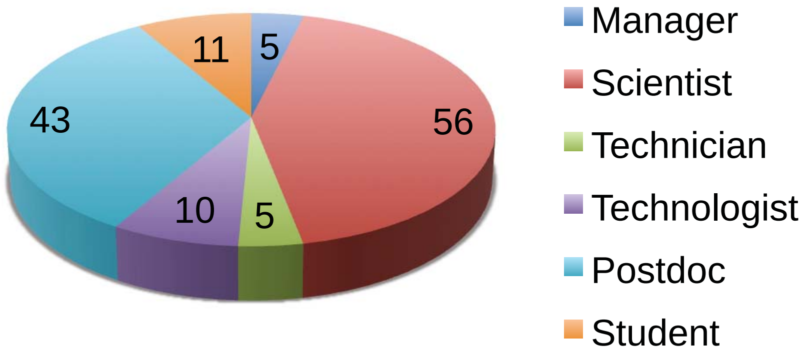
- **Actinide & correlated electron Materials: key questions**
  - How do correlations determine functionality in actinides?
  - How do we develop predictive tools to allow materials design for functionality (electronic structure → observables)?
  - What is beyond Fermi liquid theory as framework for describing interacting electrons?
  - What is the interplay between structure and correlations, and what are the consequences therein?
  - What is the effect of defects and interfaces at the nano- to mesoscale?
- **Actinide & correlated electron end states with thrusts**
  - Predictive tools to allow materials design for functionality
  - Improvements to electronic structure & EOS calculations
  - Correlated electron materials in extreme environments
  - Functionality from coupled degrees of freedom
  - Functionality from quantum-critical states
  - Superconductivity-by-design

Capability Roadmap

- **Build on current capabilities**
  - Enhanced High magnetic field measurement capability (fast vortex dynamics/imaging)
  - Combined capability for high-P, high-H, low-T (coupled to user facilities)
  - Ultra-fast/ultra-small/high-throughput modeling capability for correlated materials
  - Increased synthesis capability in complex oxides
  - Robust actinide single crystal and compounds infrastructure

- **Facility investments**
  - Establish Pu-242 capability at TFF
  - Relocate synthesis & characterization capabilities currently housed at CMR
  - Crystal growth center (consolidating far-flung LANL capabilities)
  - Co-locate experimental facilities crucial for emergent electronic materials research (theory, synthesis, characterization)

Condensed Matter Physics Personnel



Recent postdoc conversions

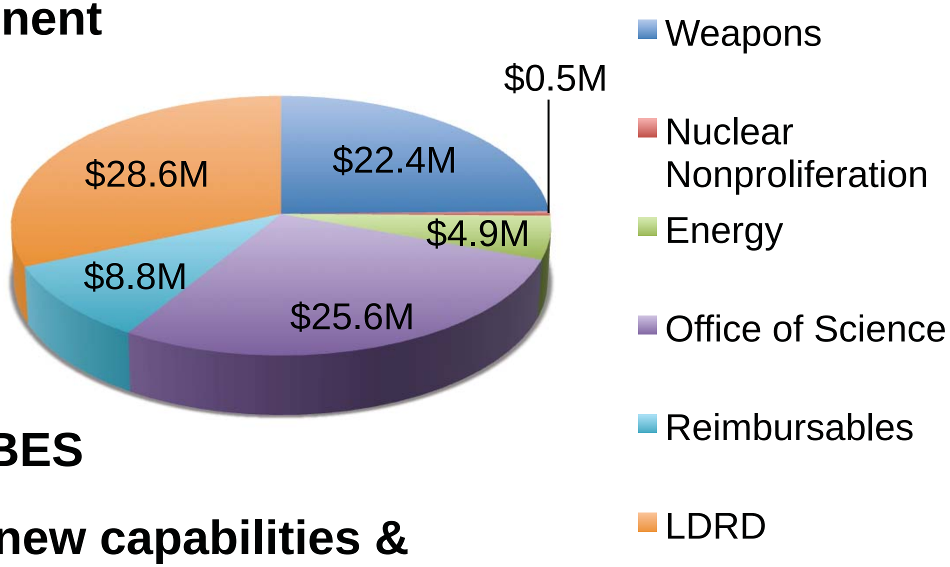
Cristiano Nisoli, T-4

Paul Tobash, MST-16

- **MPA, MST, T, C, LANSCE divisions**
- **Sizeable postdoc population**
- **Condensed matter postdoc population serves as pipeline for**
  - Condensed matter staff hires
  - LANL materials community staff hires

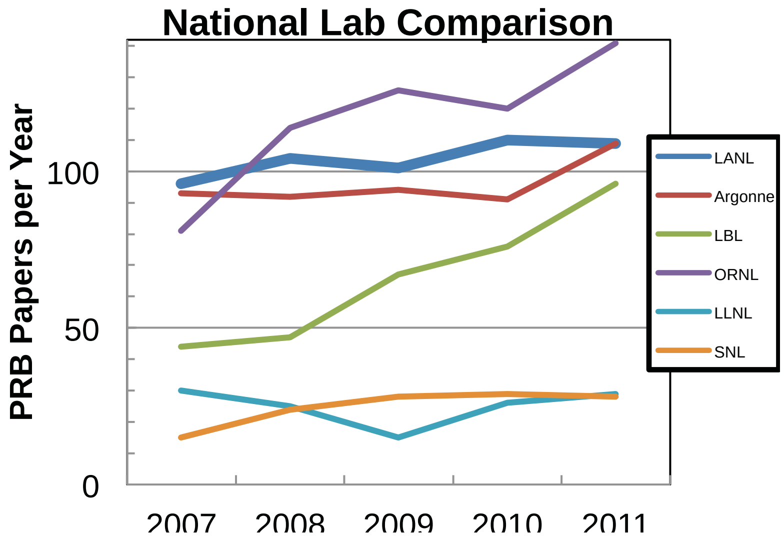
Condensed Matter Physics Portfolio

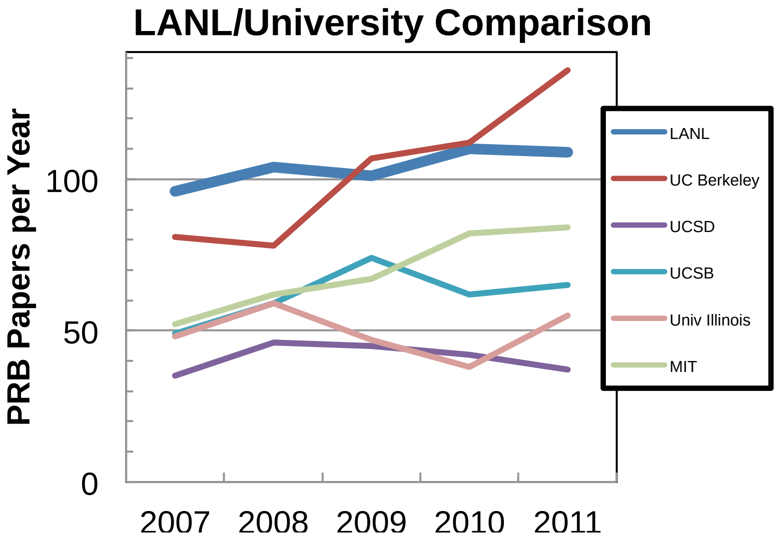
- Total funding for materials programs with a condensed matter physics component

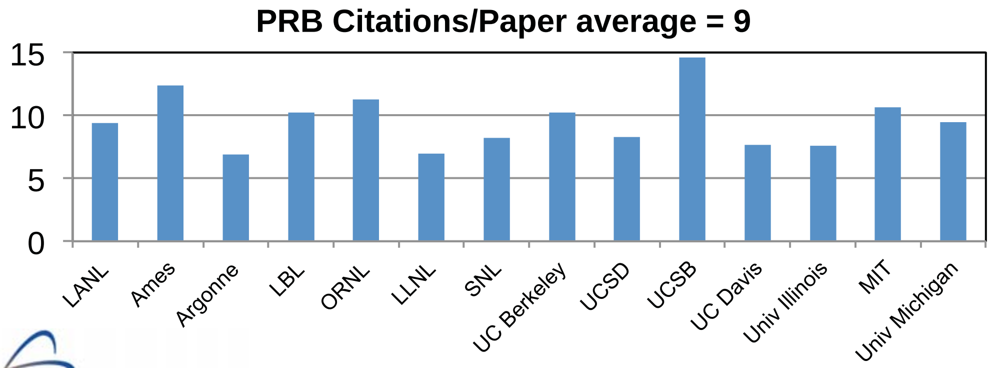


- **Office of Science: predominately BES**
- **LDRD serves as seed funding for new capabilities & competencies**
- **Reimbursable: WFO (mostly NHMFL) & CRADAs**
- **Weapons program: predominately Science Campaigns**

Impact as Measured by Publications: Physical Review B (2007-2011)


National Lab Comparison


LANL/University Comparison

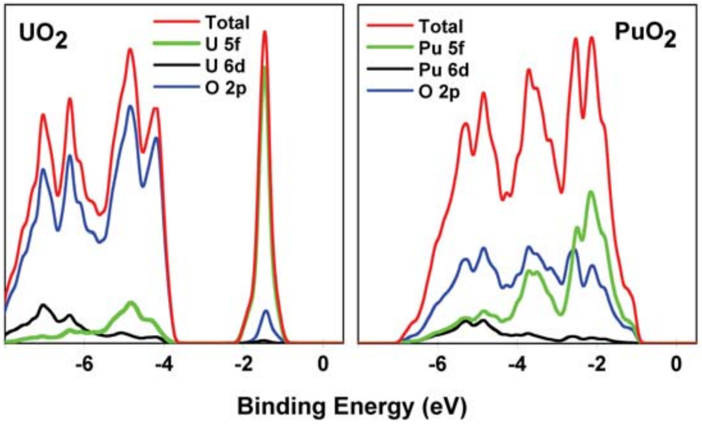

PRB Citations/Paper average = 9

- 42% of LANL Physical Review Letter articles were in condensed matter physics (175 of 415)

Electronic Structure in UO_2 & PuO_2: Hybrid Functionals and Photoemission

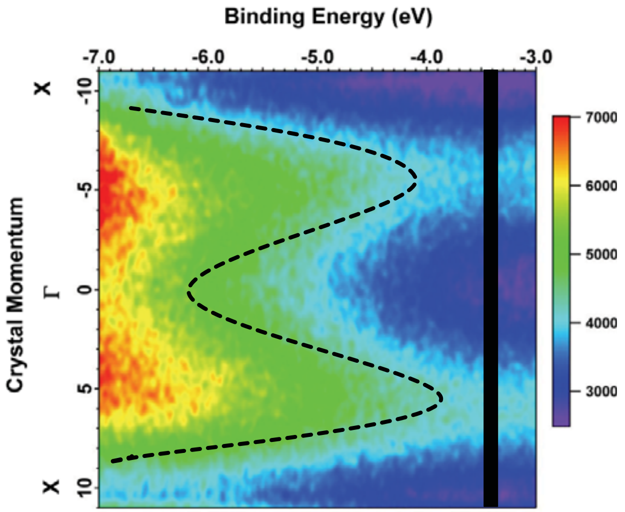
- HSE (hybrid functional) predicts strong hybridization in PuO_2 vs. UO_2, merging of O 2p and Pu 5f.
- 1st ARPES shows **k**-dep., and hybridization, 2+ eV
- Only ARPES data on PuO_2, only PuO_2 single crystals (PAD), predictive model capability.

Prodan *et al.*, Covalency in the actinide dioxides: Systematic study of the electronic properties using screened hybrid DFT. PRB **76**, 033101 (2007) (53 citations)



- Black bar – 5f dispersion in UO_2
- Dashed line – 5f dispersion in PuO_2
- Order of Magnitude difference –

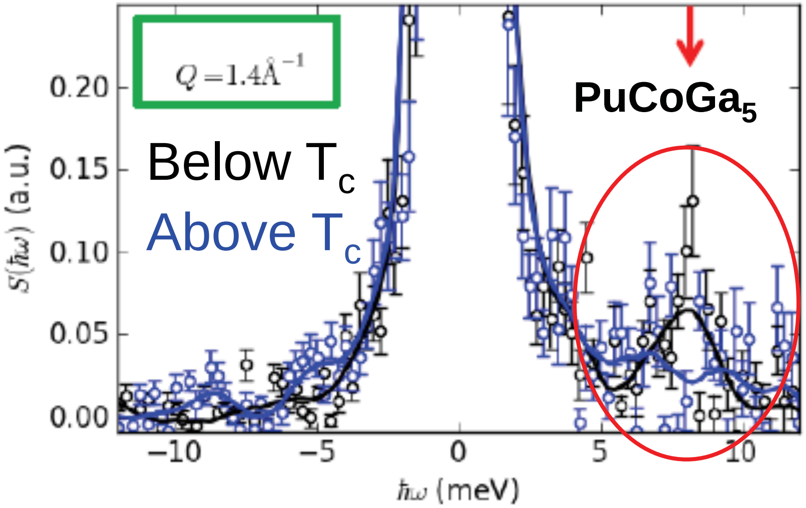
  ARPES dispersion UO_2 to PuO_2.



LDRD Pu-242 Project for Understanding 5f Electrons of Pu

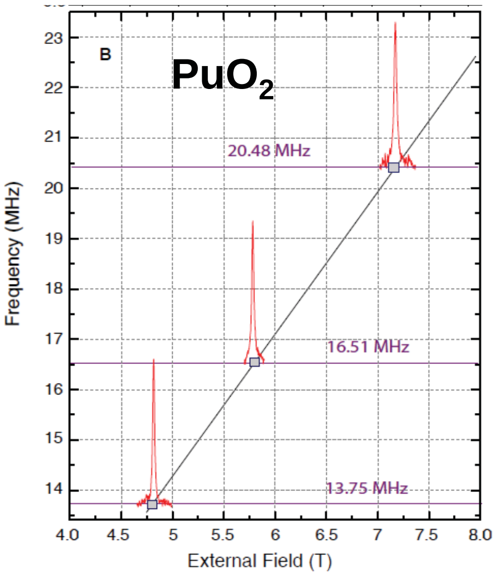
- **Neutron Scattering measurements performed on Pharos on 25 g δ-^{242}Pu sample and 15 g of ^{242}PuCoGa$_5$ single crystals**
  - Search for evidence of spin fluctuations in δ-Pu
  - Search for superconducting "spin resonance" in PuCoGa$_5$

J.L. Sarrao *et al*., Plutonium-based superconductivity with a transition temperature above 18K. Nature **420**, 297 (2002) (298 citations)



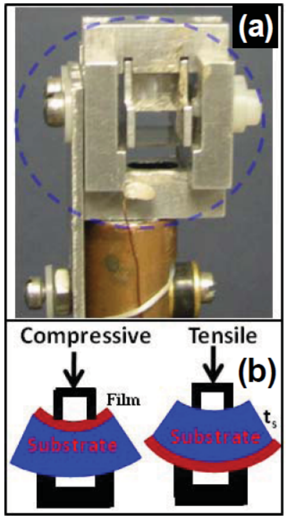
- **First observation of Pu-239 NMR signal in PuO$_2$ after 50-year search**
  - New frontier for actinide chemistry, physics, and materials science research

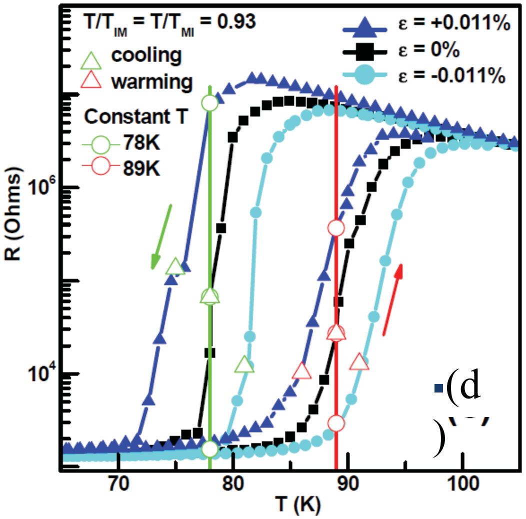
Yasuoka, *et al.,* Observation of ^{239}Pu Nuclear Magnetic Resonance. Science 2012 (in press)

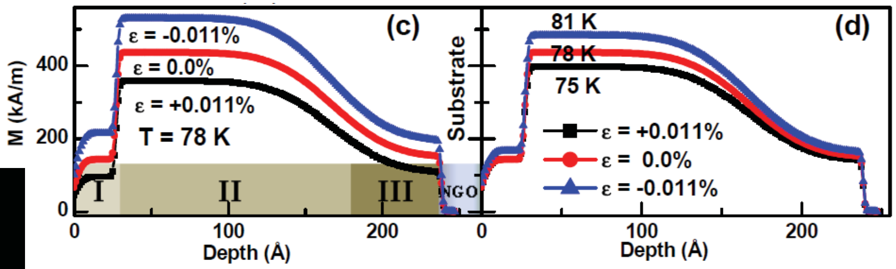


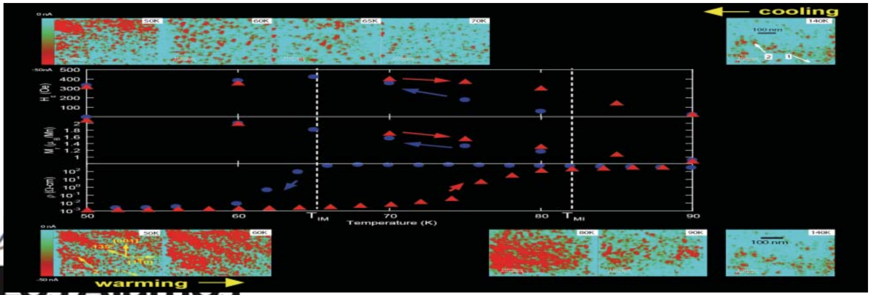
Influence of Bending Stress on a Phase-Separated Film

- **Developed capability to measure polarized neutron reflectivity and magnetotransport of a film as functions of stress, field and temperature**
- **Found that $(La_{0.5}Pr_{0.5})_{0.77}Ca_{0.23}MnO_3$ films exhibit coexistence of different magnetic phases as function of depth**
- **Found that compressive (tensile) bending stresses increase (suppress) magnetization.**





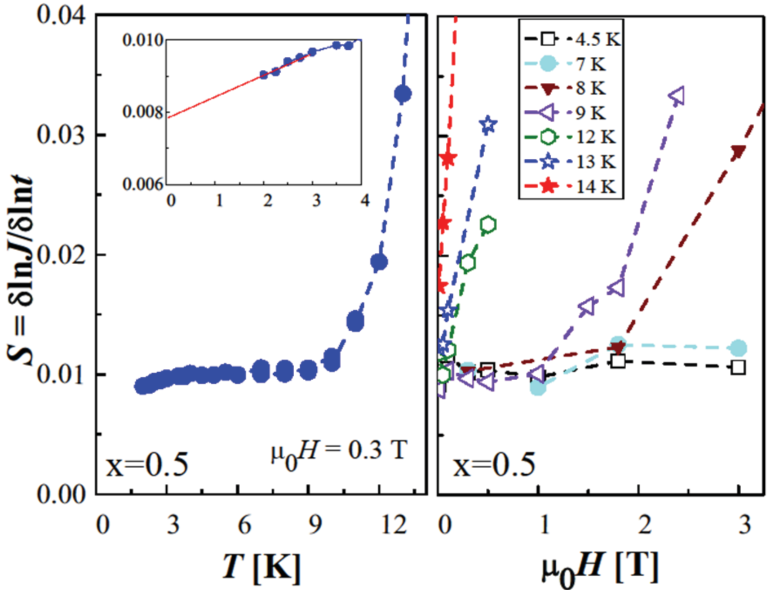




▪S. Singh, M.R. Fitzsimmons, T. Lookman, J.D. Thompson, H Jeen, and A Biwas, Phys. Rev. Letters **108**, 077207 (2012)

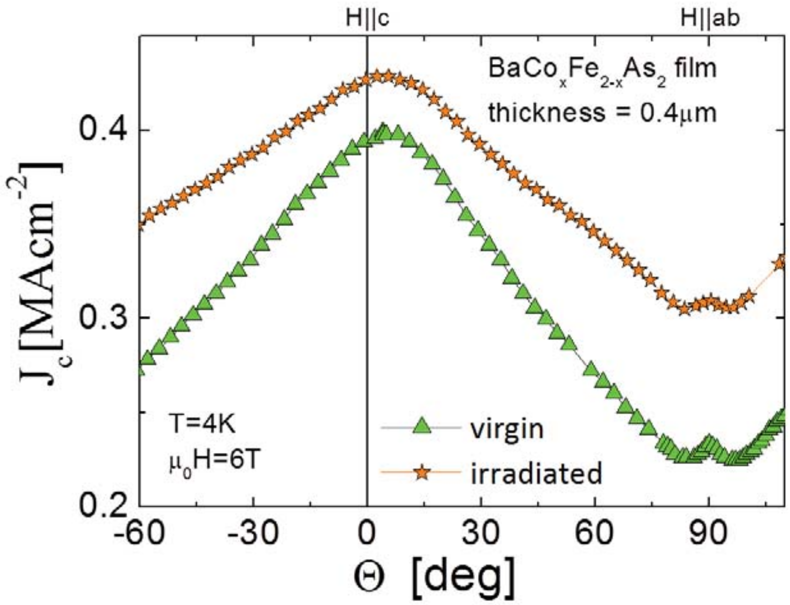
Harnessing Emergent Phenomena: Vortex Matter in Iron-Based Superconductors

Flux creep in $Ca_{1-x}Na_xFe_2As_2$ single crystals



N. Haberkorn *et al*., Effect of doping on structural and superconducting properties in $Ca_{1-x}Na_xFe_2As_2$ single crystals PRB **84**, 064533 (2011)

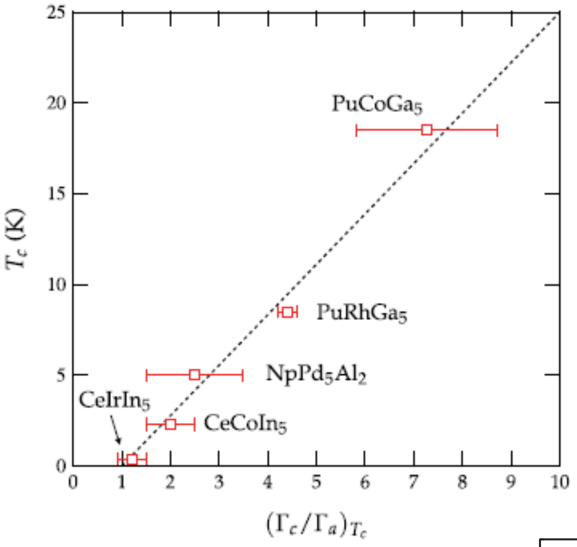
Angular dependent J_c in as-grown and proton irradiated $Ba(Fe_{1-x}Co_x)_2As_2$ films

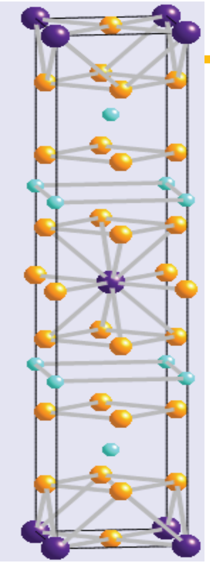


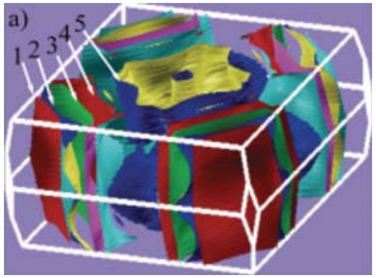
B. Maiorov *et al*., Angular and field properties of the critical current and melting line of Co-doped $SrFe_2As_2$ epitaxial films *SuST* **22**, 125011 (2009) (18 citations)

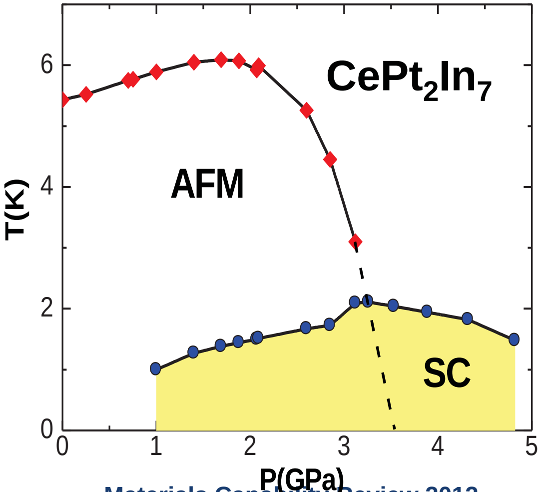
Understanding Anisotropy to Develop Design Principles for Superconductivity

- NMR discovered more microscopic origin for why layered structures enhance superconductivity S.-H. Baek *et al.*, PRL (2010)
- Our design approach led to the discovery of 3 new superconductors ($CePt_2In_7$, $PuCoIn_5$, and $PuRhIn_5$) E.D. Bauer *et al.*, PRB (2010); JPCM (2012)
- Detailed studies of these reveal discrepancies between our notions of magnetism, reduced dimensionality, bandwidth, and superconductivity M.A. Altarawneh *et al.*, PRB (2011); T. Das *et al.*, PRL (2012)







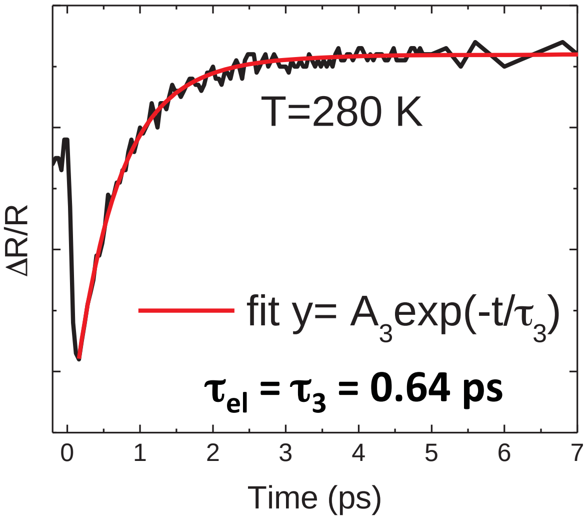


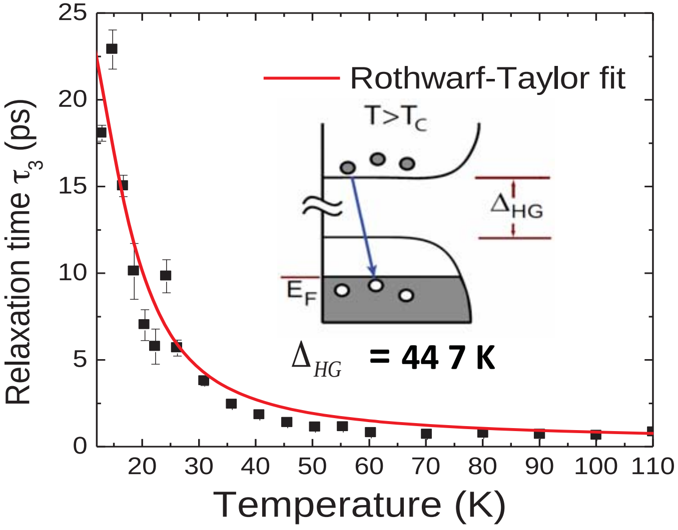
Probing Hybridization and Superconducting Gaps via Photoinduced Quasiparticles in the Heavy-Fermion Superconductor $PuCoGa_5$

- **$PuCoGa_5$:** Heavy-fermion metal with superconducting T_c = 18.5K
- 1st ultrafast experiments, transient reflectivity with 50 fs, 800-nm pulses
- **Room temperature dynamics yield electron-phonon coupling, λ**

$$\tau_{el} = \frac{\pi k_B T_e}{3\hbar\lambda\langle\omega^2\rangle}$$

  - $\lambda = 0.25 \rightarrow$ BCS $T_c = 0.03k \neq 18.5K$
  - **Rules out Phonon-mediate superconductivity**
- **First evidence for hybridization gap in $PuCoGa_5$**
  - Increase in relaxation time below 100K indicates gap opening in DOS
  - Fit to data yields hybridization gap of 44K





D. Talbayev, *et al.*,PRL **104** 227002 (2010).

Presentations and Posters

- **Presentations**
  - Vivien Zapf – “Creating magnetoelectric effects with noncoplanar spins”
  - Matthias Graf – “Electronic hot spots in the spectral function of actinides”

Presentations and Posters

- **Posters**
  - Michael Fitzsimmons (LANSCE-LC) – “Magnetic non-uniformity in $(La_{0.4}Pr_{0.6})_{0.67}Ca_{0.33}MnO_3$ films and measurement of the strain-magnetization coupling coefficient”
  - Rohit Prasankumar (MPA-CINT) & Stuart Trugman (T-4) – “Ultrafast optical probes of coupled systems”
  - Eric Bauer (MPA-CMMS) – “Electronic Inhomogeneity in heavy fermion materials”
  - Tomasz Durakiewicz (MPA-CMMS) – “New capabilities at MPA: ultrafast quasiparticle dynamics in actinides”
  - Georgios Koutroulakis (MPA-CMMS) – “First observation of ^{239}Pu nuclear magnetic resonance”
  - Doug Safarik (MST-6) – “Localized anharmonic rattling of aluminum atoms in VAl_{10}”
  - Cristiano Nisoli (T-4) – “Artificial spin ice: frustration by design and magnetic monopoles”
  - Jian-Xin Zhu (T-4) – “First-principle theory for correlated electron materials”

Creating Magnetoelectric Effects with Non-Coplanar Spins

V.S. Zapf, (NHMFL, MPA-CMMS); C.D. Batista (T-4); E.D. Bauer (MPA-CMMS); M. Fitzsimmons, (LANSCE-LC); M. Jaime (MPA-CMMS); P. Jain (MPA-CMMS, LANSCE-LC); Y. Kamiya, Y. Kato (T-4); J. W. Kim (MPA-CMMS, LANSCE-LC); I. Martin (T-4); R.D. McDonald, C. Miclea, R. Movshovich (MPA-CMMS); D. Mozyrsky (T-4); E.D. Mun (MPA-CMMS); B. Scott (MPA-MC); D. Solenov (T-4); J.D. Thompson, B. G. Ueland, F. Weickert, L. Xin (MPA-CMMS); D. Argyriou, (European Spallation Source), S.-W. Cheong (Rutgers); F. Chou (National Taiwan University); I. Fisher (Stanford); J. Gardner (NIST), B. Gaulin (McMaster, Canada); M. Kenzelmann (Paul Scherrer Institute); J. Manson (Eastern Washington University); A. Paduan-Filho (U. Sao Paulo, Brazil); F. Rivadulla (U Santiago de Compostela, Spain)

The future of our economic, energy and defense security relies on the potential to discover, understand and control new properties of materials. Magnetism underpins our ability to compute and store huge bodies of information as well as to actuate and sense. Most magnetic technologies have relied on the parallel alignment of magnetic spins. Only recently have discoveries been made that take advantage of antiferromagnetic alignment of spins to enable, for example, spintronics devices. In certain crystal structures, however, the tendency for antiparallel alignment of spins can be frustrated such that this tendency cannot be satisfied locally or globally within the material. As a result, frustration leads to complex magnetic states that can be non-coplanar. Furthermore these states can be controlled by even a small perturbation in parameters, such as composition, pressure, or temperature. It is this tunability that makes frustrated systems fundamentally interesting and highly desirable for applications. Though spin frustration has been studied extensively insulators, we focus on itinerant electrons. The coherent effect of frustrated magnetic states on itinerant electrons can generate effective magnetic fields that are orders of magnitude larger than possible in a laboratory and can be controlled by small changes in a tuning variable. Quantum magnetoelectric amplification that results from this coupling can enable entirely new technologies. In insulators as well, itinerant electrons participating in magnetic exchange can couple to the complex magnetism of local spins created by frustration, creating functionalities such as magnetic field-induced electric polarization and multiferroic behavior. Here we highlight recent progress in metals and insulators in studying the role of frustration and complex magnetism in magneto-electric coupling.

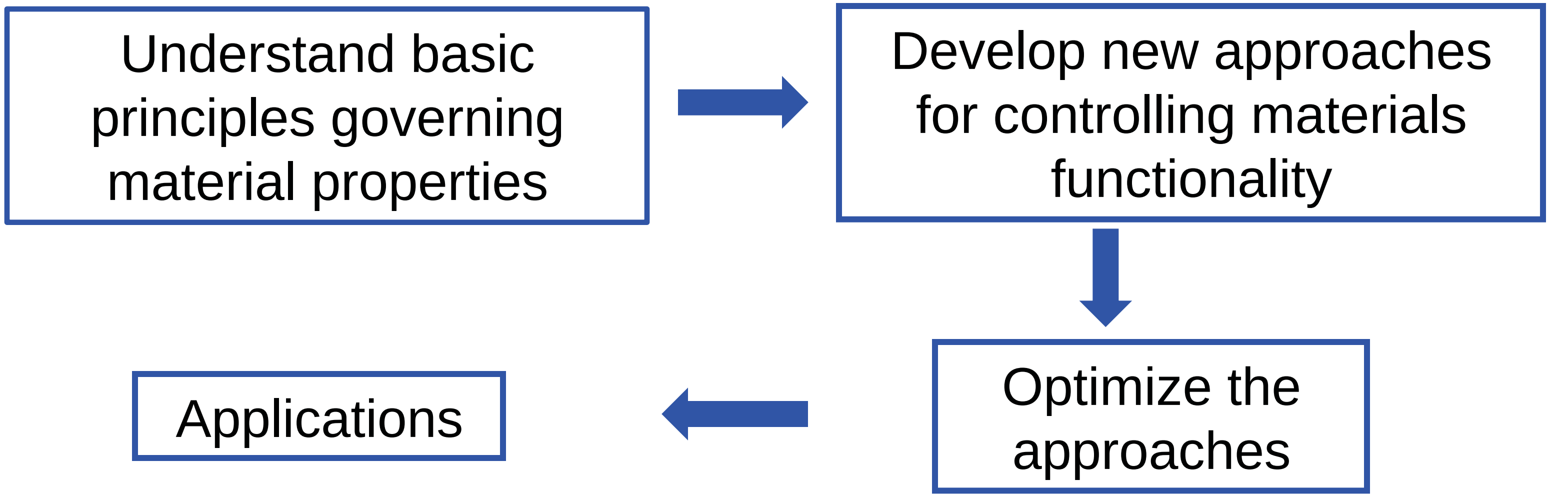
Creating Magnetoelectric Effects with Non-Coplanar Spins

Vivien Zapf, MPA-CMMS

UNCLASSIFIED

LANL Materials Strategy

The vision of controlled functionality through discovery and application of fundamental materials properties and materials synthesis and fabrication techniques, reaching from the molecular level, through nano- to microscopic scales, to bulk material



Understand basic principles governing material properties

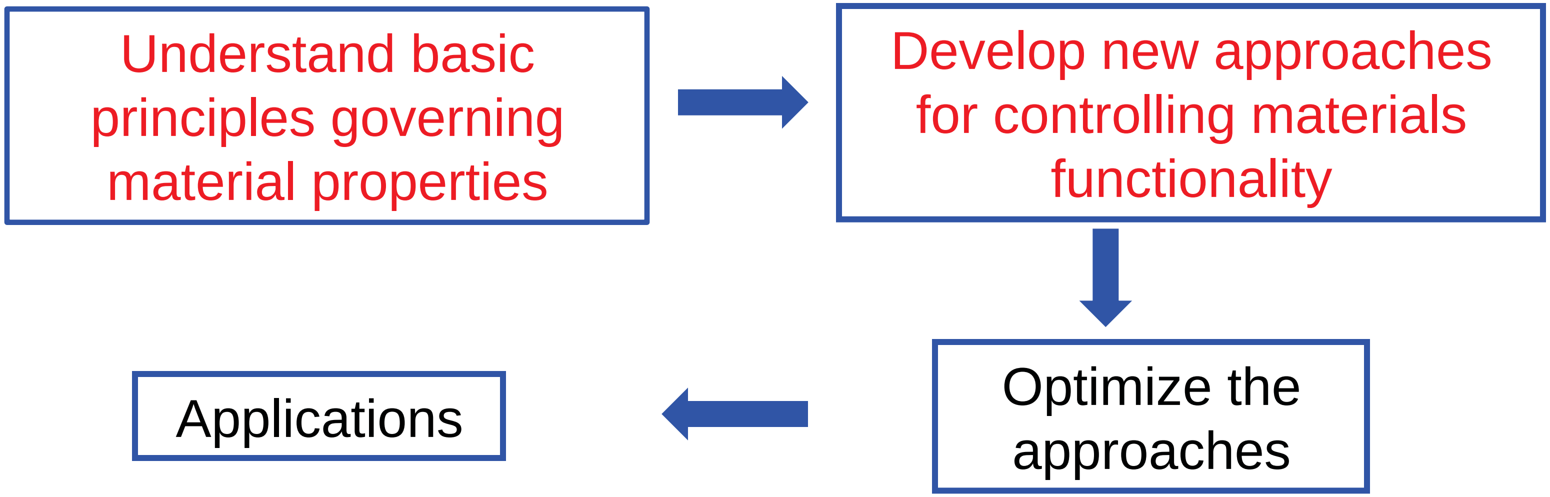
Develop new approaches for controlling materials functionality

Optimize the approaches

Applications

LANL Materials Strategy

The vision of controlled functionality through discovery and application of fundamental materials properties and materials synthesis and fabrication techniques, reaching from the molecular level, through nano- to microscopic scales, to bulk material



Understand basic principles governing material properties

Develop new approaches for controlling materials functionality

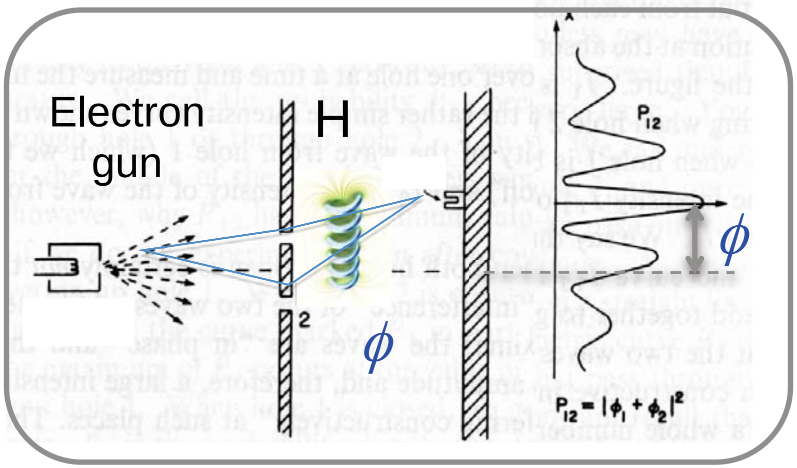
Optimize the approaches

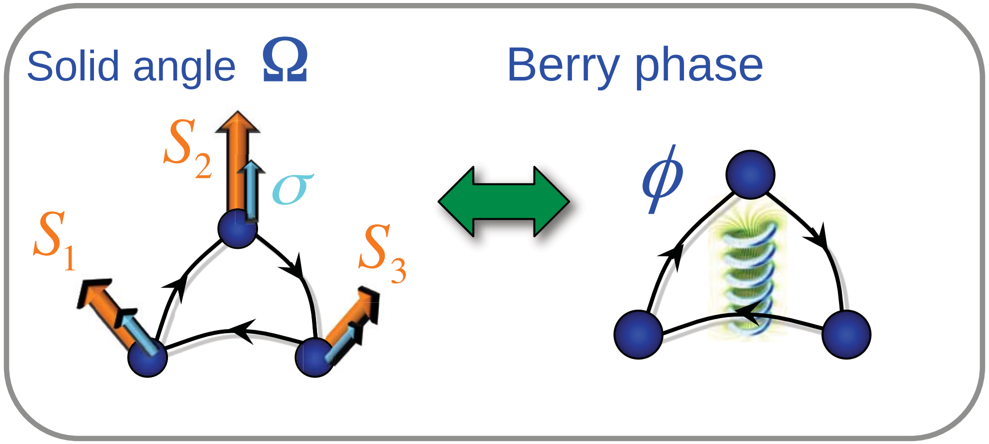
Applications

Our Approach

- **Electrons are critical for functionality**
  - They determine magnetic, electric, chemical, and structural properties of materials
- **Electrons are strongly affected by magnetic fields**
  - At the NHMFL we know that high magnetic fields can produce dramatic effects on electrons and materials properties
- **Can we create these effects at lower magnetic fields?**

Exploiting the Berry Phase: Spin Textures can Create Effective Magnetic Fields up to 10^5 Tesla

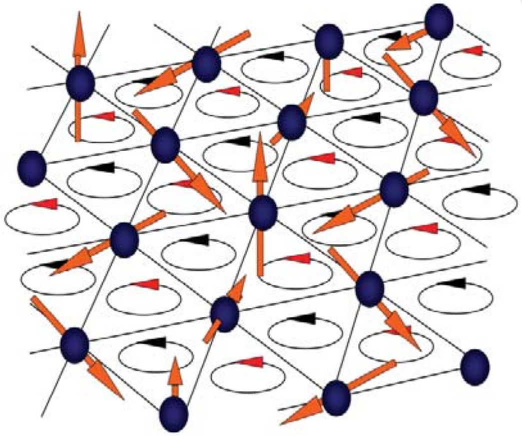


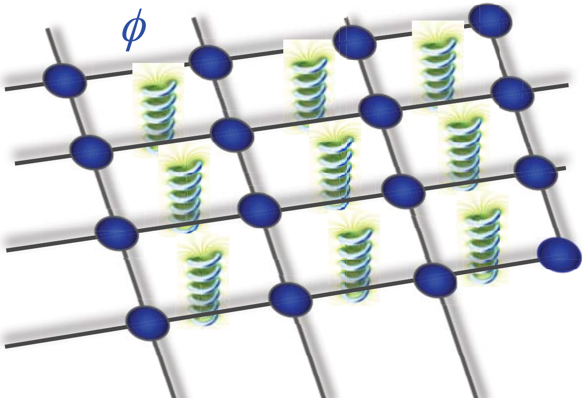


Phase of electron

$$\phi = \Omega / 2$$

Solid angle of spins

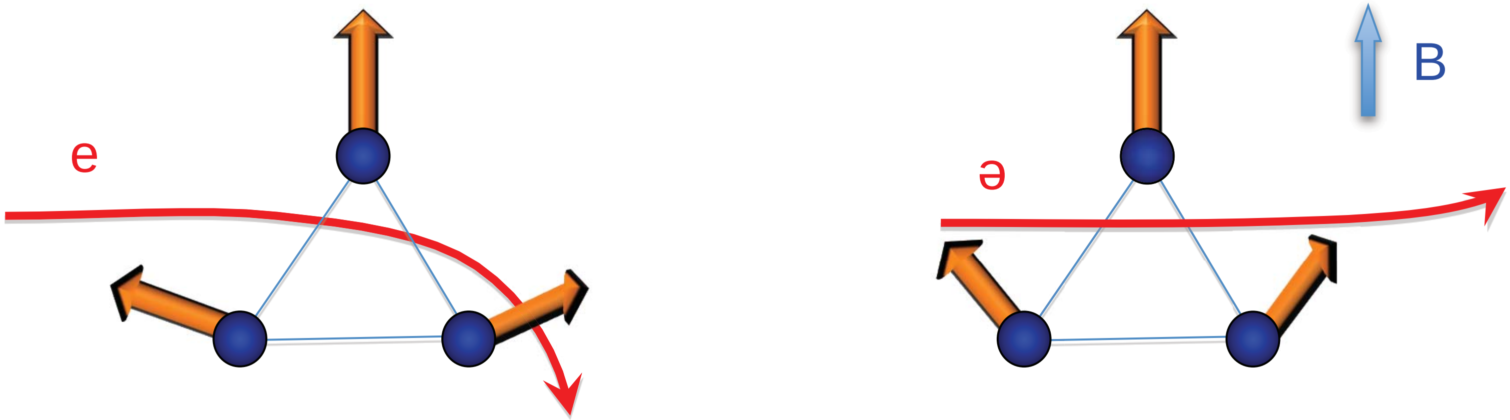




Up to 10^5 T (depending on material)

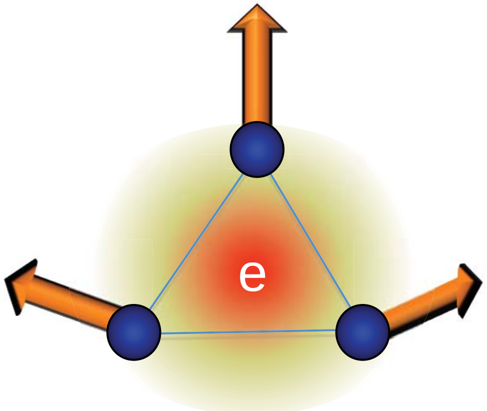
Quantum Amplification/Berry phase

Metals: B rotates **S** -> change B_{eff} -> change in conductivity and Hall

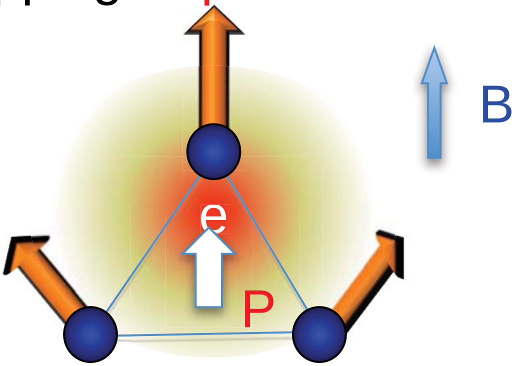


Insulators: B rotates **S** -> change in electron hopping -> polarization **P**

B = 0, P = 0

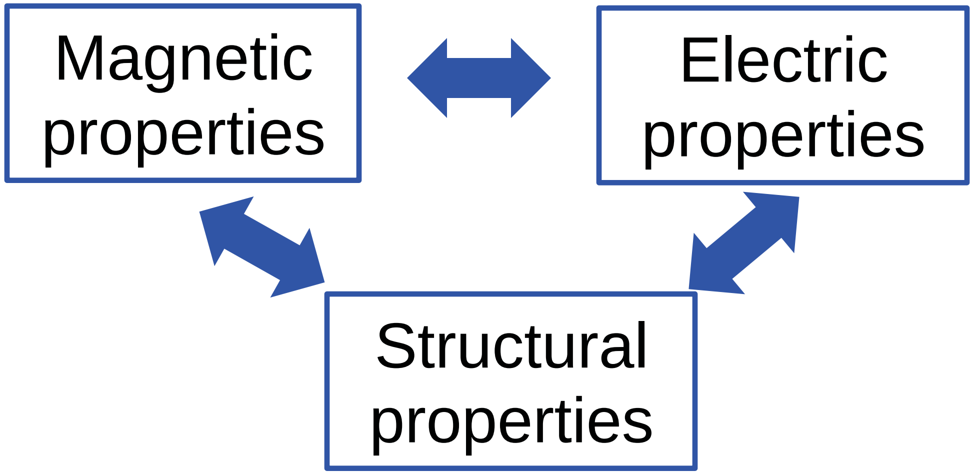


B ≠ 0, P ≠ 0



Electron in magnetic exchange

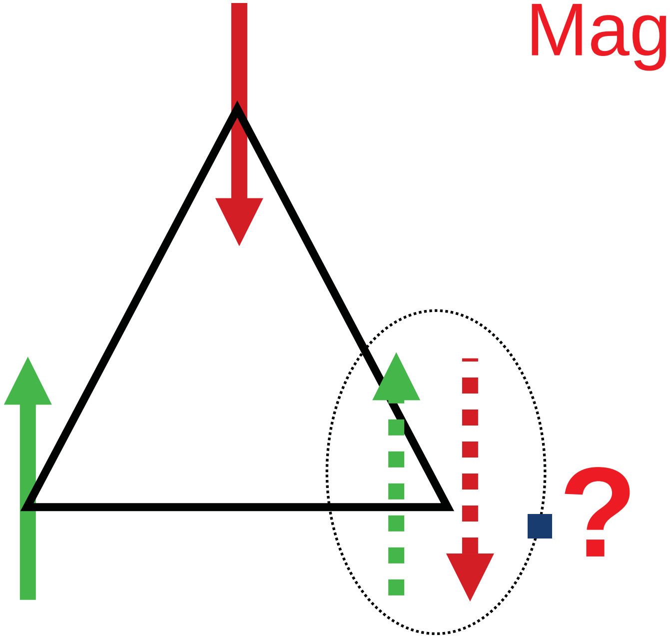
Applications of Quantum Amplification



Applications: sensors, new smart & energy-efficient circuits, spintronics

Uses: energy harvesting, metrology, national security, computation, memory

How to Create Non-Coplanar Spin Textures?

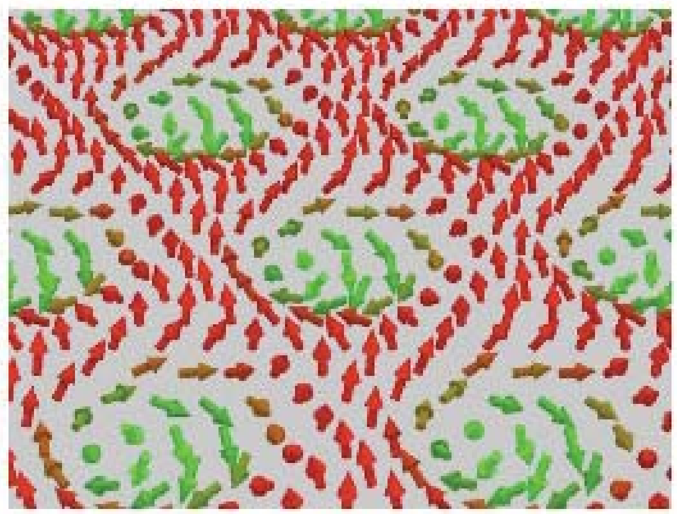


Magnetic frustration

Magnetic spins on a lattice with geometrical frustration

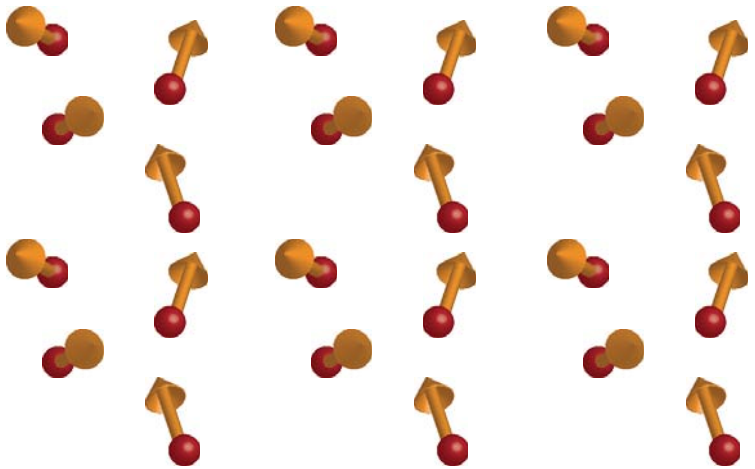
Antiferromagnetic interactions mean *each spin wants to anti-align with both of its neighbors*

Spin Textures Produced by Magnetic Frustration



MnSi, (Fe,Co)Si

S. Muhlbauer *et al.*, Science **323**, 915 (2009)



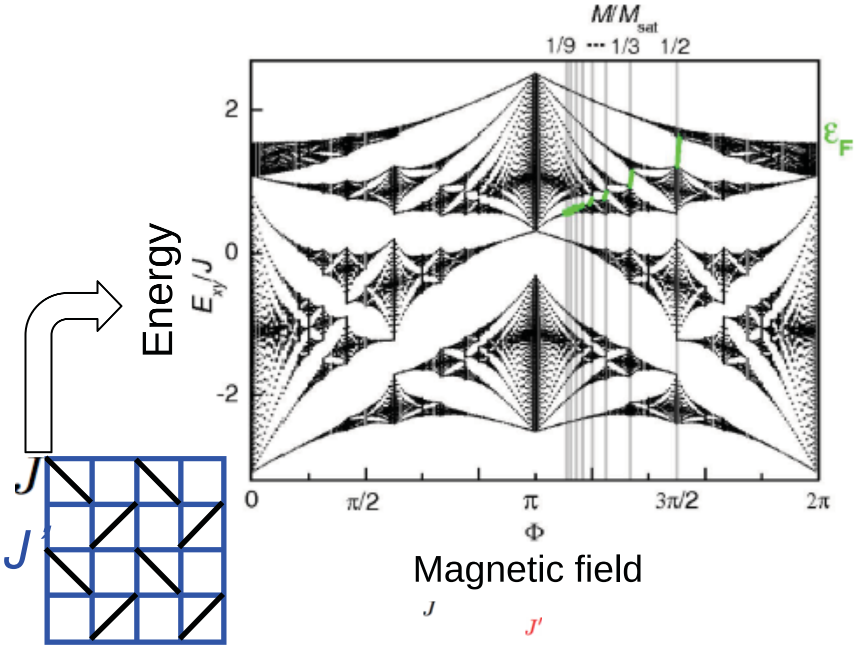
$CuCl_2$-2SO(CH_3)

V. S Zapf *et al.*, Rev. B. **82** 060402.
Editor's Suggestion (2010)

The Other Advantage of Frustration: Tuning

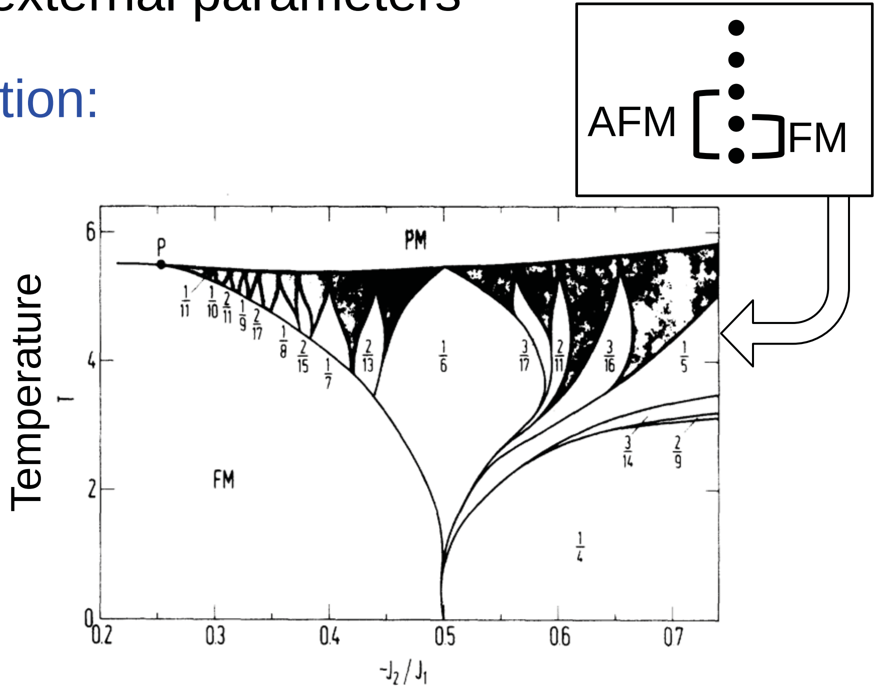
Many states close in energy:
ultra-sensitive to small changes in external parameters

Microphases emerging from frustration:



Magnetic field

Shastry-Sutherland lattice
D. R. Hofstadter, PRB **14**, 2239 (1976)



Magnetic interactions

"ANNNI" model,
W. Selke, Physics Reports **170**, 213 (1988)

People

- **Theory (T-4)**

C.D. Batista
I. Martin
D. Mozyrsky
Y. Kato (pd)
Y. Kamiya (pd)
D. Solenov (pd)

- **Physical Properties experiments (MPA-CMMS and MPA-MC)**

Brian Scott
M. Jaime
R. D. McDonald
R. Movshovich
J. D. Thompson
V. S. Zapf
J. W. Kim (pd)
E. D. Mun (pd)
B. G. Ueland (pd)
F. Weickert (pd)
Lu Xin (pd)

- **Neutron Scattering (LANSCE-LC, etc)**

M. Fitzsimmons, *LANSCE*
J. Gardner, *NIST*
M. Kenzelmann, *PSI*

- **Metals sample growth (MPA-CMMS)**

E.D. Bauer

- **Organo-metallic sample growth (external)**

P. Jain (director’s funded pd) ->
Harry Kroto *Florida State* and Tony Cheetham *Cambridge, UK*
Jamie Manson, *EWU*
Armando Paduan-Filho, *U. Sao Paulo*, *Brazil*

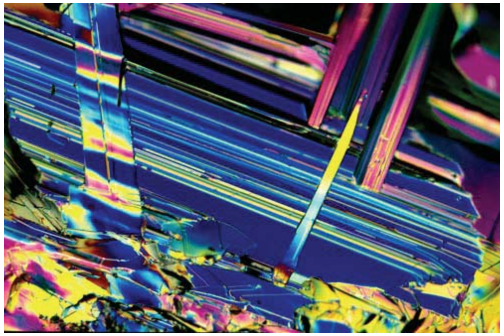
- **Oxides sample growth (external)**

Dmitri Argyriou, *European Spallation Source*
Sang-Wook Cheong, *Rutgers*
Feng Chou, *National Taiwan University*
I. Fisher, *Stanford*
B. Gaulin, *McMaster, Canada*
Y. Lee, *MIT*
Francisco Rivadulla, *U Santiago de Compostela*

Capabilities

Sample growth

(intermetallic single & polycrystals mono and tri-arc furnaces)



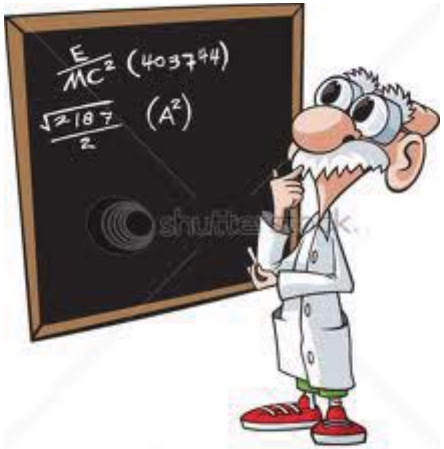
Computations

(Customized quantum & classical montecarlo, exact diagonalizations, ….)

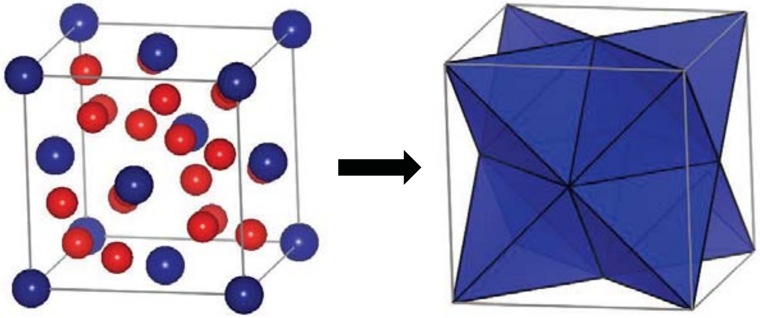
Measurements

(Sensitive physical property meas. extending to extremes of temperature, magnetic fields, pressure)

Analytics



Quantum Amplification



● U

● Cu

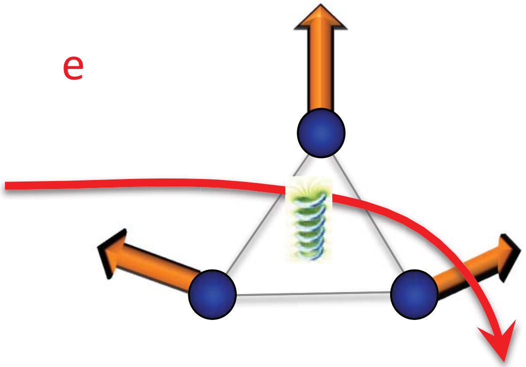
AuBe$_5$ structure

Frustrated U tetrahedra

UCu$_5$

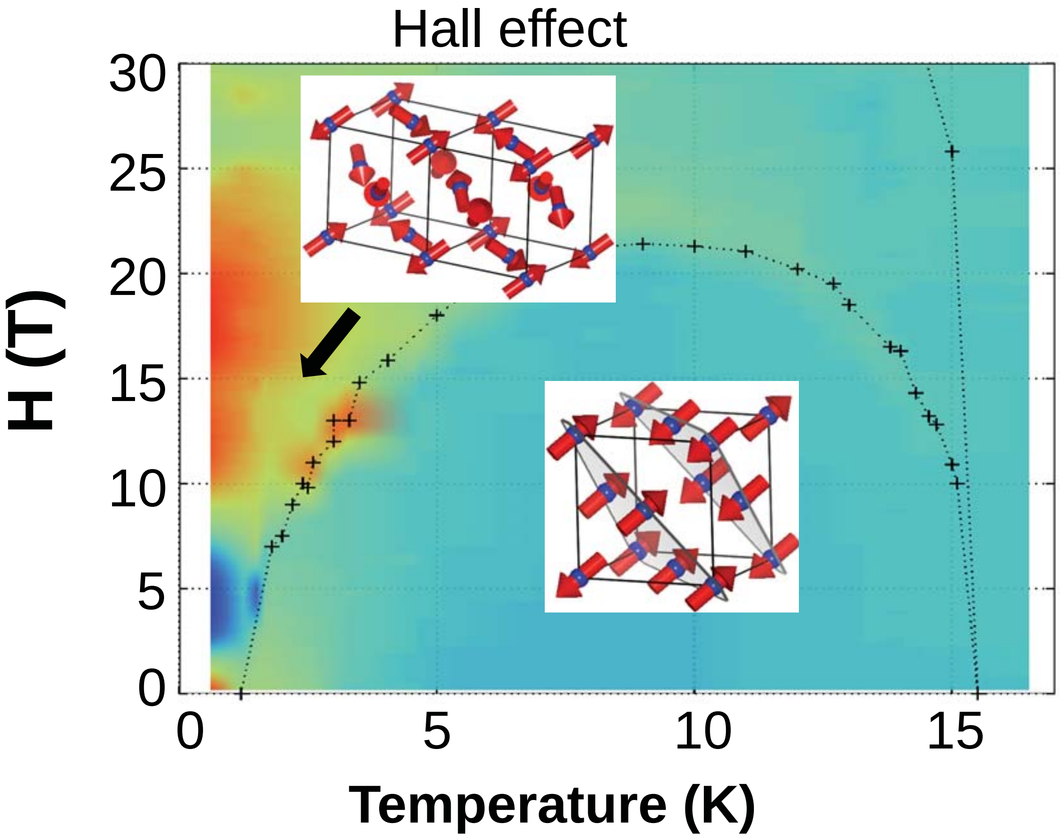
Frustration driven transition from 1-q to non-coplanar 4-q order

Geometrical Hall Effect due to REAL SPACE Berry Phase



B. G. Ueland, C. F. Miclea, Y. Kato, O. Ayala-Valenzuela, R. D. McDonald, R. Okazaki, P. H. Tobash, M. A. Torrez, F. Ronning, R. Movshovich, Z. Fisk, E. D. Bauer, I. Martin, and J. D. Thompson. Geometrical Hall effect in a magnetically frustrated metal. **Under review with Nature Communications**

Quantum Amplification

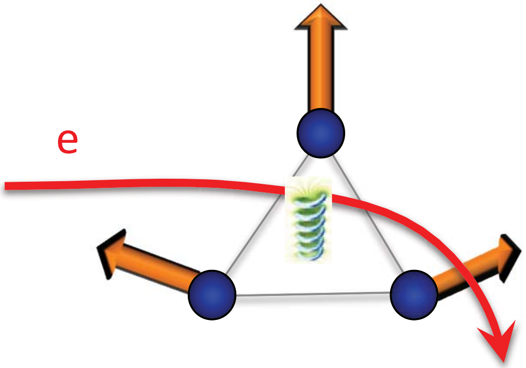


Hall effect gives 1/10 of e^2/h, effective 10^3 T

UCu$_5$

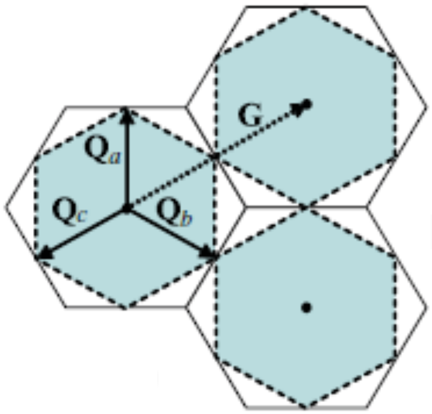
Frustration driven transition from 1-q to non-coplanar 4-q order

Geometrical Hall Effect due to REAL SPACE Berry Phase



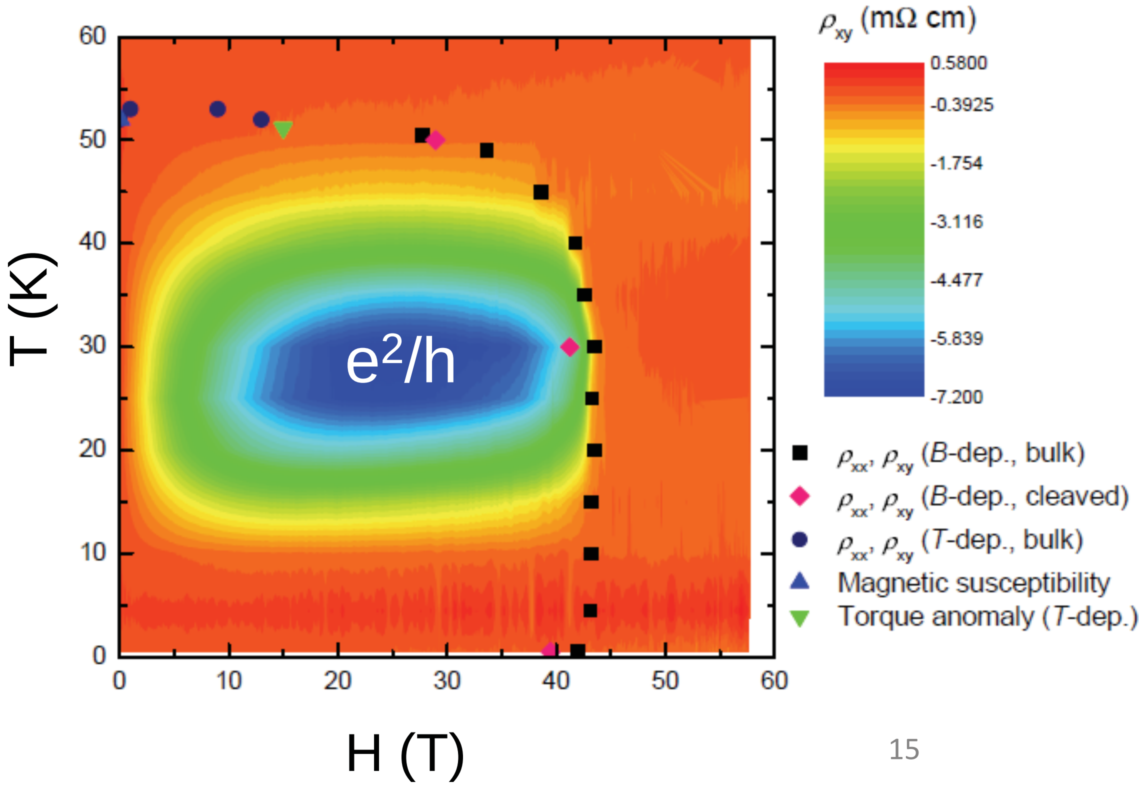
Quantum Amplification

Theory: Fermi surface nesting leading to noncoplanar ordering on triangular lattices



I. Martin, C. D. Batista,
“Itinerant electron-driven chiral magnetic ordering and spontaneous Quantum Hall effect in triangular lattice models,”
PRL **101**, 156402 (2008)

Geometrical Hall effect !?

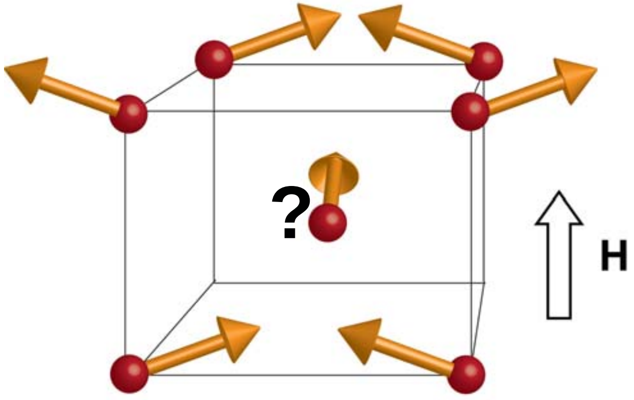


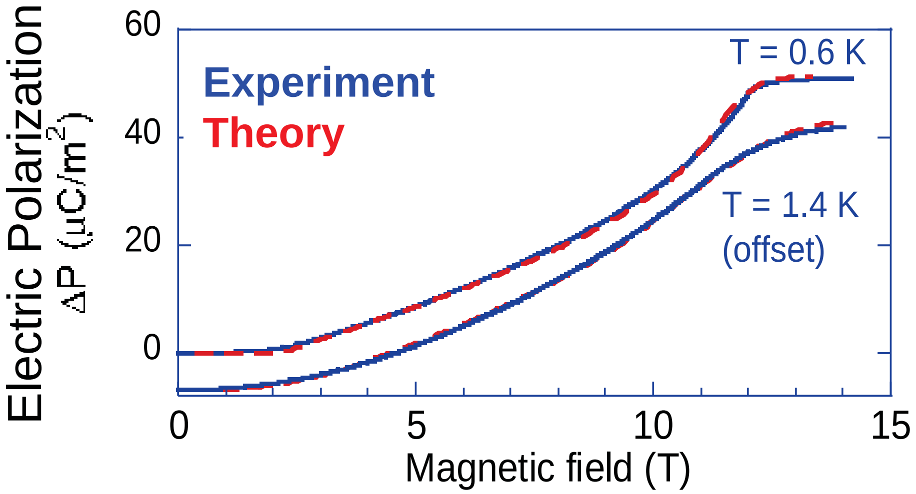
10^4 Effective Tesla

J. W. Kim, R. McDonald, V. Zapf *et al.*, in progress

Insulators: First Organo-Metallic Multiferroics

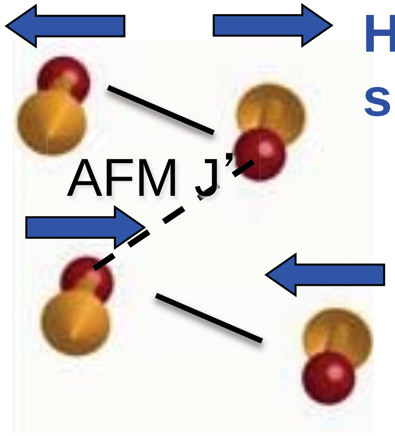
$NiCl_2\text{-}4SC(NH_2)_2$



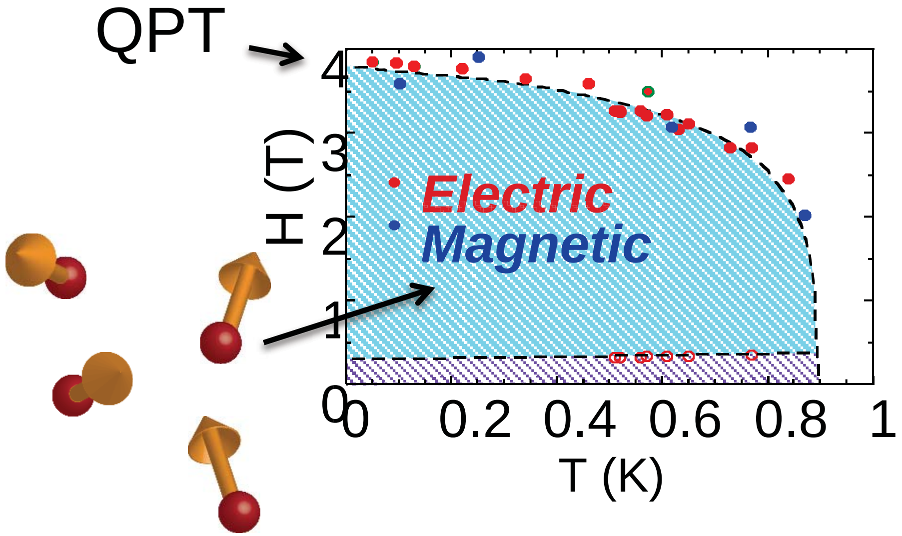


V.S. Zapf, P. Sengupta, C.D. Batista, F. Nasreen, F. Wolff-Fabris, and A. Paduan-Filho, Phys. Rev. B **83**, 140405 (2011)

$CuCl_2\text{-}2SO(CH_3)_2$

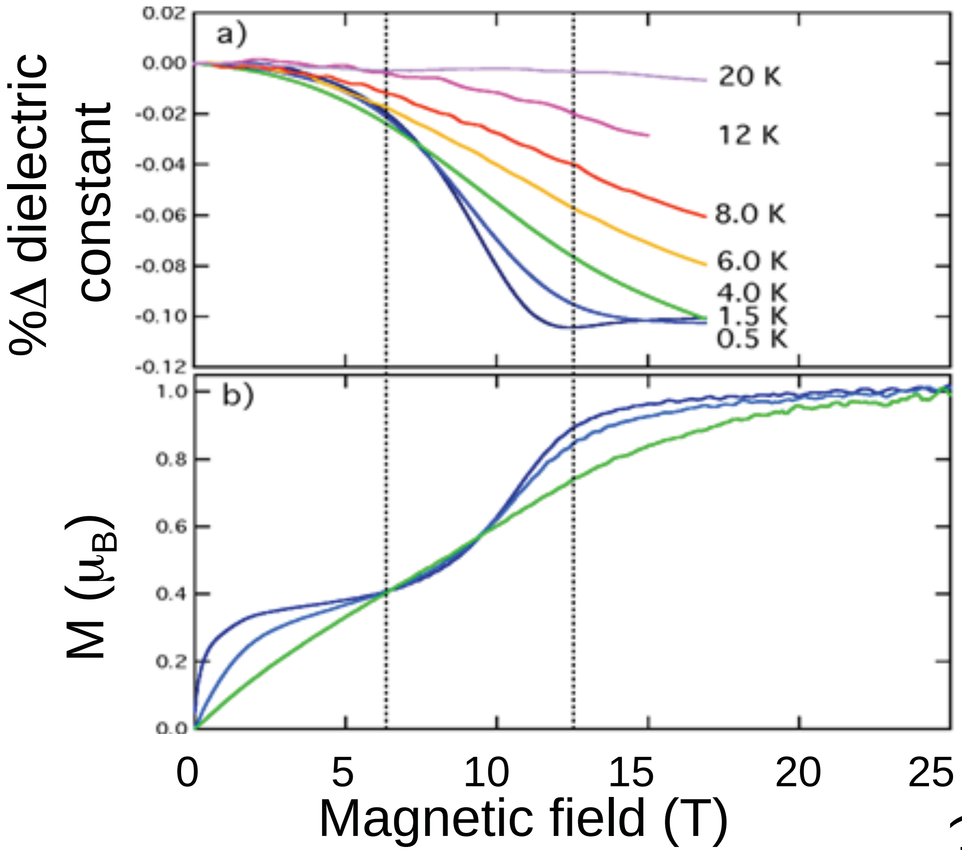


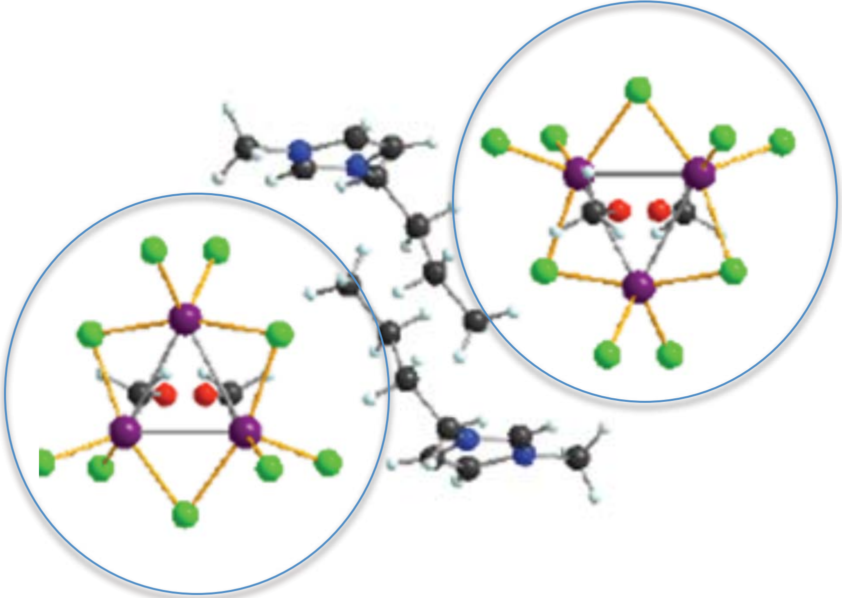
H-tuned spin-orbit



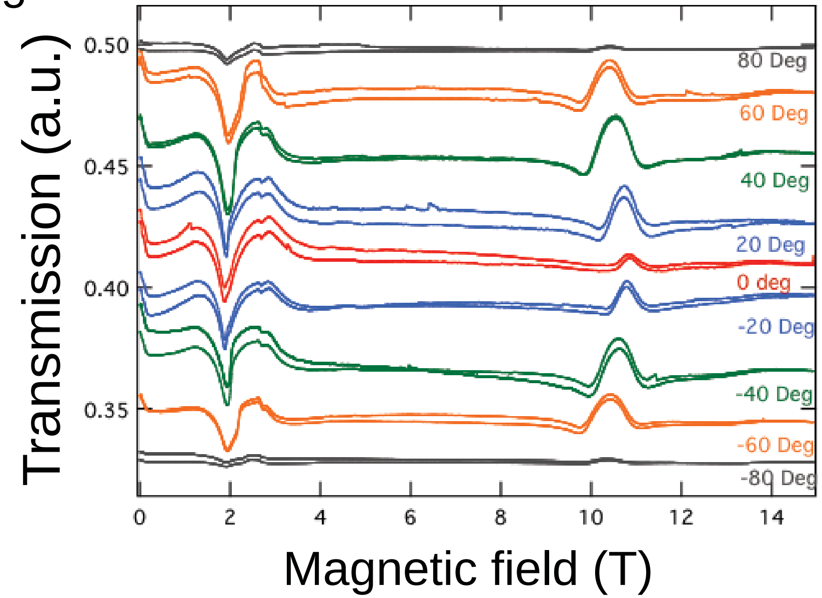
V.S. Zapf, M. Kenzelmann, F. Wolff-Fabris, F. Balakirev, and Y. Chen. Phys. Rev. B. **82**, 060402 Editor’s Suggestion (2010)

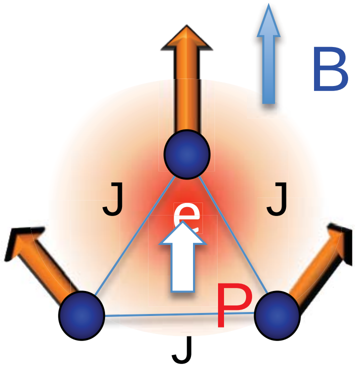
Organo-metallic Cr trimers

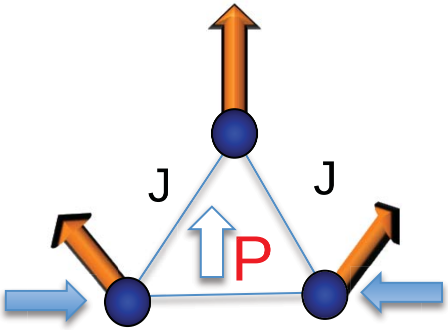




Magnetic EPR
In response to electric field





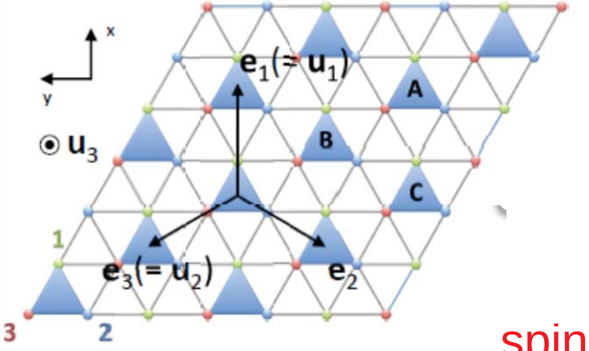


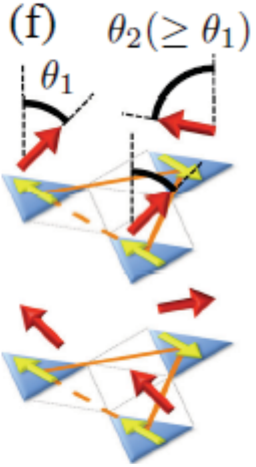
L. N. Bulaevskii, C. D. Batista, M. V. Mostovoy, and D. I. Khomskii, PRB **78**, 024402(2008); R. McDonald *et al.*

Implementation in Materials

Theory Materials

Multiferroic behavior in systems of magnetic trimers

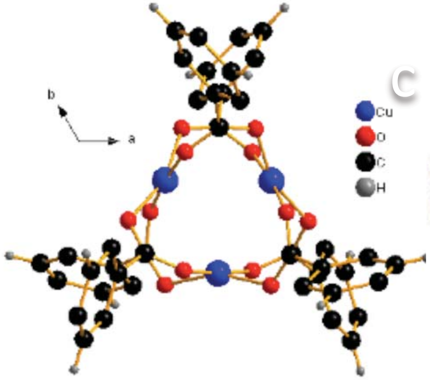


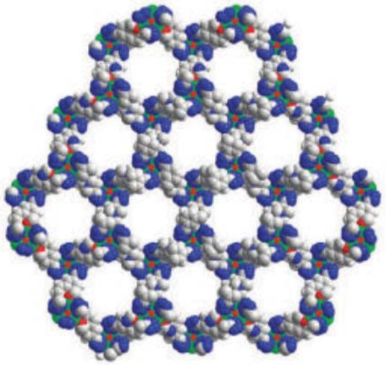


spins
orbital moments

Y. Kamiya and C. D. Batista, Multiferroic behavior in Trimerized Mott insulators (to appear in Phys. Rev. Letters)

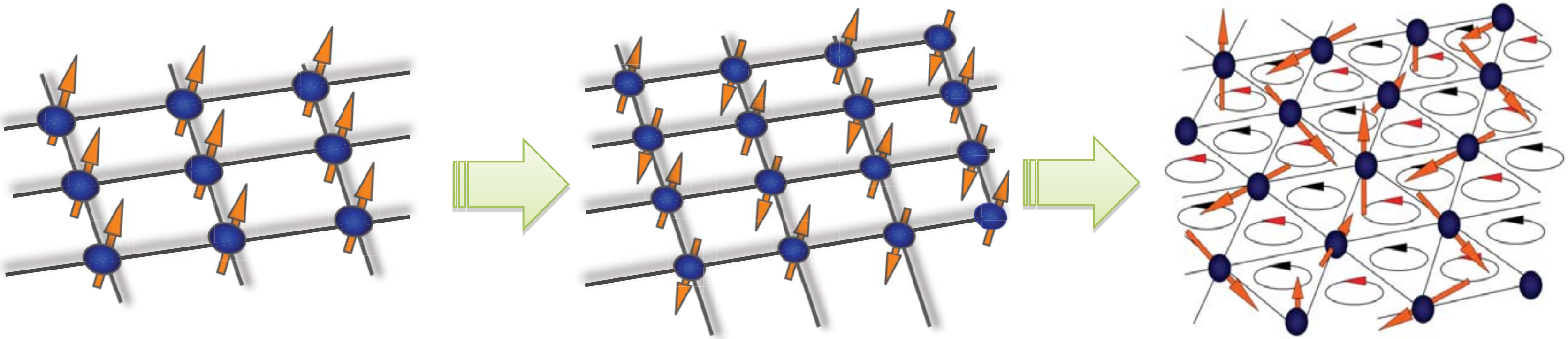
Metal-organic frameworks
Meso-scale structures for controlled design of magnetic & electric properties





The vision of controlled functionality through discovery and application of fundamental materials properties and materials synthesis and fabrication techniques, reaching from the molecular level, through nano- to microscopic scales, to bulk material

Our Approach



ferromagnet

Anti-ferromagnet

Non-coplanar magnet

Studied from prehistoric times – now

Applications: permanent magnets, hard drives, door locks, etc.

Studied from 1950s – now

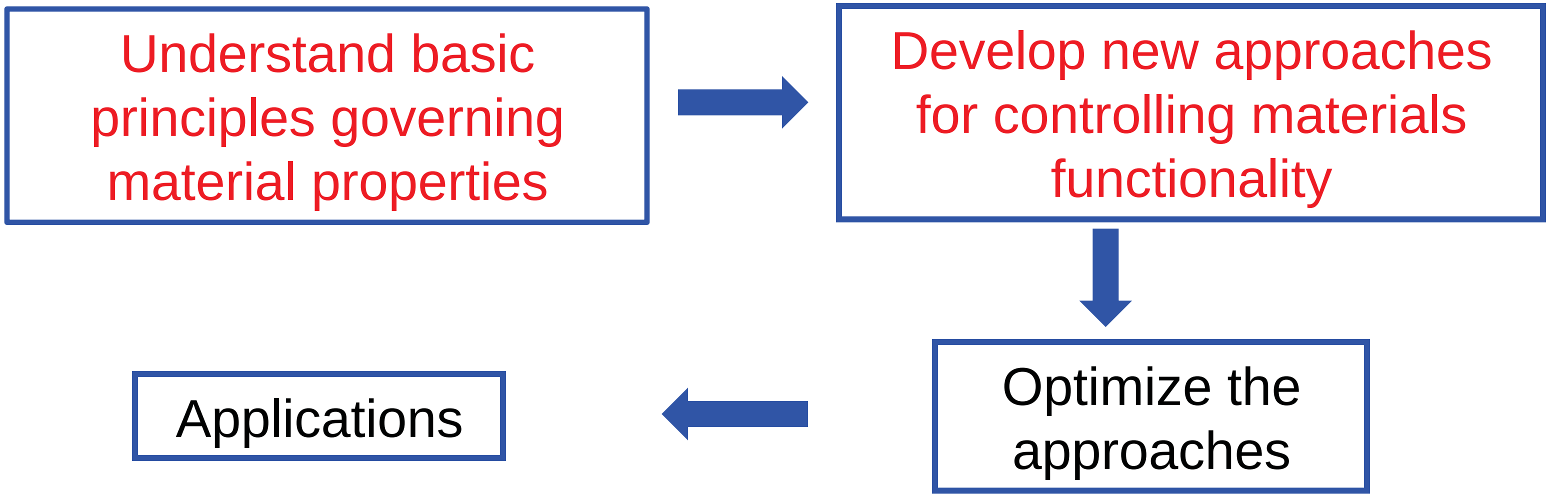
Applications: MRAM, GMR, exchange bias, spintronics, etc.

Studied from ~2000 to now

New kinds of magnetoelectric coupling, new phases of matter, chiral memory

LANL Materials Strategy

The vision of controlled functionality through discovery and application of fundamental materials properties and materials synthesis and fabrication techniques, reaching from the molecular level, through nano- to microscopic scales, to bulk material



Understand basic principles governing material properties

Develop new approaches for controlling materials functionality

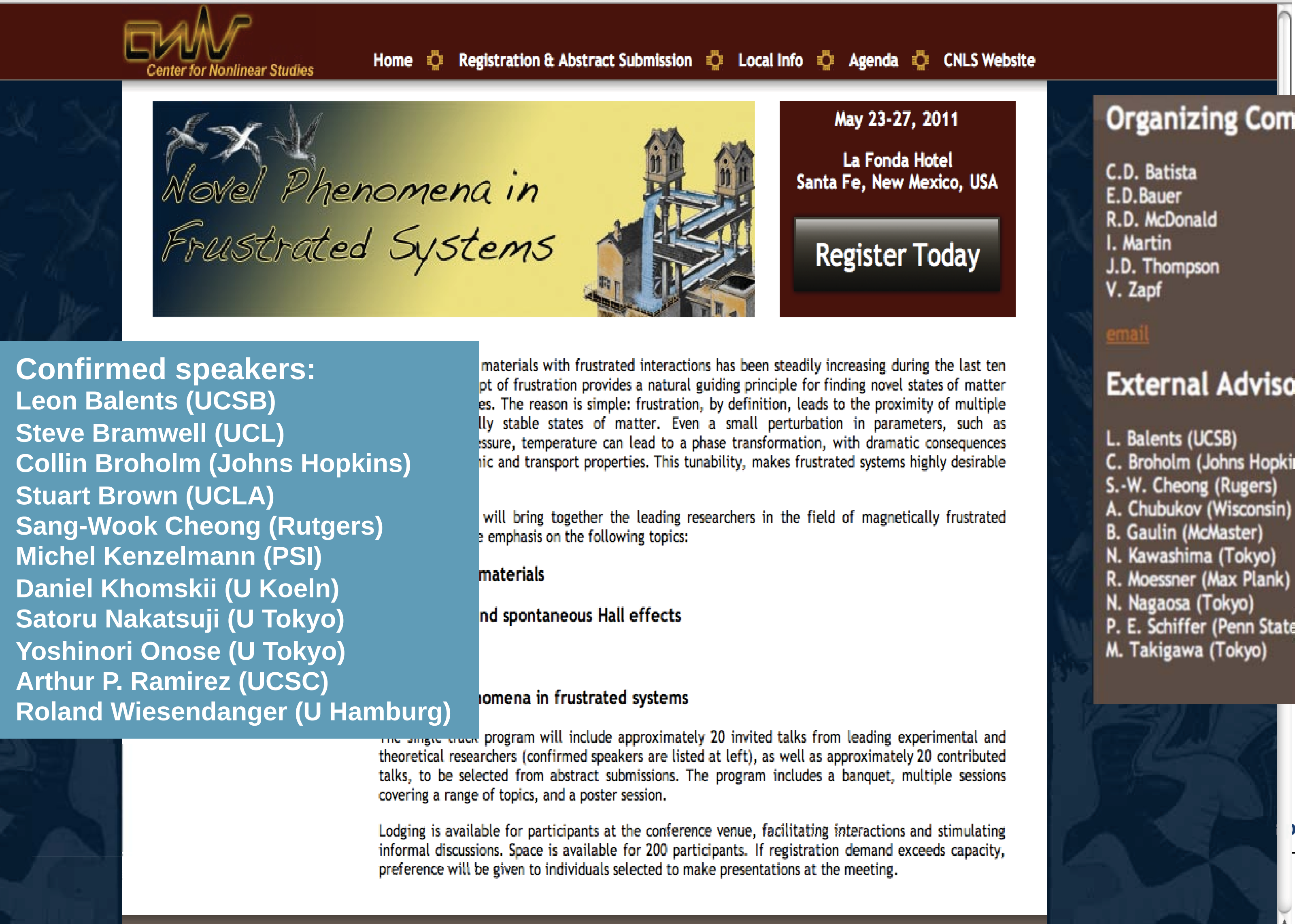
Optimize the approaches

Applications

Materials Strategy

- **We’ve developed new design principles for magnetoelectric coupling**
  - Quantum amplification in triangular lattice systems (metals)
  - Multiferroic behavior in trimers, and phase slips (insulators)
- **New classes of materials in which to see magnetoelectric coupling**
  - First actinide geometrical Hall effect (Quantum amplification)
  - Hall effect in $Na_{0.5}CoO_2$ reaches the quantum limit, effective 10^4 T @ 30 T
  - First organo-metallic multiferroics
- **Where to now**
  - Wider range of systems at higher temperatures & lower fields
  - Controlled design of MOFs
  - New theories for coupled trimers
  - Ideas about noncoplanar spins in Kondo systems

May 2011: CNLS Frustration Conference @ La Fonda Hotel: 50 Speakers, 20 International, 5 LANL



May 23-27, 2011

La Fonda Hotel
Santa Fe, New Mexico, USA

materials with frustrated interactions has been steadily increasing during the last ten
pt of frustration provides a natural guiding principle for finding novel states of matter
es. The reason is simple: frustration, by definition, leads to the proximity of multiple
lly stable states of matter. Even a small perturbation in parameters, such as
ssure, temperature can lead to a phase transformation, with dramatic consequences
ic and transport properties. This tunability, makes frustrated systems highly desirable

will bring together the leading researchers in the field of magnetically frustrated
emphasis on the following topics:

materials

nd spontaneous Hall effects

omena in frustrated systems

The single track program will include approximately 20 invited talks from leading experimental and theoretical researchers (confirmed speakers are listed at left), as well as approximately 20 contributed talks, to be selected from abstract submissions. The program includes a banquet, multiple sessions covering a range of topics, and a poster session.

Lodging is available for participants at the conference venue, facilitating interactions and stimulating informal discussions. Space is available for 200 participants. If registration demand exceeds capacity, preference will be given to individuals selected to make presentations at the meeting.

Confirmed speakers:
- Leon Balents (UCSB)
- Steve Bramwell (UCL)
- Collin Broholm (Johns Hopkins)
- Stuart Brown (UCLA)
- Sang-Wook Cheong (Rutgers)
- Michel Kenzelmann (PSI)
- Daniel Khomskii (U Koeln)
- Satoru Nakatsuji (U Tokyo)
- Yoshinori Onose (U Tokyo)
- Arthur P. Ramirez (UCSC)
- Roland Wiesendanger (U Hamburg)

Organizing Committee:

C.D. Batista
E.D.Bauer
R.D. McDonald
I. Martin
J.D. Thompson
V. Zapf

email

External Advisory Committee:

L. Balents (UCSB)
C. Broholm (Johns Hopkins)
S.-W. Cheong (Rugers)
A. Chubukov (Wisconsin)
B. Gaulin (McMaster)
N. Kawashima (Tokyo)
R. Moessner (Max Plank)
N. Nagaosa (Tokyo)
P. E. Schiffer (Penn State)
M. Takigawa (Tokyo)

Related Posters

- **Jae-Wook Kim, NHMFL poster**
  - “Multiferroic properties of materials in high magnetic fields”
- **Cristiano Nisoli, condensed matter poster**
  - “Artificial spin ice: frustration by design and magnetic monopoles”
- **Rohit Prasankumar, condensed matter poster**
  - “Ultrafast optical probes of coupled systems”

Electronic Hot Spots in the Spectral Function of Actinides

M.J. Graf, T. Das, J.-X. Zhu (T-4); T. Durakiewicz, J.J. Joyce (MPA-CMMS)

Predicting and modeling materials properties of correlated electron systems, like the actinides, is an important, yet inherently challenging problem. Current first-principles electronic structure codes fail to describe the electronic properties of actinides, because they neglect crucial many-body interactions arising from electron-electron correlations. Overcoming this problem requires an integrated theory and experiment effort, on which we embarked.

We propose that the "genetic" information of correlated electron materials regarding their duality between localization and itinerancy is encoded in electronic hot spots of the spectral function. By studying theoretically and experimentally these areas of increased intensity, we expect to lay the foundation for the control of materials functionality toward new design principles.

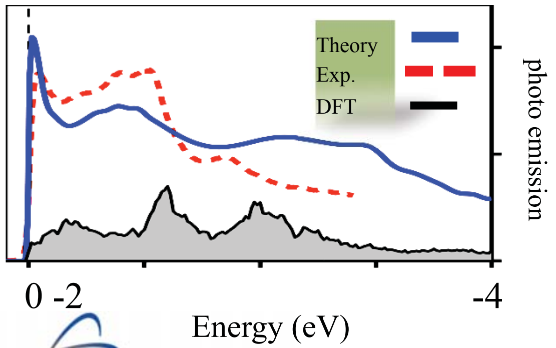
Highlights will be presented of recently performed first-principles based multiband spin-fluctuation calculations within the self-consistent random-phase approximation for intermetallic actinides. The correlation effects generate anomalies in the dispersion, which give rise to the peak-dip-hump structure in photoemission spectra. We identified these anomalies in momentum-energy space with the electronic hot spots and found that they are adequately described by the coupling between itinerant electrons and spin fluctuations. In the case of uranium and plutonium based actinides, fluctuations arise from the particle-hole continuum of the spin-orbit split 5f states. Theoretical predictions were validated by high-precision angle-resolved photoemission spectroscopy (ARPES), which images dispersion anomalies in the spectral function.

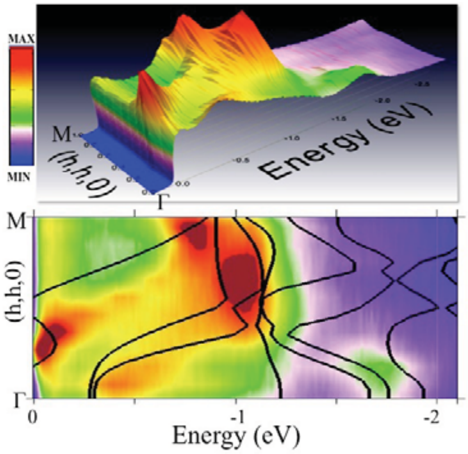
Electronic Hot Spots in the Spectral Function of Actinides

**Matthias Graf[1], Tanmoy Das[1], Jian-Xin Zhu[1],
Tomasz Durakiewcz[2], John Joyce[2]**

[1] T-4

[2] MPA-CMMS





Outline

- **Tie to LANL mission and materials strategy**
- **Motivation and background**
  - Toward design principles for controlled functionalities in correlated electron materials
  - Understanding dynamic correlation effects
- **Problem and approach**
  - Standard density functional theory is inadequate to capture dynamic electronic correlation effects of metals (band renormalization, heavy masses, …)
  - First-principles approaches combined with many-body methods for correlations
  - High-precision angle-resolved photoemission spectroscopy (ARPES)
- **Technical highlights**
  - Prediction and validation of electronic hot spots for actinides
- **Summary and outlook**

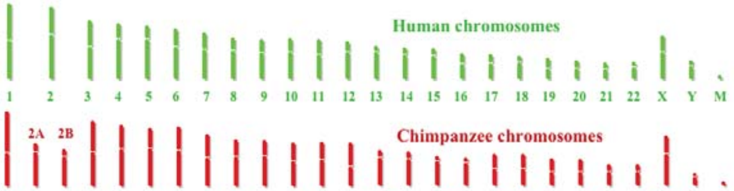
Tie to LANL mission and materials strategy

- **Strategic investment plan – Institutional priorities**
  - Plutonium science – actinide centric research
  - Technology capabilities for MaRIE – ultrafast techniques
  - Materials: discovery science to strategic applications
    - FY13 Priority: discovery science leading to understand/control actinide matter
    - Emergent phenomena: discover/understand/control to create functionality
    - Integration of synthesis, characterization and theory
    - FY13 Opportunity – Materials Genome Initiative
    - Understanding the genetic make-up of actinides for control/functionality & design principles

- **Theory and modeling predictions validated through experiments**
  - Long-term synergies between T, MPA & MST divisions
  - Building international leadership

Motivation and background

- **Foundational challenge:** We do not control the electronic structure of correlated electrons in metals
  - Treatment of dynamic correlation effects is crucial
- **Exploiting ‘hot spots’ as the ‘genes’ of the material**
  - Find the “2-6%” of hot spots that are important (human vs. chimpanzee genome)
  - Knowing how electronic differences are expressed will be the game changer



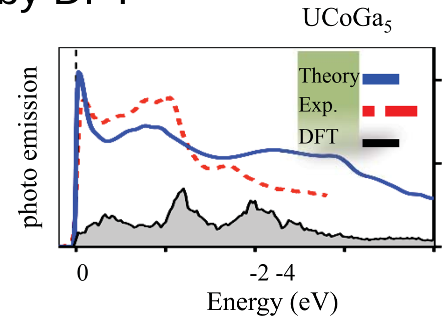
- **Integration of theory and experiment is essential for success**
  - Theory can predict hot spots and provide maps for measurements
  - Experiment can target hot spots and validate predictions
  - Need many-body methods coupled with DFT; high-precision probes for characterization, validation and discovery; synthesis to make high-quality crystals

Problem and approach

- Standard density functional theory (DFT) is inadequate to capture dynamic electronic correlation effects in metals (band renormalization, heavy masses, …)

- Band renormalization
  - Velocity - slope in dispersion: $$v_i = -\frac{1}{\hbar}\partial_{k_i} E(k)$$
  - Mass – curvature in dispersion: $$m_{ij}^{-1} = \frac{1}{\hbar^2}\partial_{k_i}\partial_{k_j} E(k)$$
  - Lifetime effects – broadening and shadow bands: $$\Delta E(k)$$

- Peak-dip-hump structure in photoemission is *not described* by DFT
- Electron mass of heavy fermions is *not described* by DFT
- Magnetic ordering vector is *not always described* by DFT
- Optical conductivity, tunneling conductance, …, is *not always described* by DFT



Materials to test approach

- The intermetallic actinide families Pu-115 and U-115 provide an excellent test bed for dynamic correlations and electronic hot spots

($PuCoGa_5$, $PuRhGa_5$, $PuCoIn_5$ and U*M*Ga_5 with *M*=Co, Fe, Ni, Ru, Rh, Pd, Os, Ir, Pt)

Why Pu-115 and U-115?

- Electronic correlation effects lead to mass enhancement and different ground states
- Fermi surface dimensionality in family changes from 3D to 2D favoring magnetism and superconductivity
- Crystals cleave with good surface properties for ARPES
- U-115 compounds allow access to national user facilities to test approach

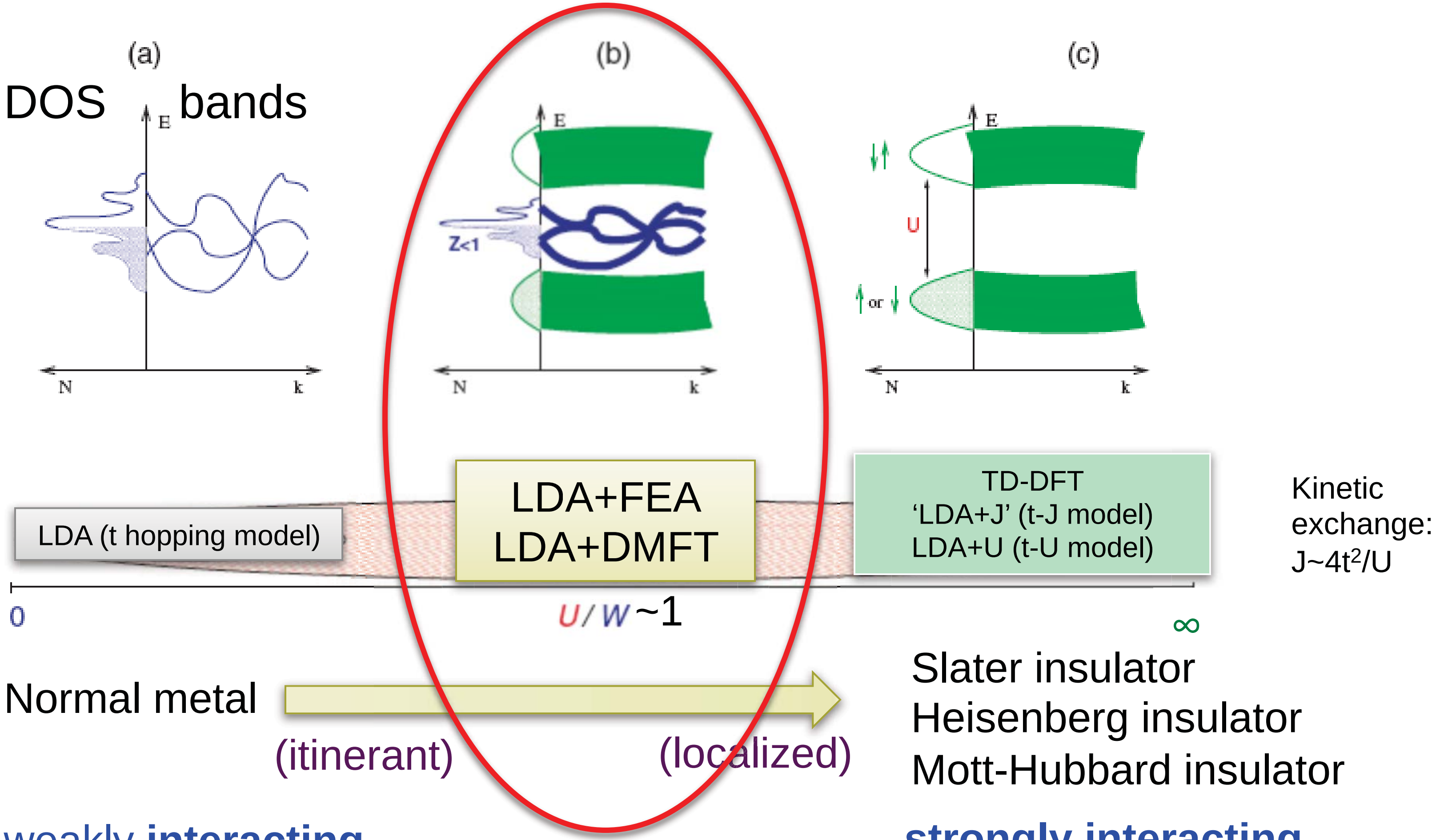
Approach: Materials specific modeling of correlation effects in metals

- **LDA/GGA of DFT** (local density/generalized gradient approx. of density functional theory): **momentum space anisotropy**
  - Full-potential codes correctly describe semi-core states (6s, 6p orbitals of 5f electron materials)
  - Relativistic full-potential codes correctly describe spin-orbit coupling

- **FEA** (fluctuation exchange approximation): electronic correlations of spin, charge and lattice fluctuations with bath of itinerant electrons
  - Start from <u>itinerant</u> picture of band electrons

- **DMFT** (dynamical mean-field theory): electronic correlations of single quantum impurity or “on-site f electron” with bath of itinerant electrons
  - Start from <u>localized</u> picture of single-site electron coupled to band electrons

Approach: First-principles based methods for electronic correlation effects



DOS bands

LDA (t hopping model)

LDA+FEA
LDA+DMFT

TD-DFT
'LDA+J' (t-J model)
LDA+U (t-U model)

Kinetic exchange:
$J \sim 4t^2/U$

0 $U/W \sim 1$ ∞

Normal metal

(itinerant) (localized)

Slater insulator
Heisenberg insulator
Mott-Hubbard insulator

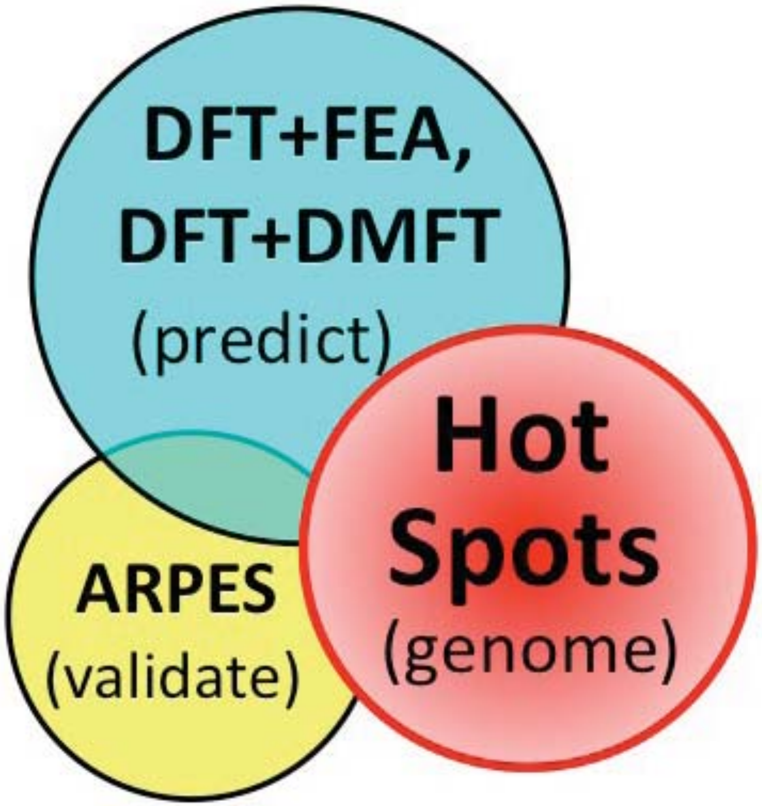
weakly **interacting**

strongly interacting

Integration of theory and experiment

- **Integration is essential for success – needed for validation and improvement of methods and techniques**

Probing momentum, energy and temperature



(see posters by Zhu & Durakiewicz)

Theory coupled with ARPES

- **D**ensity **F**unctional **T**heory
- **F**luctuation **E**xchange **A**pproximation
- **D**ynamical **M**ean-**F**ield **T**heory

One-electron DFT

Correlation self-energy

$$\boxed{G^{-1} = G_0^{-1} - \Sigma}$$

electron-phonon

particle-hole fluctuations (spin, charge, …)

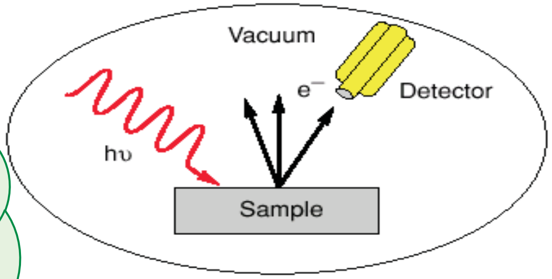
$$\left.\begin{array}{ll}(1) & \Sigma_{FEA}(k,\omega;T)\\ (2) & \Sigma_{DMFT}(\omega;T)\end{array}\right\}\ \boxed{\text{Compare predictions}}$$

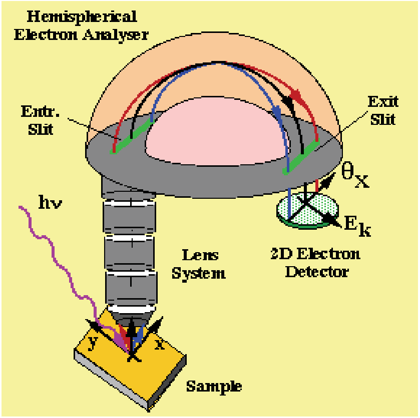
theory

+

experiment

Angle-**R**esolved **P**hoto-**E**mission **S**pectroscopy (**ARPES**)

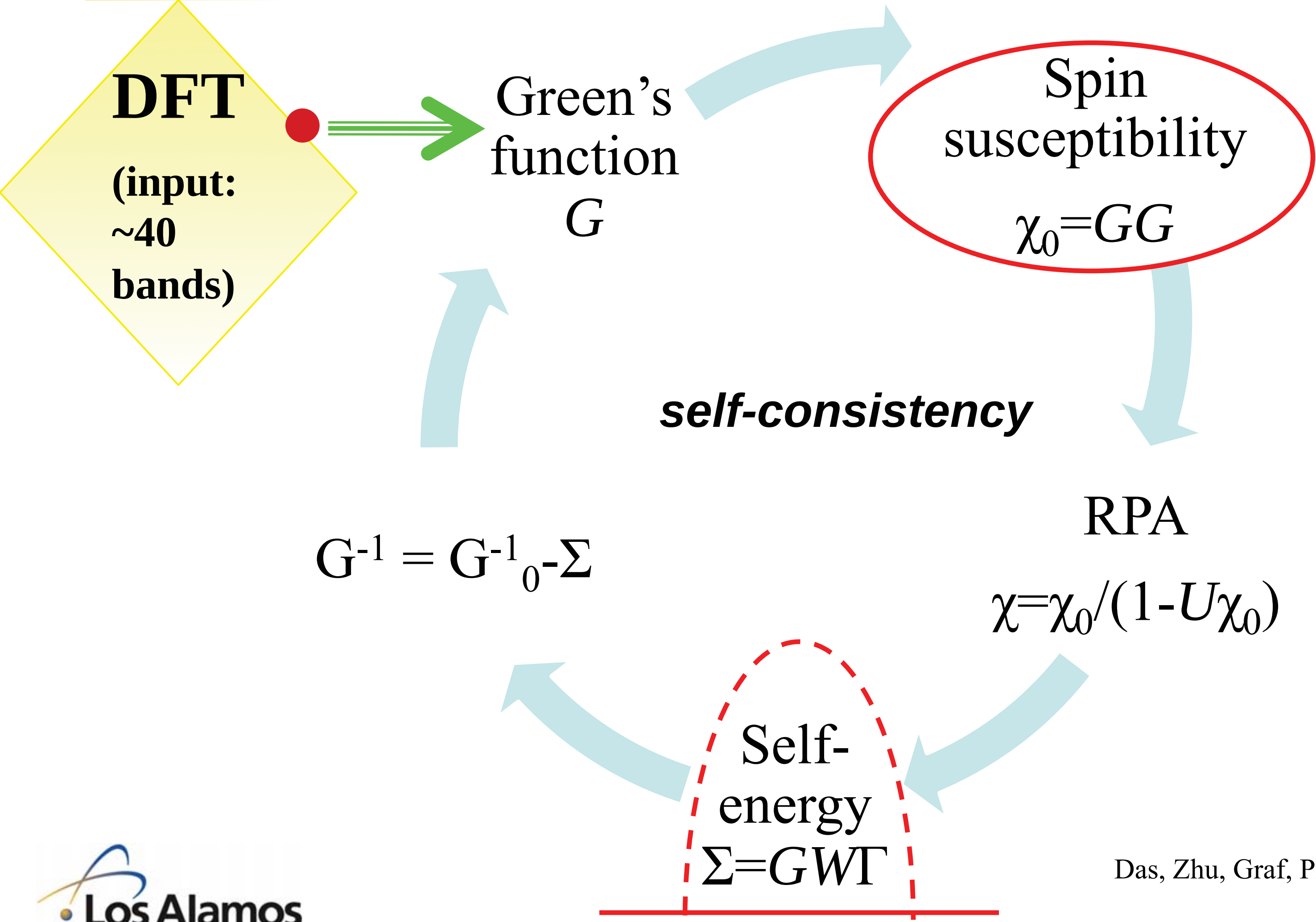




Spectral function (*k*-resolved density of states)

$$\boxed{A(k,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G(k,\omega)}$$

Theory approach – DFT+GW model (intermediate coupling/renormalized RPA)



DFT

(input: ~40 bands)

Green's function G

Spin susceptibility

$\chi_0 = GG$

self-consistency

RPA

$\chi = \chi_0/(1-U\chi_0)$

Self-energy

$\Sigma = GW\Gamma$

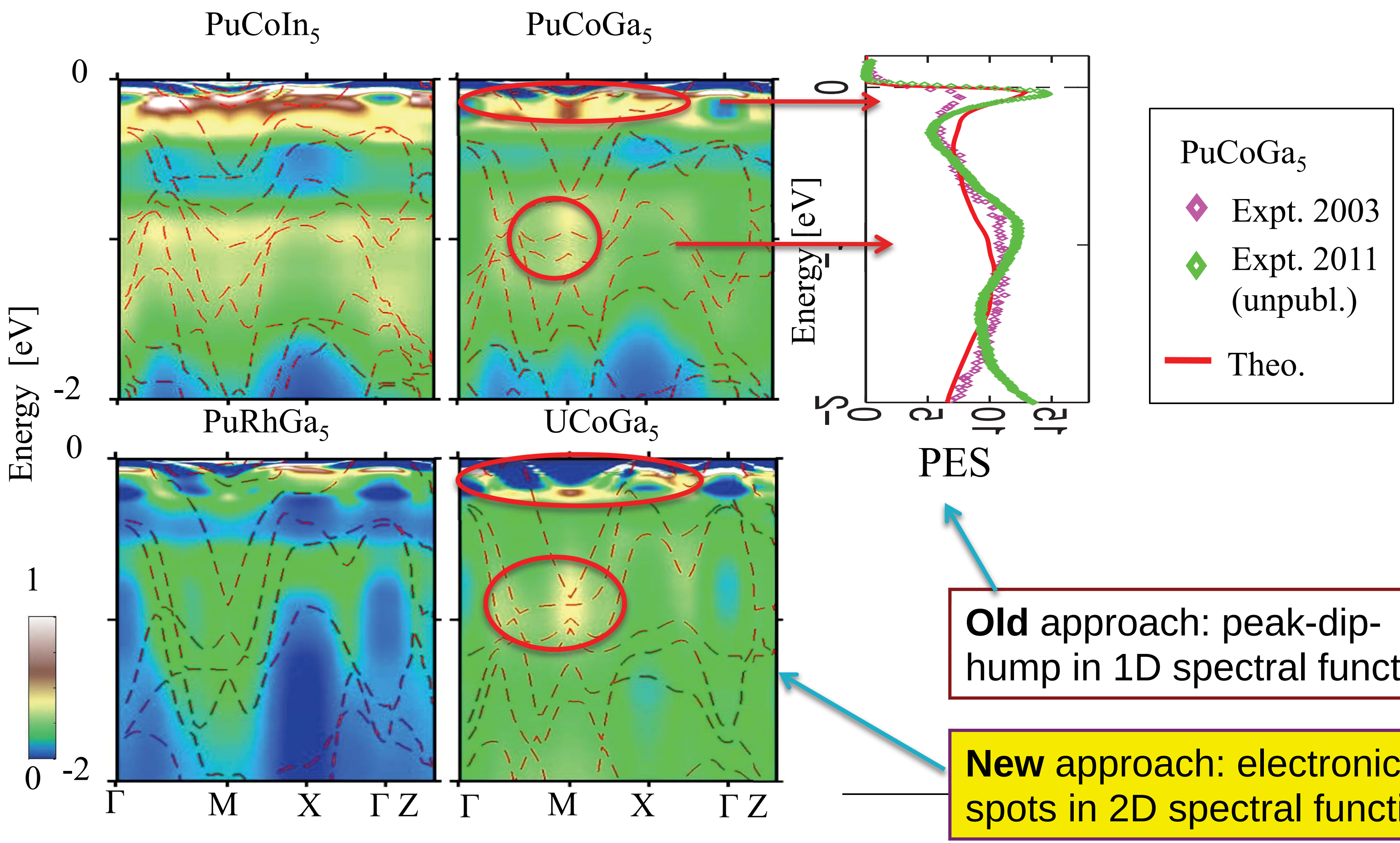
$G^{-1} = G^{-1}_0 - \Sigma$

Das, Zhu, Graf, PRL **108**, 017001 (2012)

We ***predicted*** hot spots in intermetallic actinides Pu-115 and UCoGa$_5$ based on DFT+FEA!

Technical highlights

Das, Zhu, Graf, PRL 108, 017001 (2012)

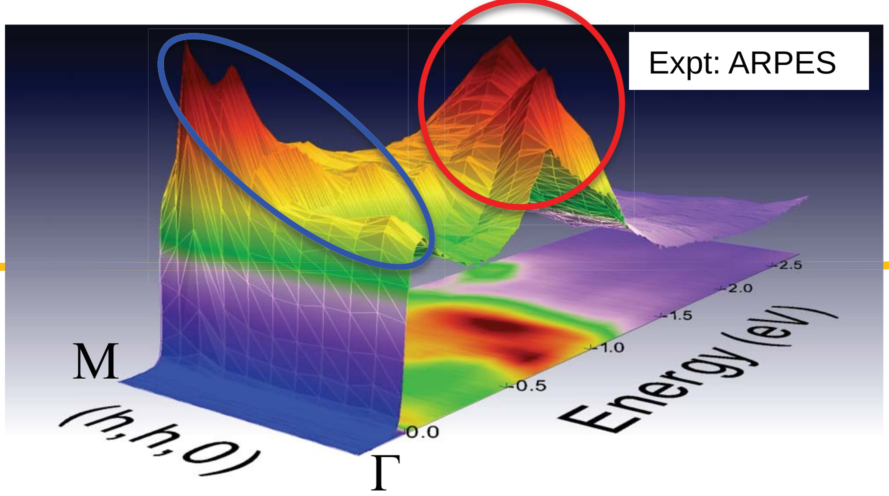


Old approach: peak-dip-hump in 1D spectral function

New approach: electronic hot spots in 2D spectral function

More technical highlights

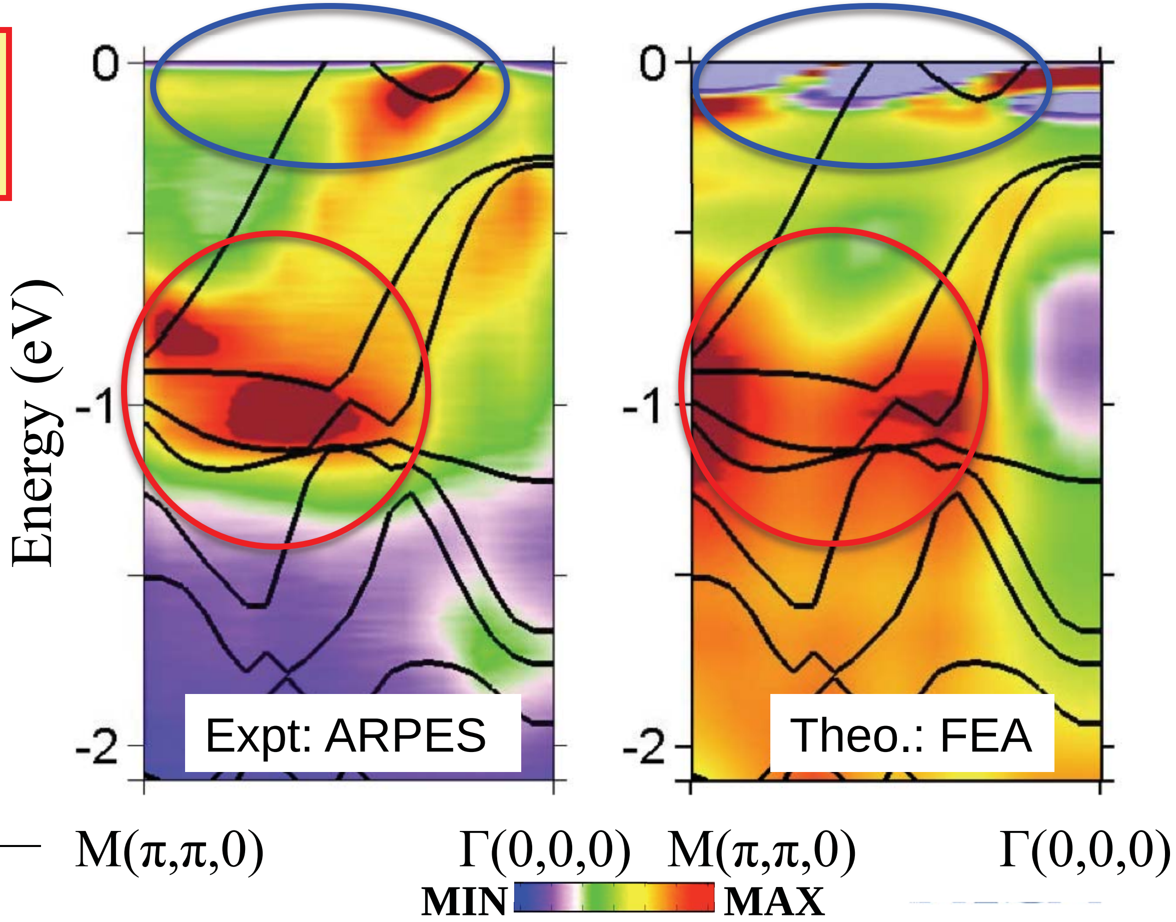
- FEA **predicted** hot spots
- ARPES **confirmed** hot spots



Hot spots already in the 'vegetable' $UCoGa_5$

Hot spots = "genes in the genome"

First low and high energy kinks observed in an actinide! (analog to 'waterfall' phenomenon in high-T_c cuprates)



(Das, Durakiewicz, Zhu, Joyce, Sarrao, Graf; submitted to PRX)

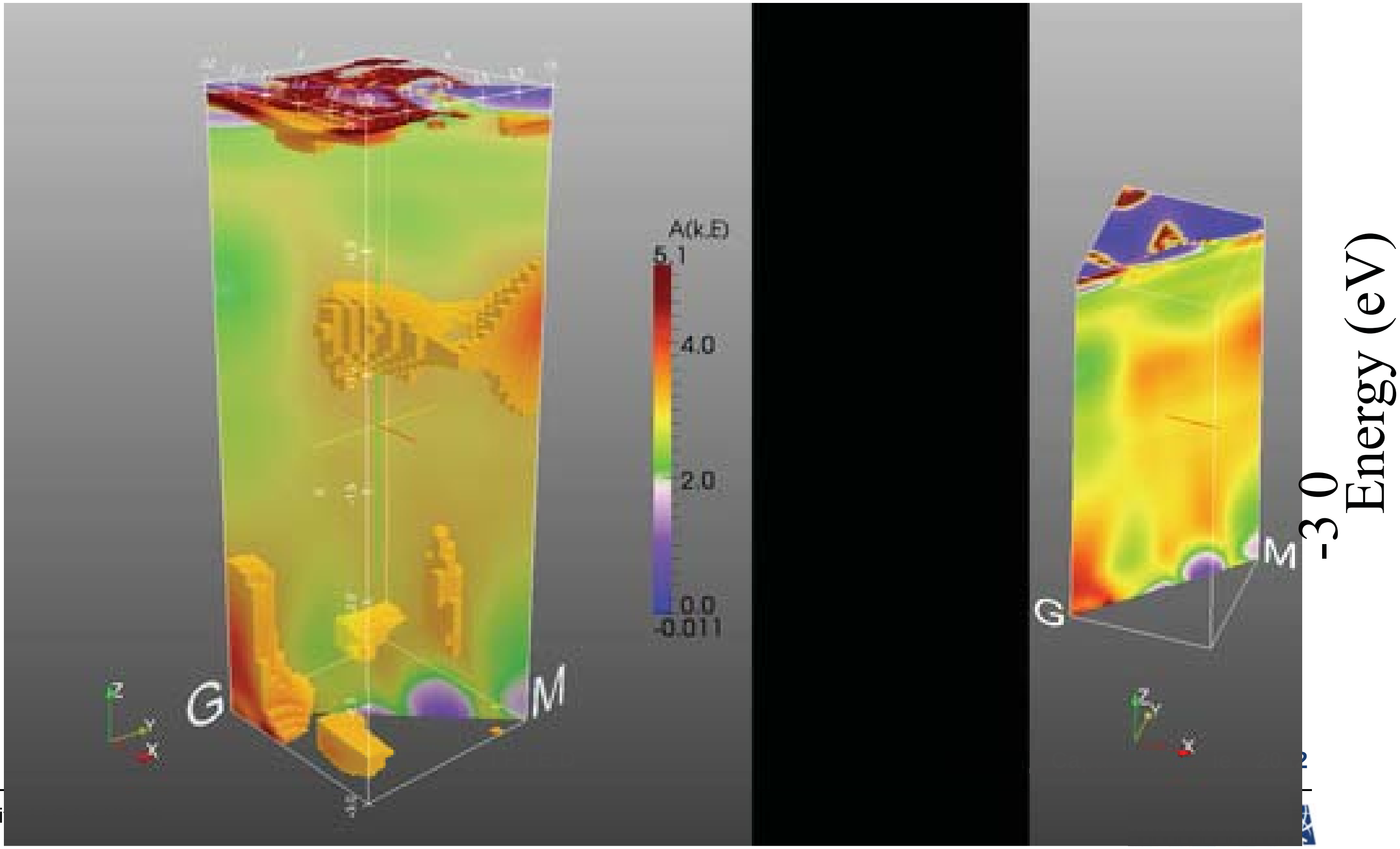
Regions of electronic hot spots in spectral function

FEA calculated $\boxed{A(k,\omega) = -\frac{1}{\pi}\operatorname{Im} G(k,\omega)}$ for **UCoGa$_5$**

Providing *k*-E maps of hot spots to be validated through experiment

Brillouin zone:
k$_z$=0

Goal:
Sequencing
and
understanding
hot spots



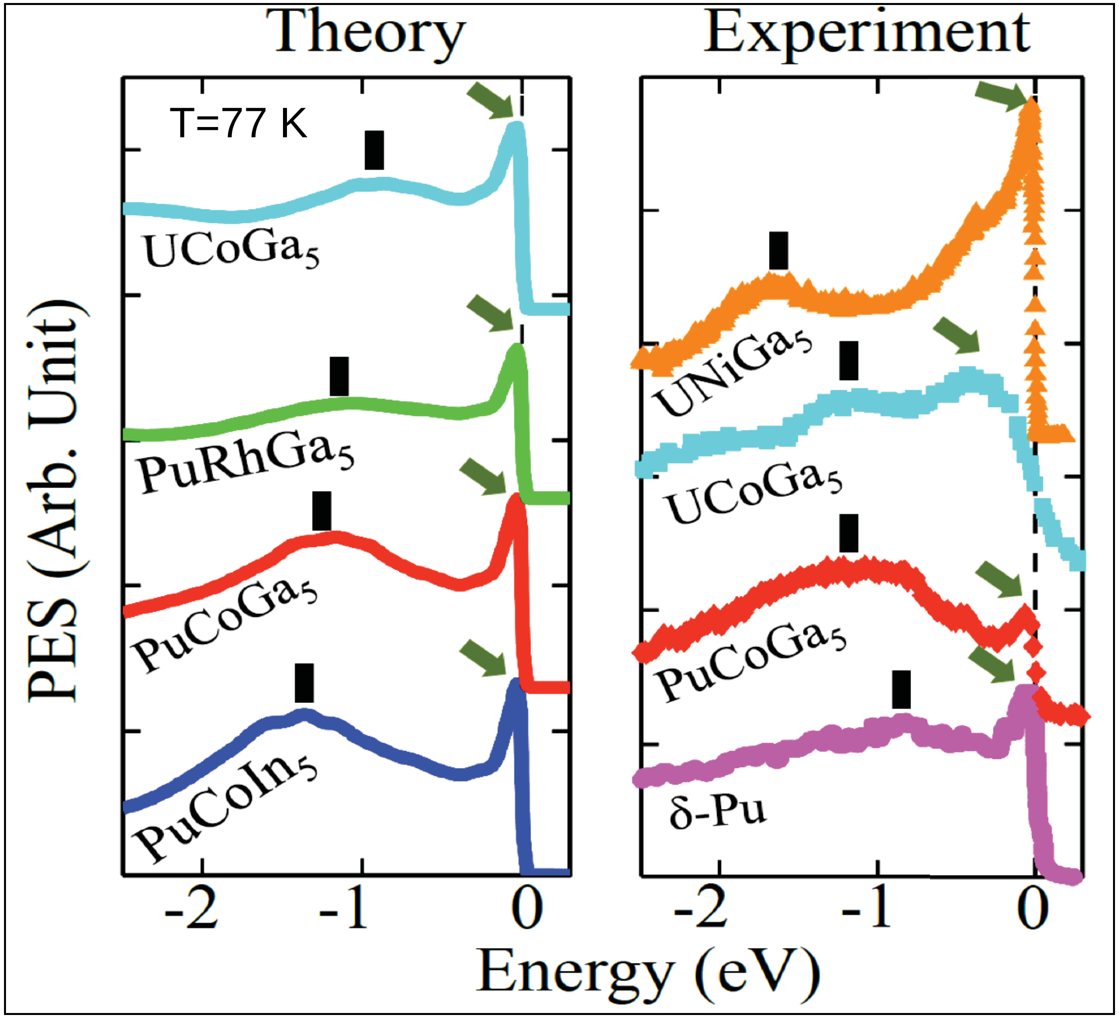
(Das, Zhu, Durakiewicz, Joyce, Graf; submitted to MRS)

Universality of electronic hot spots in actinide metals

Peak-dip-hump

=

hot spots of 1D spectral function

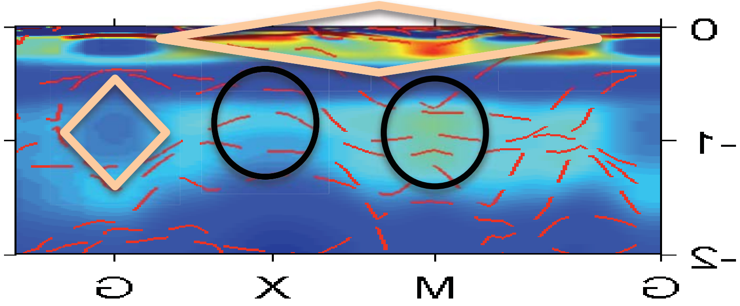


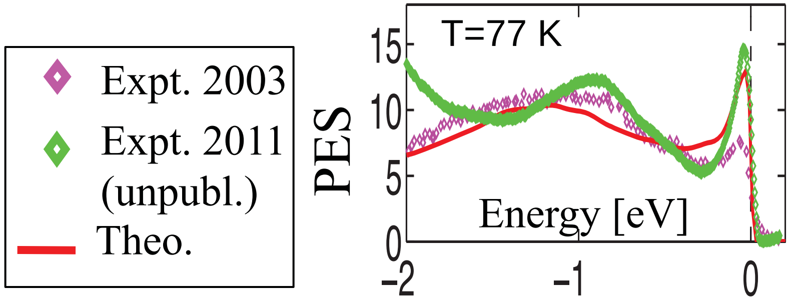
(Das, Zhu, Durakiewicz, Joyce, Graf; submitted to MRS)

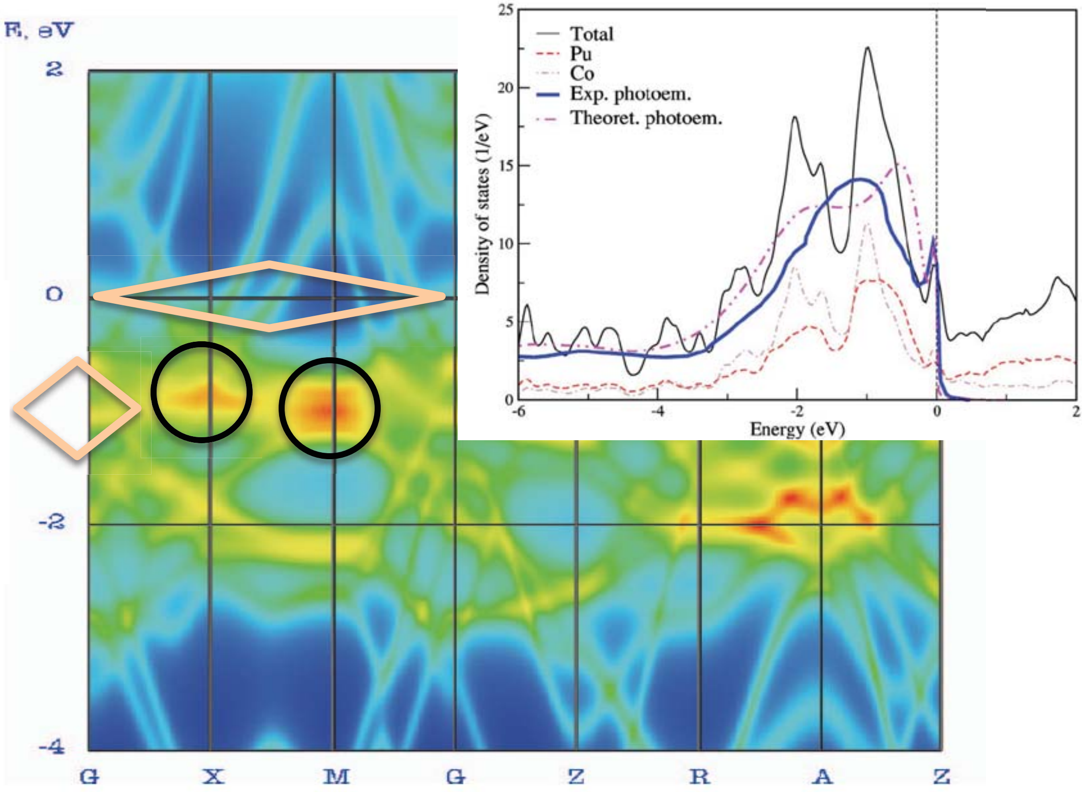
Comparing FEA with DMFT method in $PuCoGa_5$

- Different self-energies give rise to different hot spots
- Validation of methods through experiment is crucial

○ agreement
◇ disagreement



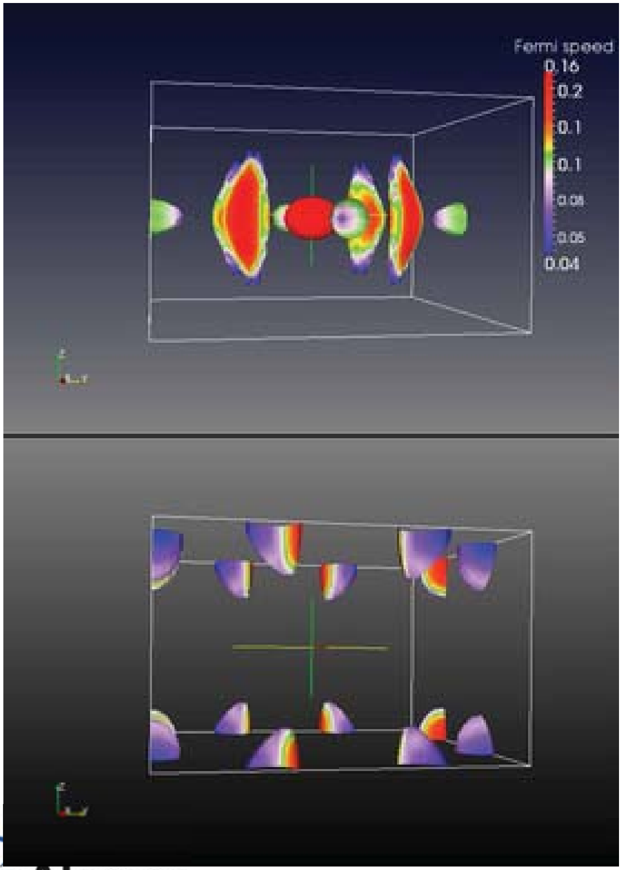




Pourovskii, Katsnelson, Lichtenstein PRB **73**, 060606(R) (2006)

Connecting hot spots to Fermi surface topology

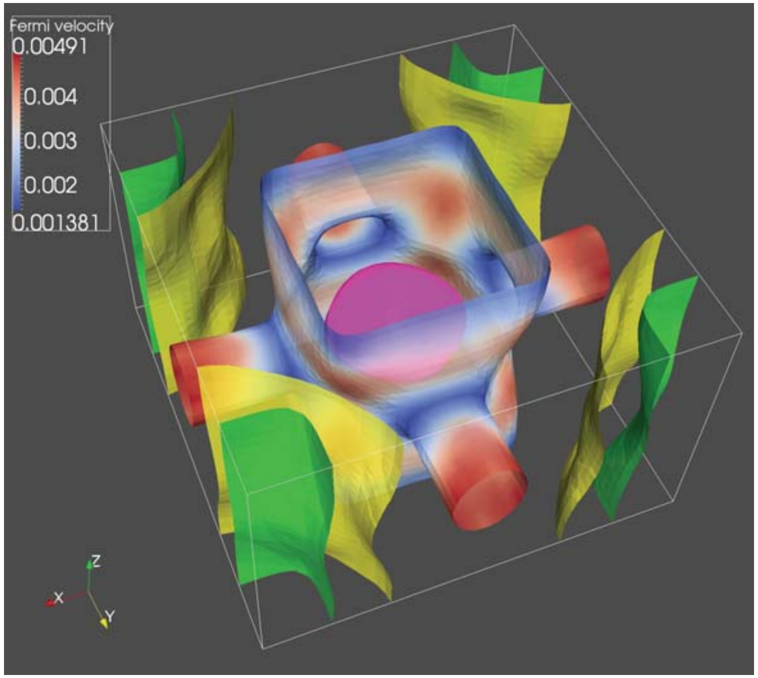
$UCoGa_5$
(2 bands)



Very different fermiology, but similar hot spots due to spin fluctuations between spin-orbit split states

(see poster by Zhu)

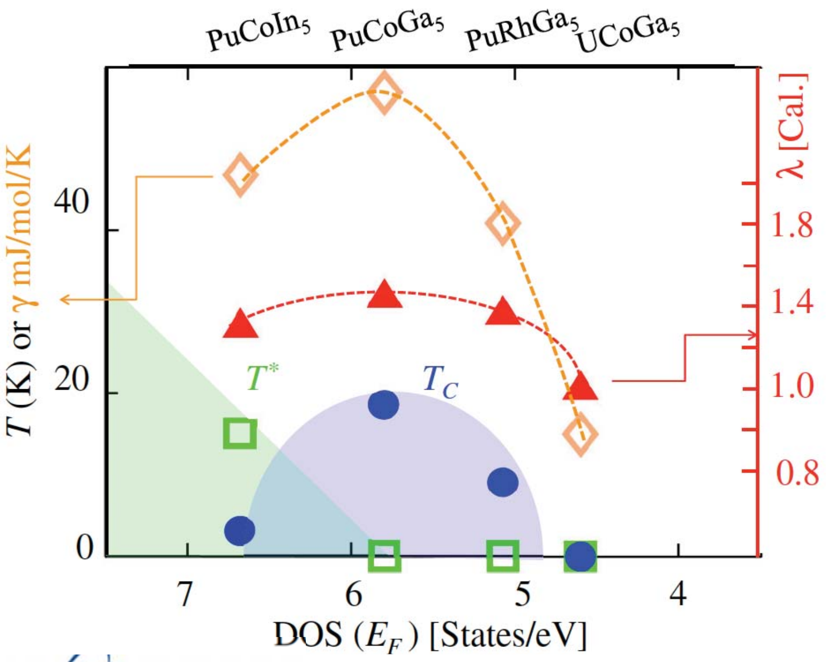
$PuCoGa_5$
(4 bands)

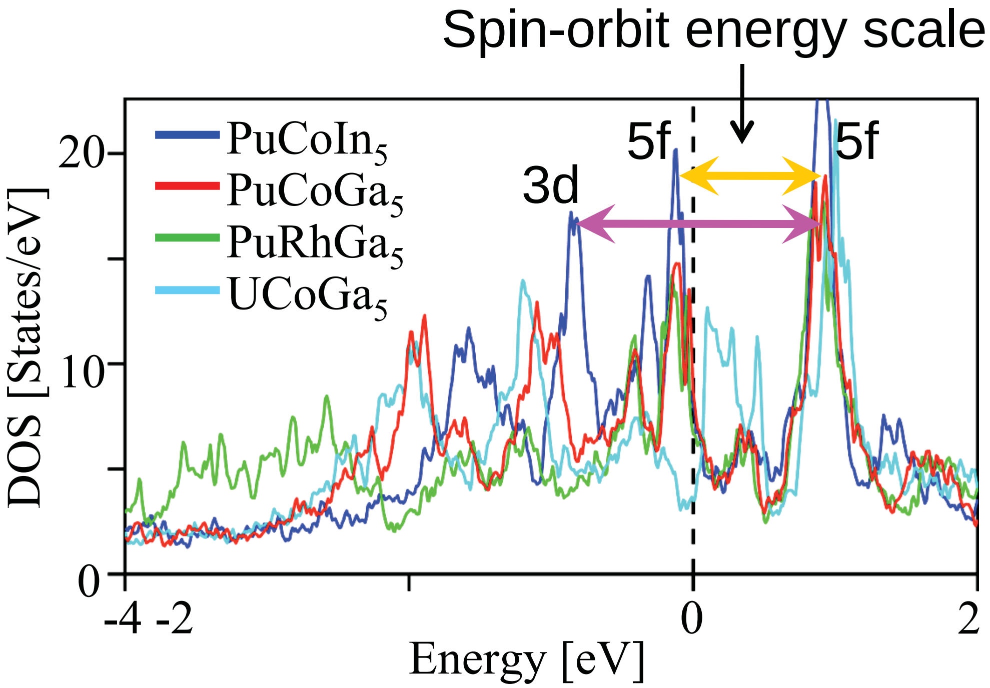


(Das, Zhu, Graf; unpublished)

Connecting hot spots to functionality

- **Mass renormalization due to hot spots near Fermi energy**
- **Superconductivity controlled by which hot spots?**



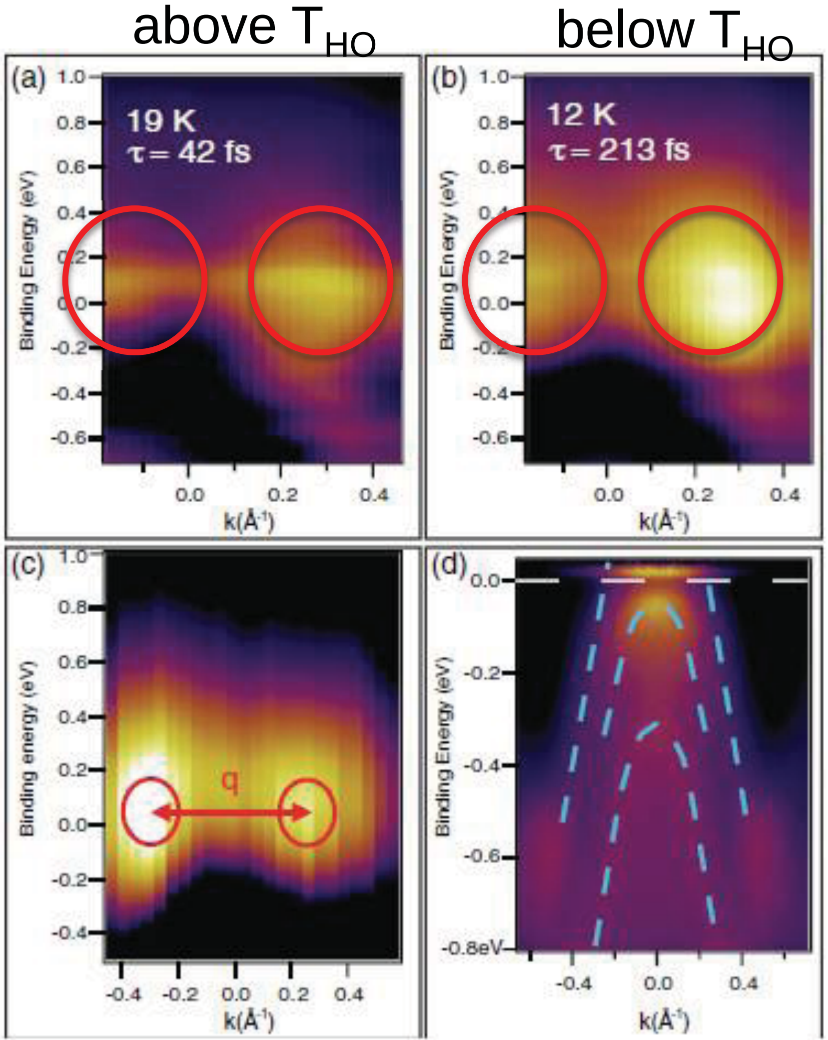


Connection with ultrafast time-resolved ARPES

- **Ultrafast hot spot dynamics in URu_2Si_2**

(see poster by Durakiewicz)

A ‘first’ in f-electron systems (Dakovski, …, Durakiewicz, PRB **84**, 161103 (2011))



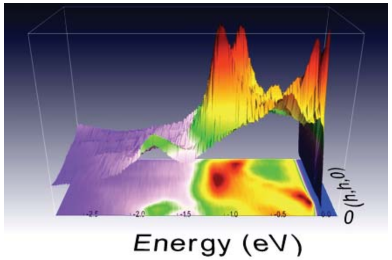
- Probing the hidden order phase transition
- Pumping the unoccupied f states
- Electronic hot spots change across phase transition
- Massive renormalization and change in quasiparticle lifetime

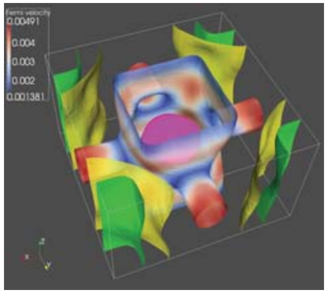
Direct measurement of correlation self-energy:

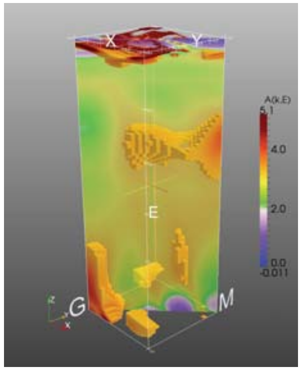
$$\boxed{1/\tau \sim \mathrm{Im}\,\Sigma}$$

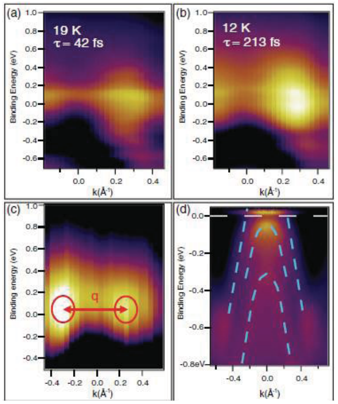
Summary and outlook

- We are developing capabilities and tools for sequencing of hot spots in actinides and correlated electron systems
- We are developing computational and experimental tools needed that are adequate to study the complexity of real materials
- Fluctuations integrated with first-principles methods offer an alternate path for treating dynamic correlations
- Validation of theory through experiment is essential to accelerate discovery and capability development









Magnetic Non-Uniformity in $(La_{0.4}Pr_{0.6})_{0.67}Ca_{0.33}MnO_3$ Films and Measurement of the Strain-magnetization Coupling Coefficient

M.R. Fitzsimmons (LANSCE-Lujan Center); S. Singh (Bhabha Atomic Research Center; T. Lookman (T-4), M. Hawley (MST-7); J.D. Thompson (MPA-CMMS); H. Jeen (ORNL); M.A. Roldan (Universidad Complutense de Madrid); M. Varela (ORNL); A. Biswas (University of Florida)

We have characterized the non-uniformity of chemical and magnetic properties of $(La_{0.4}Pr_{0.6})_{0.67}Ca_{0.33}MnO_3$ (LPCMO) films grown on $NdGaO_3$ using polarized neutron reflectometry (PNR). Our data indicate that the films exhibit coexistence of different magnetic phases as a function of depth. The variation of magnetism with depth is correlated with a variation of chemical composition with depth. Using PNR we also measured the magnetization depth profile of the LPCMO film as a function of applied bending stress. From these measurements we were able to obtain values for the coupling coefficients relating strain to the variation of the magnetization depth profile. Our results suggested that application of elastic compressive (tensile) bending stress increases (suppresses) magnetization. We will discuss the implications of our results on the prevailing theories of the role of strain on phase separation in manganites.

Work was supported by the Office of Basic Energy Science, U.S. Department of Energy, BES-DMS funded by the Department of Energy's Office of Basic Energy Science and the National Science Foundation (DMR-0804452) (HJ and AB). Los Alamos National Laboratory is operated by Los Alamos National Security LLC under DOE Contract DE-AC52-06NA25396.

Ultrafast Optical Probes of Coupled Systems

*R.P. Prasankumar, S.A. Trugman, J. Lee, Y.-M. Sheu, J. Qi, Q.X. Jia, Y.-S. Park, D. Talbayev, D.A. Yarotski (MPA-CINT); C.D. Batista (T-4); C.L. Zhang, Z. Lee, H.T. Yi, S.-W. Cheong (Rutgers University); X.S. Xu (Oak Ridge National Laboratory); J. Bonca (J. Stefan Institute);
A.J. Taylor (MPA-DO)*

A variety of interesting materials, such as high-temperature superconductors, colossal magnetoresistance manganites, and multiferroic oxides display strong coupling between the different order parameters (e.g., magnetic, lattice, and electronic) that govern their properties. To fully understand these unique materials, advanced experimental and theoretical techniques capable of dynamically unraveling the interplay between these degrees of freedom on an ultrafast timescale are needed. Here, we theoretically treat the quantum dynamics of electron-phonon coupled systems far from equilibrium, beginning with a Hamiltonian and solving the time-dependent Schrodinger equation in a many-body Hilbert space. Aided by the insight obtained from these theoretical studies, we then use ultrafast optical spectroscopy (UOS) to experimentally study the coupling between magnetic, electronic, and phonon degrees of freedom in multiferroic oxides.

As a first example, we studied the canonical multiferroic oxide $BiFeO_3$ (BFO), which has enormous potential for applications since it is both ferroelectrically and antiferromagnetically ordered at room temperature. Our UOS experiments revealed the timescale for carrier relaxation and potential coupling to spin and phonon degrees of freedom. We also observed photoluminescence from BFO for the first time, revealing the important role of radiative recombination in carrier relaxation.

In a second example, UOS was also used to study the multiferroic oxide $LuFe_2O_4$, which has strong magnetoelectric (ME) coupling originating from charge order near room temperature. These experiments revealed that quantum charge fluctuations may be the mechanism underlying ME coupling in this material. Overall, our studies demonstrate the utility of UOS in probing the coupling between different order parameters in coupled systems on an ultrashort timescale.

Electronic Inhomogeneity in Heavy Fermion Materials

E.D. Bauer, X. Lu, C. Miclea, F. Ronning, V. Sidorov, R. Movshovich, J. Thompson, (MPA-CMMS); T. Park (Sungkyunkwan University); Y. F. Yang (Institute of Physics); M. Graf, A. Balatsky, I. Martin (T-4); Z. Fisk (UC-Irvine)

We present two new results exploring electronic inhomogeneity in heavy fermion materials. In $CeRhIn_5$, a significant temperature difference between resistively and thermodynamically determined transitions into the superconducting state is observed in its coexistent antiferromagnetism and unconventional superconducting phase under pressure. Anisotropic transport near the superconducting transition reveals the emergence of textured superconducting planes that appear without a change in translational symmetry of the lattice. $CeRhIn_5$ is not unique in exhibiting these behaviors, indicating that textured superconductivity may be a general consequence of coexisting orders in correlated electron materials.

We have also discovered a new manifestation of electronic inhomogeneity in a strongly correlated f-electron system, using $CeCoIn_5$ as an example. A thermodynamic analysis of its superconductivity shows that nonmagnetic impurities (Y, La, Yb, Th, Hg and Sn) locally suppress unconventional superconductivity, generating an inhomogeneous electronic “Swiss cheese” due to disrupted periodicity of the Kondo lattice. Our analysis may be generalized to include related systems, suggesting that electronic inhomogeneity should be considered broadly in Kondo lattice materials.

New Capabilities at MPA: Ultrafast Quasiparticle Dynamics in Actinides

T. Durakiewicz, Y. Li, E.D. Bauer (MPA-CMMS); G.L. Dakovski, S.M. Gilbertson, G. Rodriguez (MPA-CINT); A.V. Balatsky, J.-X. Zhu, S.A. Trugman (T-4); K. Gofryk (MST-6); P.H. Tobash (MST-16); A. Taylor (MPA-DO); J.L. Sarrao (SPO-SC); P. M. Oppeneer (Uppsala Univ.); P.S. Riseborough (Temple Univ.); Y.Q. An, S.D. Conradson (MST-8)

Every time we add a new dimension to an experimental method, we open a window to novel, unexpected and fascinating phenomena. Here we show the results of our focused effort of adding time-domain to the powerful experimental techniques of Angle Resolved Photoelectron Spectroscopy (ARPES) and reflectivity. The novel tools are applied to actinides and help us understand the details of the electronic structure of the correlated f-electron materials.

In the famous hidden order system URu_2Si_2 we investigate the massive renormalization of the Fermi surface at specific k values. The application of time-resolved ARPES allowed a direct measurement of the momentum-resolved quasiparticle lifetime which was shown to increase by an order of magnitude at the hidden order transition. Time-resolved ARPES together with the ultrafast reflectivity results provided evidence for forming a multiple gap structure, including the hybridization gap, pseudogap and HO gap. The work was published so far in: PRB **84**, 161101(R) (2011); PRB **84**, 161103(R) (2011); PRB **84**, 241102(R) (2011).

The novel femtosecond pump-probe methods provide unique information about the dynamics of 5f quasiparticles, and open novel possibilities in addressing the long-standing questions about the role of near-Fermi level band renormalization in establishing the physical properties of the correlated materials.

First Observation of ^{239}Pu Nuclear Magnetic Resonance

H. Yasuoka, G.Koutroulakis, H. Chudo, E.D. Bauer, J. D. Thompson (MPA-CMMS); S. Richmond, A.I. Smith (MST-16); D.K. Veirs (MET-1); G.D. Jarvinen (Seaborg); D.L. Clark (INST-OFF)

The spin-1/2 plutonium-239 nucleus in principle should be active in nuclear magnetic resonance spectroscopy. However, its signal has eluded detection for the past fifty years. Here, we report observation of a ^{239}Pu resonance from a solid sample of plutonium dioxide, PuO_2, subjected to a wide scan of external magnetic field values ($B_0 = 3$ to 8 T) at a temperature of 4 Kelvin. By mapping the external field dependence of the measured resonance frequency, we determined the nuclear gyromagnetic ratio $^{239}\gamma_n(PuO_2)/2\pi$ to be 2.856 ± 0.001 MHz/T. Assuming a free-ion value for the Pu^{4+} hyperfine coupling constant, we estimated a bare $^{239}\gamma_n/2\pi$ value of approximately 2.29 MHz/T, corresponding to a nuclear magnetic moment of $\mu_n \approx 0.15\mu_N$ (where μ_N is the nuclear magneton).

Our finding puts an end to a fifty-year long search for Pu NMR and opens new frontiers for the study of plutonium in the fields of solid state physics, chemistry, and nuclear materials science. In view of the technological importance of plutonium compounds in nuclear fuels, power generation for interplanetary exploration, and long-term storage of nuclear wastes, the ability to probe local structure, nuclear spin-relaxation processes, and electronic environment of the nucleus by ^{239}Pu NMR should prove particularly powerful.

Localized Anharmonic Rattling of Al Atoms in VAl_{10}

D. Safarik (MST-6); T. Klimczuk (MST-8, now Institute for Transuranium Elements); A. Llobet (LANSCE-LC); D. Byler (MST-8); J. Lashley (MST-6); J. O'Brien, N. Dilley (Quantum Design)

In the present study we used diffraction, thermodynamic, and transport measurements to study the rattling of the Al guest atoms in VAl_{10}. The mean-square displacement of the rattling atom shows an unusual concave-down temperature dependence. This is characteristic of an anharmonic vibration whose frequency increases with amplitude, akin to a particle in a box. We find that the rattling is best described in terms of a sixth-order interatomic potential, with negligible contributions from harmonic and quartic terms. The rattler has a low characteristic temperature of $\theta_{RM} = 21$ K, and couples strongly to the acoustic phonons and conduction electrons. The strong coupling is clear from the large value of the Grüneisen parameter, which reaches $\Gamma \approx 43$ at 5 K. Below 6 K the electrical resistivity varies as T^3, which we explain in terms of electron scattering from damped sixth-order vibrations. We also find VAl_{10} to be a weak-coupling, type-II superconductor with $T_c = 1.53$ K and an upper critical field of $H_{c2} = 800$ Oe. Our results suggest that the effect of rattling on physical properties depends on the particular *shape* of the anharmonic potential. Manipulating the rattling site chemistry and geometry is therefore one possible avenue to controlling functionality.

Artificial Spin Ice: Frustration by Design and Magnetic Monopoles

C. Nisoli (T-4); X. Ke (ORNL); R.F. Wang, J. Li, V. Crespi, P. Schiffer (Penn State)

Frustration is ubiquitous in the physical sciences, and nowhere does it occur more simply, and has it been studied in more detail, than in correlated spin systems. In disordered magnetic materials it leads to spin-glass phenomena, in highly ordered materials, geometrical frustration has opened a window on a wide range of fundamentally new exotic behaviors. In spin ice in particular, the spin system appears to retain macroscopic entropy even in the low temperature limit and enters a topological "Coulomb phase". In the past five years, a new manifestation of frustrated magnetism has emerged in the "Artificial Spin Ice" materials. These systems are lithographically created from thin ferromagnetic films to consist of nanoscale structures that define individual ferromagnetic domains, whose geometry is chosen such that the magnetostatic interactions among the domains are frustrated. They have opened new possibilities in the study of frustrated magnetism, since the moments can be individually observed and their interactions can be tailor-designed. Experimental studies have unearthed intriguing connections to the out-of-equilibrium physics of disordered systems and non-thermal 'granular' materials, while revealing strong analogies to spin ice materials and their magnetic monopole excitations. Continuous synergy between experiments and theory is facilitated by connections to classic models of frustrated magnetism, hitherto little-studied aspects of which find an experimental realization in these systems.

First-Principles Theory for Correlated Electron Materials

J.-X. Zhu (T-4); R. Yu (Rice University); M. J. Graf, A.V. Balatsky (T-4); S. Qi (Rice University)

Emergent phenomena in correlated electron materials arise from competing interactions between various degrees of freedom. To enable a controlled design of materials with desirable electronic functionalities, a full understanding of dynamic correlation effects and their resulting electronic properties is needed. For that purpose, we develop theoretical methods to explore emergent phenomena in these materials. The methods are based on the integration of density functional theory with low-energy effective models and quantum many-body approaches to incorporate self-consistently electron-electron correlations by including DMFT and FLEX methods.

We applied this suite of new theoretical and modeling capabilities to recently discovered iron-based superconductors and plutonium-based superconductors. In our first example, we present electronic structure calculations for $La_2O_2Fe_2OSe_2$, which show band narrowing due to an expanded lattice as compared with the iron pnictides. The enhanced electronic correlations promote the Mott localization of electrons, which is also evidenced experimentally. The spin exchange parameter values are evaluated from the first-principles total energy calculations. These values allow us to place the compound in a magnetic phase diagram.

Our second example is the study of electronic properties in the newly discovered $K_{0.8}Fe_{1.6}Se_2$ compound. It shows that electronic correlations can also be enhanced by the presence of iron vacancy order. The close proximity to the Mott insulating state motivates us to use a strong-coupling model to discuss the superconducting pairing symmetry in this series of compounds. Based on these results, we propose to measure the local electronic states around a single non-magnetic impurity to identify the pairing symmetry.

As a third example, we present results of our LDA+DMFT study of the electronic structure and band renormalization in the superconductor $PuCoIn_5$ in comparison to $PuCoGa_5$, Here, we establish trends between electronic properties and functionalities in an attempt to understand why the former system has a lower superconducting transition temperature.

Materials Capability Review Committee Members

GARY S. WAS
Committee Chairperson
University of Michigan

Gary S. Was received his ScD from MIT in 1980. He is the Walter J. Weber, Jr. Professor of Sustainable Energy, Environmental and Earth Systems Engineering, and holds appointments in nuclear engineering and radiological sciences, and materials science and engineering at the University of Michigan. His research is focused on materials for advanced nuclear energy systems and radiation materials science, including environmental effects on materials, radiation effects, ion beam surface modification of materials and nuclear fuels. He has worked extensively in experiments and modeling of the effects of irradiation, corrosion, stress corrosion cracking and hydrogen embrittlement on iron- and nickel-base austenitic alloys. He has led the refinement of models for radiation induced segregation to account for composition dependent processes, and developed the first comprehensive thermodynamic and kinetic model for chromium carbide formation and chromium depletion in nickel-base alloys. Most recently his group has led the development of proton irradiation as a technique for emulating neutron irradiation effects in reactor structural materials and has conducted some of the first stress corrosion cracking experiments of austenitic and ferritic alloys in supercritical water. He has published more than 340 papers in archival journals or refereed conference proceedings, and a graduate textbook on radiation materials science. He is a Fellow of the American Nuclear Society, ASM International, NACE International and the Materials Research Society.

BARBARA JONES
Committee Vice Chairperson
IBM Almaden Research Center

Barbara Jones received her PhD in physics from Cornell University in 1988. She is the group leader of Theoretical and Computational Physics at IBM Almaden Research Center. Her research interests include analytic and computational studies of strongly correlated electrons and quantum magnetism especially at the atomic scale, current-induced magnetization reversal and spin torque, Griffiths phase and disorder effects in heavy fermions, and the thermodynamics of viral evolution. Jones has served on several committees including the National Academies Solid State Sciences as chair, *Phys. Rev. B* editorial board, and the Argonne Center for Nanoscale Materials Advisory Board.

DIMITRI BASOV
University of California, San Diego

Dimitri Basov serves as the chair of the Department of Physics, UCSD. He received his PhD from the Lebedev Physics Institute, Academy of Sciences of Russia in 1991. His research employs infrared spectroscopy to investigate novel physics of novel electronic and magnetic materials. “Infrared” here is used colloquially since in fact the instruments allow them to cover much broader frequency range extending continuously from sub-THz to UV light. Current research directions include: physics of strongly correlated electron systems, magnetic semiconductors, molecular and organic nano-electronics, electromagnetic metamaterials, and charge dynamics in grapheme. Basov is a Fellow of the American Physical Society and has received the Humboldt Research Award (2009) and the Frank Isakson Prize (2012.)

MICHAEL KAUFMAN
Colorado School of Mines

Michael Kaufman joined the CSM faculty as professor of metallurgical and materials engineering and director of the electron microscopy laboratory. He received his BS in metallurgical engineering from the University of Illinois in Urbana-Champaign and subsequently worked as a research engineer at the United Technologies Research Center where he also attended the University of Connecticut. He then returned to the University of Illinois for his PhD in metallurgical engineering and subsequently worked for two years in the Metallurgy Division at the National Institute of Science and Technology (formerly NBS) in Gaithersburg, MD. Thereafter, he was appointed an assistant professor of materials science and engineering at the University of Washington where he spent three years before joining the faculty in materials science and engineering at the University of Florida where he spent 14.5 years in various capacities including associate chair. Kaufman than relocated to the University of North Texas as chair of the Materials Science and Engineering Department where he also served as interim director of UNT's Center for Advanced Research and Technology. His primary research interests are in the area of structure-property-processing relationships in metals, intermetallics and composites, conventional and rapid solidification—all with an emphasis on characterization using advanced analytical techniques, particularly analytical and high resolution transmission electron microscopy. Kaufman has more than 100 publications, has mentored 19 PhD and 23 MS students and has managed research grants of over $5M from both federal sources (AFOSR, ONR, ARL, NSF, and DOE) and private companies (GM, Alcoa, GE, Howmet, etc.) He is a Fellow of ASM and a professional engineer.

RICHARD LESAR
Iowa State University

Richard LeSar has served as chair and professor of the Department of Materials Science and Engineering at Iowa State University since 2006. He received his PhD in chemical physics from Harvard and his BS in chemistry from the University of Michigan. His work focuses on the development and application of theory, modeling, and simulation of materials structures and properties. He has interest in modeling at many scales, with recent applications of electronic structure calculations (perovskites), atomistic simulations (molecular and metallic systems) and mesoscale simulations (dislocation dynamics). His work is currently focused in two areas: (1) employing dislocation simulations to guide the development of new theories of plasticity and (2) development of coarse-grained descriptions of biomolecules for simulating large-scale molecular processes. He is a member of the US Air Force Scientific Advisory Board, member of the editorial board of the *Annual Reviews of Materials Research* and has served as an editor of *Computational Materials Science*. LeSar served as the co-chair of the Gordon Conference on Physical Metallurgy in 2004. He received the Associated Western Universities (AWU) Department of Energy Distinguished Lecturer "Grand Challenges in Computational Materials Science" award in 1995, the NATO Travel Award in 1985, the Gomberg Prize in Chemistry from the University of Michigan in 1974, and was the James B. Angell Scholar at the University of Michigan in 1974.

JEFFREY LYNN
National Institute of Standards and Technology

Jeffrey Lynn is a NIST Fellow and team leader for Condensed Matter Physics in the NIST Center for Neutron Research at the National Institute of Standards and Technology in Gaithersburg, MD. His primary responsibilities are in the area of condensed matter physics research, and for the triple-axis neutron spectrometers at the NCNR. He is responsible for the new BT-7 double-focusing thermal triple axis instrument recently commissioned, and for a second new thermal triple axis instrument under development. He also has a longstanding relationship with the University of Maryland, and is an adjunct professor of physics. He received his PhD in physics from the Georgia Institute of Technology in 1974.

CHRISTINE ORME

Lawrence Livermore National Laboratory

Christine Orme is a senior scientist at Lawrence Livermore National Laboratory working in the Physical and Life Sciences Directorate. She received her PhD in physics from the University of Michigan. Orme is a Fellow of the American Physical Society and won the Presidential Early Career Award for Science and Engineering (PECASE) and the Office of Science Early Career Scientist and Engineer Award. She was elected to the Materials Research Society Board of Directors and is involved in planning and organizing many programs and conferences. Her research interests are in shape control in metal and metal-oxide nanostructures, biomineralization, biomimetic synthesis, physics of assembly, corrosion, and *in situ* methods for investigating interfacial dynamics.

THOMAS P. RUSSELL

Air Force Office of Scientific Research

Thomas P. Russell, a member of the Senior Executive Service, is director of the Air Force Office of Scientific Research, Arlington, VA. He guides the management of the entire basic research investment for the Air Force. Russell leads a staff of 200 scientists, engineers, and administrators in Arlington and foreign technology offices in London, Tokyo, and Santiago, Chile. Each year, AFORSR selects, sponsors, and manages revolutionary basic research that impacts the future Air Force. AFOSR interacts with leading scientists and engineers throughout the world to identify breakthrough opportunities; actively manages a $510 million investment portfolio encompassing the best of these opportunities; and transitions the resulting discoveries to other components of the Air Force Research Laboratory, to defense industries and to other federal agencies. The office's annual investment in basic research is distributed among more than 200 academic institutions, 150 businesses, and 200 research efforts within the AFRL. Russell's government career began as a research scientist at the Naval Surface Warfare Center, White Oak Laboratory, Md. In 1994, he joined the Naval Research Laboratory, serving as a research scientist and head of the High-Energy Materials Section within the Chemistry Division. In September 2000, he was assigned to the Naval Surface Warfare Center, Indian Head Division, where his assignments included director, Chemistry and Detonics Division, Research Department; head, Research and Technology Department; acting technical operations manager; and head, Research, Development, Testing and Evaluation Directorate. In August 2006, he was selected as the director of the Aerospace and Material Sciences Directorate, AFOSR. He was responsible for the Air Force basic research program in aerospace, chemical and material sciences. Russell has been a visiting scientist at the National Institutes of Standards and Technology, an adjunct professor at the Washington State University Shock Dynamics Laboratory, and a part-time faculty member at Montgomery College. His principal fields of interest are energetic materials, decomposition/combustion chemistry, detonation physics/chemistry, high-pressure chemistry/physics, and spectroscopy. He has authored more than 100 publications and inventions in these areas. Russell was appointed to the Senior Executive Service in 2006. He earned his PhD in chemistry from the University of Delaware in 1990.

ADAM SCHWARTZ
Lawrence Livermore National Laboratory

Adam Schwartz is the division leader for Condensed Matter and Materials Division in the Physical and Life Sciences Directorate at the Lawrence Livermore National Laboratory in Livermore, California. His research focuses on the fundamentals of plutonium aging, phase transformations and phase stability of Pu alloys, electronic structure of actinide elements, and dynamic properties of materials. These research efforts are supported by the National Nuclear Security Administration. He holds BS and MS degrees in metallurgical engineering from University of Pittsburgh, and a PhD degree in materials science and engineering from University of Pittsburgh. In addition to serving as the division leader, he is the deputy program leader for Dynamic Materials Properties within the Science Campaigns and the deputy program leader for physics and engineering models in the Advanced Simulation and Computing Program. Prior to these activities, he led the Plutonium Aging and Pit Lifetime Program at LLNL, was major technical effort leader for Pu aging, was principal investigator on numerous projects, and was a post-doctoral research associate at LLNL.

LANS Science and Technology Committee Representatives

ALEXANDRA NAVROTSKY
University of California, Davis

Alexandra Navrotsky is interdisciplinary professor of ceramic, earth, and environmental materials chemistry at the University of California, Davis. She holds an interdisciplinary appointment in the departments of chemical engineering and materials science; chemistry; land, air, and water resources; and geology. Her areas of specialization are physics and chemistry of minerals, geochemistry, solid-state chemistry, and materials science. Before joining UC Davis, Navrotsky was a professor in the Department of Geological and Geophysical Sciences at Princeton University and held the Albert G. Blanke Jr. Professorship in the Department of Chemistry. Earlier, she was a research associate at Technische Hochschule, Clausthal, Germany, Institut fur Theoretische Huttenkunde; a research associate in the Department of Mineralogy and Geochemistry at Pennsylvania State University; and then a faculty member in the Department of Chemistry at Arizona State University. Navrotsky was named Fellow of the Mineralogical Society of America, the American Geophysical Union, and the Geochemical Society and was elected to the National Academy of Sciences. She has received the Mineralogical Society of America Award and the Arizona State University Graduate College Distinguished Research Award. She has also served as president of the Mineralogical Society. She was named Doctor Honoris Causa of Uppsala University in Sweden.

ROCHUS (ROBBIE) E. VOGT
California Institute of Technology

Rochus (Robbie) E. Vogt is the R. Stanton Avery Distinguished Service Professor and professor of physics, emeritus at the California Institute of Technology (Caltech), where he began his service in1962. Vogt has served as chairman of the faculty, as chairman of the Physics, Mathematics, and Astronomy Division, and as vice president and provost at Caltech. A recipient of the NASA Exceptional Scientific Achievement Medal, Vogt was chief scientist at Caltech's Jet Propulsion Laboratory in 1977-78 and was acting-director of Caltech's Owens Valley Radio Observatory in 1980-81. He served as the director and principal investigator of the Caltech-MIT Laser Interferometer Gravitational-Wave Observatory (LIGO)

Project from 1987 to 1994. He is a US citizen, born near Heidelberg, Germany in 1929, studied as a Fulbright Fellow, and earned his doctorate in 1961 at the University of Chicago, which has honored him with the Alumni Association's Professional Achievement Award. Before coming to Caltech, he worked at the Enrico Fermi Institute for Nuclear Studies at the University of Chicago. His research career has focused on astrophysical aspects of cosmic radiation, gamma-ray astronomy, and gravitational-wave astronomy. Vogt has done extensive consulting work with government and industry. He has been a member of NASA's Physical Sciences Committee, and of the University of California (UC) Scientific & Academic Advisory Committee for the Los Alamos and Lawrence Livermore National Laboratories. He currently serves on the UC President's Council on the National Laboratories and chairs its Science and Technology Panel. He also serves on the LANS LLC Science and Technology Committee. He has served as vice chairman of the board of directors of the California Association for Research in Astronomy; he also serves on the board of directors of International Rectifier Corporation, a semiconductor company. In 1982, Vogt was honored as Caltech's first R. Stanton Avery Distinguished Service Professor. He and his wife Micheline live in Pasadena, California. They have two daughters.

Materials Capability Review Theme Leaders and Presenters

ALAN BISHOP

Science, Technology, and Engineering (PADSTE)
Principal Associate Director

Alan Bishop is an internationally recognized leader in theory, modeling, and simulation for condensed matter, statistical physics, and nonlinear science. In September 2011 he accepted the position of acting Principal Associate Director for Science, Technology, and Engineering for Los Alamos National Laboratory. As PADSTE, he leads the divisions of Chemistry, Life, and Earth Sciences; Engineering and Engineering Sciences; Experimental Physical Sciences; Information Technology; and Theory, Simulation, and Computation.

Bishop has made major contributions in the areas of soliton mathematics and applications, quantum complexity, structural and magnetic transitions, collective excitations in low-dimensional organic, inorganic and biological materials, and complex electronic and structural materials with strong spin-charge-lattice coupling.

A naturalized U.S. citizen, Bishop was born in Staffordshire, England and was educated at the University of East Anglia and the University of Cambridge where he earned a doctorate degree in theoretical solid state physics at the Cavendish Laboratory. After postdoctoral periods at Oxford, Cornell, and teaching at London universities, he came to work at Los Alamos Scientific Laboratory (LASL) in January 1979 taking a staff position in the Materials and Statistical Physics Theory group of the Theoretical Division. He was a founding member of the Los Alamos Center for Nonlinear Studies. After a two-year period as the acting/deputy chairman of the Center for Nonlinear Studies and 14 years as the group leader of the Condensed Matter Theory group at Los Alamos, he became the director of the Theoretical Division in August 1999. With the transition from the University of California to Los Alamos National Security, LLC, management of Los Alamos National Laboratory on June 1, 2006, Bishop became the associate director for Theory, Simulation, and Computation, encompassing the divisions of Computer, Computational, and Statistical Sciences; High Performance Computing; and Theoretical, as well as the Center for Nonlinear Studies.

He is a Fellow of the American Physical Society, The Institute of Physics, and the American Association for the Advancement of Science, a recipient of the Department of Energy's E.O. Lawrence Award, a Humboldt Senior Fellow, and a Los Alamos Laboratory Fellow.

ELLEN CERRETA

Materials Science in Radiation and Dynamic Extremes (MST-8)
Team Leader

Ellen Cerreta is a team leader in MST-8 and has been a technical staff member at Los Alamos within Structure/Properties Relations Group of the Materials Science and Technology Division since January 2003. Prior to that, she was a postdoctoral associate within the same division. Cerreta received her BS in aerospace engineering from The University of Virginia and her PhD in materials science and engineering from Carnegie Mellon University in 2001. Since coming to Los Alamos, she has focused on the correlation of microstructure to mechanical response of metals and alloys, with the support of BES, the national defense and energy programs, and Laboratory Directed Research and Development (LDRD). She is a member of the Mechanical Extremes Thrust in the Center for Materials in Irradiation and Mechanical Extremes EFRC. In 2010, Cerreta assumed the role of co-PI for an LDRD/DR project, "Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage". Finally, Cerreta is an adjunct faculty member in The Institute of Shock Physics at Washington State University and a recent member of the board of directors (Membership Director) of The Minerals, Metals, and Materials Society.

DAVID FUNK

Weapons Experiments (WX-DO)
Division Leader

David Funk came to the Laboratory as a postdoctoral fellow in 1989. After becoming a staff member in 1991, he has held positions as team leader (2001-05), deputy group leader (2005-06), program manager (2006-08), deputy division leader (2006-08), Campaign 2 (C2) program manager (2006-09), Dynamic Plutonium Experiments (DPE) program manager (2008-09), division leader of Hydrodynamic Experiments (2009-10), and is currently the division leader for Weapons Experiments (as well as the Hydro Program manager). His research interests have included unravelling the atomic and molecular scale details of detonation and shock physics; physics of reaction dynamics (chemical dynamics); controlling intramolecular energy redistribution; ultrafast laser technology; optical diagnostics; and the quantum mechanics of small molecular systems. Funk has published throughout his career (co-author of 89 papers and 5 book chapters; ~1100 citations which represents an h-index of 20). He holds two patents for his research and development work and was the chair of the topical group on the Shock Compression of Condensed Matter (2007). He has mentored 10 postdoctoral and undergraduate students and has been a principal investigator or co-investigator for several Laboratory Directed Research and Development projects. He holds a BS in chemistry (St. John's University, 1983) and a PhD in physical chemistry (University of Utah, 1988).

TIMOTHY C. GERMANN

Physics and Chemistry of Materials Group (T-1)
Scientist

Since joining Los Alamos in 1997, Timothy C. Germann has used large-scale classical molecular dynamics simulations to investigate shock, friction, detonation, and other materials dynamics issues using BlueGene/L, Roadrunner, Cielo, and other NNSA supercomputer platforms. He is Director of the ASCR "Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx)," and has led the high strain-rate team in the BES "Center for Materials in Mechanical and Irradiation Extremes (CMIME)," an Energy Frontier Research Center (EFRC).

Germann earned dual BS degrees (computer science & chemistry) from the University of Illinois at Urbana-Champaign in 1991, and a PhD in chemical physics from Harvard University in 1995, where he was a DOE Computational Science Graduate Fellow (performing a summer practicum in 1994 in the Center for Materials Science at LANL).

He has co-authored more than 130 peer-reviewed scientific publications with more than 2200 citations, and is chair-elect of the APS Division of Computational Physics. He has received an IEEE Gordon Bell Prize for high-performance computing (1998; also a finalist in 2005 and 2008), three LANL Distinguished Performance Awards (2005, 2007, and 2009), two NNSA Defense Programs Awards of Excellence (2006 and 2007), the LANL Fellows Prize for Research (2006), and the LANL Distinguished Copyright Award (2007); and is a Fellow of the American Physical Society (2011).

MATTHIAS J. GRAF

Physics of Condensed Matter and Complex Systems (T-4)
R&D Scientist

Matthias J. Graf is a condensed matter theorist in the group T-4 of the Theoretical Division at the Los Alamos National Laboratory. He has led various small investigator and large team LDRD projects, and mentored postdoctoral researchers and summer students.

His research interests include the theory of thermodynamic, transport, and electromagnetic properties, effective low-energy models for competing orders, and many-body effects in correlated electron systems. His work spans the fields of lattice dynamics, pair-density function analysis, ultrafast optical and angle-resolved photoemission spectroscopies, energy transfer in novel scintillators, heavy-fermion and high-temperature superconductors, vortex motion, as well as fundamental materials properties of actinides and plutonium. Matthias has served on or chaired several committees for the LDRD program office and the MaRIE planning. He authored over 80 peer-reviewed articles, published and submitted, with over 1,300 citations.

Graf received his PhD in theoretical condensed matter physics from the University of Bayreuth (Germany) in 1995. He started his scientific career with an appointment as a postdoctoral researcher at the Department of Physics and Astronomy at Northwestern University followed by an appointment in 1998 at the Center for Materials Science, LANL. He became a staff member in 2000.

NEIL HARRISON

National High Magnetic Field Laboratory – Pulsed Field Facility (NHMFL-PFF)
Condensed Matter and Magnet Science (MPA-CMMS)
Scientist

Neil Harrison has been at Los Alamos National Laboratory since 1996 and is a world leader in high magnetic field condensed matter research with approximately 3000 citations. He was a recipient of the Los Alamos Fellows Prize in 2005 and elected as a Fellow of the American Physical Society in 2006. Currently, Harrison in the principal investigator of the "Science at 100 tesla" Basic Energy Sciences project.

DANIEL HOOKS

Shock and Detonation Physics group, DE-9
Project Leader

Daniel Hooks is a scientist in the Shock and Detonation Physics group, DE-9. He is the project leader for High Explosives Science for NNSA Science Campaign 2, an experimental project focused on performance, safety, and materials development of energetic materials. His research interests are fundamental properties of molecular materials (including explosives) and crystal growth. Hooks earned materials science and engineering degrees at the University of Wisconsin – Madison (BS, 1995) and the University of Minnesota (PhD, 2000).

MICHAEL HUNDLEY

Condensed Matter & Magnet Science (MPA-CMMS)
Group Leader

Michael Hundley is group leader of Condensed Matter & Magnet Science (MPA-CMMS), Los Alamos National Laboratory's core experimental condensed matter group and home to the National High Magnetic Field Laboratory's Pulsed-Field Facility. Hundley received his PhD in condensed matter physics from the University of California, Berkeley in 1988. As a LANL Director's Postdoctoral Fellow he researched correlated electron physics in cuprate superconductors and Kondo insulators. Hundley was converted to full-time technical staff member in the Condensed Matter & Thermal Physics group in 1991. His research interests include correlated electron physics, magnetism, and heavy-fermion materials and his experimental expertise involves low-temperature investigation of thermodynamic and electronic transport properties. He is the co-author of more than 220 peer-reviewed publications that have been cited more than 7,000 times. He organized two MRS symposia focusing on the science and technology of magnetic transition-metal oxide compounds, and was lead editor for an MRS proceedings volume that resulted from one of those symposia.

BRIAN JENSEN

Shock and Detonation Physics (WX-9)
Team Leader

Brian Jensen is an experimental physicist and team leader in the WX-9 Shock and Detonation Physics group. He graduated from Washington State University's Institute for Shock Physics where his dissertation involved the use of dynamic x-ray diffraction to examine shock induced elastic-plastic deformation in LiF crystals at the atomic and continuum levels. In WX-9, his team focuses on the physics of materials (such as iron, cerium, and actinides) at extreme conditions, which includes equation-of-state, phase transitions and kinetics, strength, and structure. He has been a principle investigator for many projects including the Large-Bore Powder-Gun project – a highly visible experimental effort to be conducted at the Nevada Test Site U1a underground complex. Current research includes experiments to study of multiphase properties of cerium (equation-of-state, strength, and transition kinetics) and the development of an ultrafast (ns) experimental capability using dynamic Laue and phase contrast imaging at the Advanced Photon Source (Argonne National Laboratory). His work has been presented at numerous professional conferences and workshops and in print as peer-reviewed publications, laboratory reports, and conference proceedings.

DENIECE R. KORZEKWA

Nuclear Materials Science (MST-16)
Group Leader

Deniece Korzekwa is group leader of the Materials Science and Technology: Nuclear Materials Science group (MST-16) at Los Alamos National Laboratory. She has a BS in metallurgical engineering from the Colorado School of Mines and an MS in multidisciplinary engineering from Purdue University. Korzekwa started at LANL in 1986 and worked on the MST-6 foundry team where she served as the technical lead for a combined experimental and modeling program for casting and solidification processes until 2009 when she moved to MST-16. Her primary research interest has been on solidification and fluid flow modeling of uranium and plutonium casting processes. Much of her work has focused on better understanding and quantification of boundary conditions, especially those at the metal/mold interface and electromagnetic heating of mold assemblies.

CHARLES MCMILLAN

Los Alamos National Laboratory
Director

Charles McMillan has more than 22 years of scientific and management experience in weapons science and stockpile certification, hands-on experience in both experimental physics and computational science, and demonstrated success at balancing mission performance with security and safety. McMillan previously led the Laboratory's weapons physics organization since 2006, when Los Alamos National Security, LLC, began managing the Laboratory. Prior to joining the Los Alamos, McMillan served in a variety of research and management positions at Lawrence Livermore National Laboratory in California.

McMillan is married with three college-age children. He is an avid photographer and an accomplished musician, playing both the piano and organ as well as the recorder. His interest in early music dates back to his high school days when he considered majoring in music. Although he continues to perform ensemble music his intellectual fascination with science led him to study mathematics and physics and he continues to practice an active interest in astronomy and telescopes.

He holds a doctorate in physics from the Massachusetts Institute of Technology and a bachelor's degree in mathematics and physics from Columbia Union College. He has been awarded two DOE Awards of Excellence, one of which for development of an innovative holographic tool that enhances the ability to predict nuclear performance.

CHUCK MIELKE

National High Magnetic Field Laboratory – Pulsed Field Facility (NHMFL-PFF)
Condensed Matter and Magnet Science (MPA-CMMS)
Director
Deputy Group Leader

As the director of the National High Magnetic Field Laboratory – Pulsed Field Facility, Chuck Mielke draws more than 20 years of experience of research in condensed matter physics in high magnetic fields. Mielke received his PhD in condensed matter physics from Clark University under the advisement of Prof. C. C. Agosta. As part of Mielke's thesis research he built a 50 tesla pulsed magnet system in the early 1990s and used it to complete his PhD thesis research (in 1996) of the superconducting and normal state of organic molecule based superconductors and metals. Specializing in the determination of the Fermi surface of metals using pulsed magnetic fields which drew him towards the development of ultra-high field systems such as explosively driven flux compression generators and the "single-turn" method for reaching extreme magnetic fields well beyond 100 tesla. In 2003 Mielke became the Head of the Pulsed Field User Program for the NHMFL in Los Alamos. In 2009, Mielke became the interim director for the Pulsed Field Facility and was chosen to lead the facility full time. The NHMFL-PFF program consists of about 30 people whom are part of the group MPA-CMMS where Mielke also serves as the deputy group leader. The complexity of actinide behavior in high magnetic fields is currently an active area of his lab involvement today.

WILLIAM PRIEDHORSKY

Laboratory-directed Research and Development (LDRD-PO)
Program Director

William Priedhorsky has been on the staff of Los Alamos National Laboratory since 1978, and he was honored to be named a Laboratory Fellow in 1997. He is program director for the Laboratory-directed Research and Development program, a $140M/annual investment in flagship Laboratory research. His research interests include new technologies to stymie the spread of weapons of mass destruction, whether nuclear, chemical, or biological, as well as astrophysics.

Priedhorsky received a BA in physics summa cum laude and Phi Beta Kappa from Whitman College in 1973, and a PhD in physics, specializing in x-ray astronomy, from the California Institute of Technology in 1978. After joining Los Alamos as a staff member in 1978, he developed x-ray diagnostics for laser fusion research, and discovered copious hard x-rays from CO_2 laser-plasma interaction, which unfortunately boded poorly for the future of the Los Alamos laser fusion program. In 1981, he joined the Space Astronomy and Astrophysics Group, and discovered a wealth of eruptions and long-term cycles in cosmic neutron stars and black holes using data from the Los Alamos Vela 5B satellite, as well as developing instrumentation for the detection of nuclear materials in space. He discovered what was then the closest double star in the sky, and the novel phenomenon of quasi-periodic oscillations in the brightest x-ray star in the sky, Scorpius X-1. Notably, he led the development of photon-counting optical imagers for remote ultralow light imaging, a project that continues to this day as “Remote Ultralow Light Imaging.” He conceived and led the development of ALEXIS, Los Alamos’s first small satellite, launched in 1993, and the MOXE x-ray all sky monitor, which sadly never went to space, because of the collapse of the Russian space program after the fall of the USSR. From 1995 to 1999, he was lead project leader for Proliferation Detection Technology, responsible for the Lab’s projects in active and passive remote sensing, as well as Laboratory’s efforts in Hard and Deeply Buried Target Defeat. From 1999 to 2007 he was chief scientist in the Nonproliferation and International Security Division, the International, Space, and Response Divisions, and the Threat Reduction Directorate, responsible for the health of basic and applied research in space science, proliferation detection, treaty monitoring, nuclear safeguards, and international technologies. With Chris Morris of Physics Division, he originated the idea of using cosmic-ray muons to detect nuclear material. In 2005, he received the Leo Szilard Award of the American Physical Society for his part in their study of boost-phase missile defense, and was named a Fellow of the Society in 2006. Whitman College awarded him its alumnus of the year award in 1995. He has been a Max Planck Fellow, a visiting scientist at the Danish Space Research Institute, a Lyle Fellow at the University of Melbourne, Australia, and coordinator (elected head) of the Los Alamos National Laboratory Fellows. Priedhorsky is an avid outdoorsman and past president of the Los Alamos Mountaineers.

ANTONIO REDONDO

Theoretical Division (T-DO)
Division Leader

Antonio Redondo received a BSc in physics from Utah State University in 1971 and a MSc and PhD in applied physics from the California Institute of Technology in 1972 and 1977, respectively. He came to Los Alamos National Laboratory as a technical staff member in the Electronics and Electrochemical Materials and Devices group in 1983. He joined the Theoretical Division in 1994 as group leader of the Theoretical Chemistry and Molecular Physics group. During 2005 and 2006 he was group leader of the Theoretical Biology and Biophysics group in the Theoretical Division and became division leader in June 2006. He is an adjunct professor in the Computational Science Research Center at San Diego State University and in the Chemical Engineering Department at the University of California at Santa

Barbara. He is a Fellow of the American Association for the Advancement of Science and the World Technology Network. His current interests are in the development of mathematical and numerical models for soft matter and biomaterials properties; the development and application of mathematical and numerical methods for atomistic, coarse-grained and agent-based modeling of condensed matter system and modeling and simulation in biofuels.

JOHN L. SARRAO

Science Program Office-Office of Science (SPO-SC)
Program Director

John Sarrao is the program director for Los Alamos National Laboratory's Office of Science Programs, a $100M/y portfolio, and for MaRIE (Matter-Radiation Interactions in Extremes), LANL's signature facility concept that will provide transformational materials solutions for national security challenges. Since 2002, John has held leadership positions of increasing responsibility within LANL's materials community. He has also served on a number of US Department of Energy Basic Energy Sciences Advisory Committee (BESAC) subcommittees, helping to set strategic directions for materials research. Sarrao received his PhD in physics from the University of California, Los Angeles in 1993 based on thesis work performed at LANL. He returned to LANL as a technical staff member in 1997, following postdoctoral research with Zachary Fisk at the University of California, San Diego and the National High Magnetic Field Laboratory in Tallahassee, Florida. His primary research interest is in the synthesis and characterization of correlated electron systems, especially actinide materials. He is the coauthor of more than 520 publications, including 56 papers in *Physical Review Letters*, *Nature*, and *Science*. These publications have been cited more than 10,000 times (h=50). He was the 2004 winner of the LANL Fellows Prize for Research, in part for his discovery of the first plutonium superconductor and is a Fellow of the American Association for the Advancement of Science (AAAS), the American Physical Society (APS), and Los Alamos National Laboratory.

SUSAN SEESTROM

Experimental Physical Sciences (ADEPS)
Associate Director

Susan Seestrom brings to this position a combination of strong science credentials and management skills developed during her 20-year tenure at LANL. In her recent role as associate director of Weapons Physics, Seestrom led six LANL divisions that executed program work in experimental, simulation, and weapons physics assessment. She directed the major line organization responsible for carrying out research and development for the weapons program and technical work in support of stockpile certification and assessment. She oversaw the operation of complex facilities, including the Dual-Axis Radiographic Hydrodynamic Test Facility, the Los Alamos Neutron Science Center, and the U1a laboratory at the Nevada Test Site.

Previously, Seestrom led the Physics Division at LANL for three years after serving as a deputy group leader in the Neutron Science and Technology group. Seestrom's personal research efforts focused on nuclear structure with medium energy probes and fundamental physics with neutrons. Together with Laboratory scientist Tom Bowles, Seestrom led the effort to develop an ultracold neutron source that culminated in demonstration of the world's most intense source of such neutrons. She received a Distinguished Performance Award for this work in 2001.

Seestrom holds PhD and BS degrees in physics from the University of Minnesota. She has published 135 papers and has had 1,663 career citations. She is a Fellow of the American Physical Society.

ANTOINETTE (TONI) TAYLOR

Materials Physics and Applications (MPA-DO)
Division Leader

Antoinette Taylor is leader of the Materials Physics and Applications Division at LANL. Prior to this position she was director of the Center for Integrated Nanotechnologies, a joint Sandia/LANL Nanoscience Research Center funded through BES. Her research interests include the investigation of ultrafast dynamical nanoscale processes in materials and the development of novel optics-based measurement techniques for the understanding of new phenomena. She has published ~300 papers in these areas, written three book chapters and edited five books. She is a former director-at-large of the Optical Society of America, topical editor of *Journal of the Optical Society B: Optical Physics*, and member of the Solid State Science Committee, Board of Physics and Astronomy, the National Academies and chaired the National Academies' Committee on Nanophotonics Applicability and Accessibility. She is a vice-chair, Division of Laser Science of the American Physical Society and chairs the Joint Council of Quantum Electronics. She is a LANL Laboratory Fellow and a Fellow of the American Physical Society, the Optical Society of America and American Association for the Advancement of Science. In 2003, Taylor won the inaugural Los Alamos Fellows Prize for Outstanding Leadership in Science and Engineering.

DAVID F. TETER

Materials Science & Technology (MST-DO)
Division Leader

David Teter is the Materials Science and Technology (MST) division leader. MST Division provides world-leading, innovative, and agile materials science and technology solutions for national security missions.

After finishing his doctoral thesis at the University of Illinois in 1996, he began a postdoctoral Appointment at Los Alamos National Laboratory researching hydrogen storage and solid-state phase transformations in Pd-based alloys. In 1997 he was converted to a full-time technical staff member in the Metallurgy Technology group (MST-6). As a staff member, he expanded his research interests into the areas of alloy design, hydrogen storage, hydrogen-induced phase changes, solid-state phase transformations and aging phenomena of weapons materials.

In 2002 Teter became a weapons project leader for metals issues. In this role, he was responsible for the technical direction and planning of the program leading to several key decisions regarding material re-use and remanufacturing. This project led to his next role in 2006 as the project leader for the Enhanced Surveillance CSA/Case effort. The main focus of this program is to understand and quantitatively predict lifetimes of materials, components and assemblies. This project combines fundamental scientific research of aging mechanisms and kinetics with engineering assessments of performance.

Concurrently, Teter was the team leader for the Alloy Design and Development team from 2003 to 2005, which primarily investigated processing-structure-property relationships of materials as they relate to engineering and physics requirements. From 2005 to 2010, Teter was the deputy group leader of MST-6 where he led a diverse technical organization, which uses materials technology to support national security. Most recently he served as the MST deputy division leader from 2010 to 2012.

Teter also serves as the chair for the M4 (Making, Measuring and Modeling Materials) pillar of the Matter-Radiation Interaction in Extremes (MaRIE) experimental facility, which is vital to many national security challenges and is a critical component of the LANL Materials Strategy. The M4 control synthesis and design of materials, and address the decadal materials challenges of the future. Teter is also president of the Materials Science and Engineering Alumni Board at the University of Illinois.

DAVID WATKINS

Materials Physics and Applications (MPA-DO)
Deputy Division Leader

David Watkins is deputy division leader for the Materials Physics and Applications Division. Watkins got his BS in physics at New Mexico Tech, and his MS and PhD in physics from the University of Washington. He joined the staff at Los Alamos in 1979 to work on nonlinear optics for the laser fusion and isotope separation programs. He later worked on the Strategic Defense Initiative, exploring issues of high-power laser beam propagation through the atmosphere. As part of this effort, Watkins spent a year at the Royal Signals and Radar Establishment in Great Britain as part of a technical exchange on the Strategic Defense Initiative. Following this appointment, he returned to Los Alamos and became involved in the management of the Electronic and Electrochemical Materials Group (now MPA-11). To facilitate the energy research carried out in this group, Watkins developed and managed more than 20 cooperative research agreements with industry and played a key role in increasing the size of the fuel cell research program at Los Alamos. He next took on the challenge of program manager for Laboratory Directed Research and Development at Los Alamos. In this position, he worked to foster a strong program in basic research at LANL that enhances the scientific vitality of the Laboratory in critical, mission-relevant, areas of research and development. He returned to MPA Division with the goal of contributing to a leading research organization engaged in the critical issue of energy security.

VIVIEN ZAPF

National High Magnetic Field Laboratory - Pulsed Field Facility (NHMFL-PFF)
Condensed Matter and Magnet Science (MPA-CMMS)
Scientist

Vivien Zapf works on quantum magnetism and multiferroic behavior at the National High Magnetic Field Laboratory, part of the MPA-CMMS group. She completed her PhD at UCSD in 2003, was awarded a Milliken Postdoctoral fellowship at Caltech, and then joined LANL first as a Director's funded postdoc and then as a staff member in 2006. There she worked on quantum magnetism, establishing the existence of Bose-Einstein condensation in certain spin systems and developing thermodynamic measurement techniques at dilution refrigerator temperatures and 20 T. She went on to discover multiferroic behavior in new classes of organo-metallic materials and developed electric polarization measurements in fast pulsed magnetic fields. She is interested in the interplay between magnetism, electric properties and structure of materials. She is the recipient of the Lee Oscheroff Richardson prize in low-temperature physics and has published 75 papers with ~ 1000 citations. She currently serves as the P.I. on the LDRD/DR project "Understanding and Controlling Complex States Emerging from Frustration."