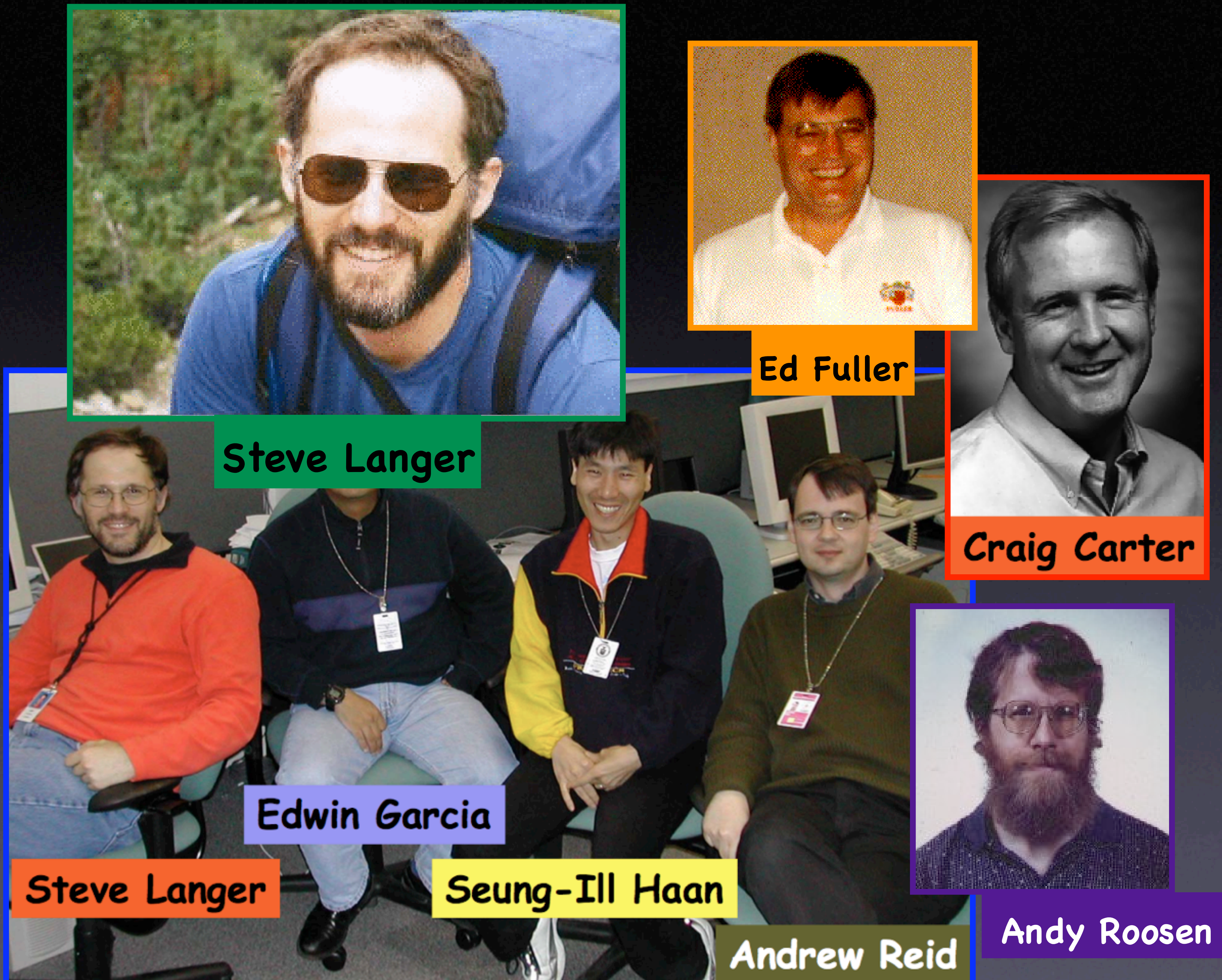
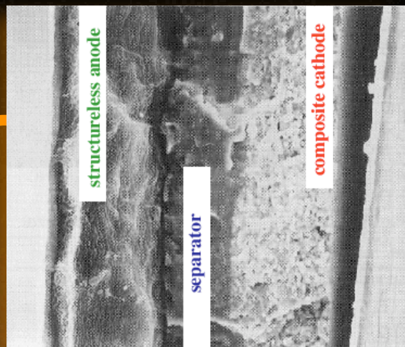
OOF Extensions and Applications to Multifunctional Materials and Devices: An Overview

R. Edwin García


Steve Langer
Ed Fuller
Craig Carter
Edwin Garcia
Steve Langer
Seung-Ill Haan
Andrew Reid
Andy Roosen

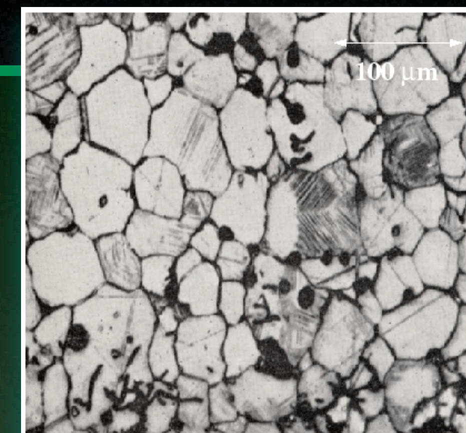
Outline

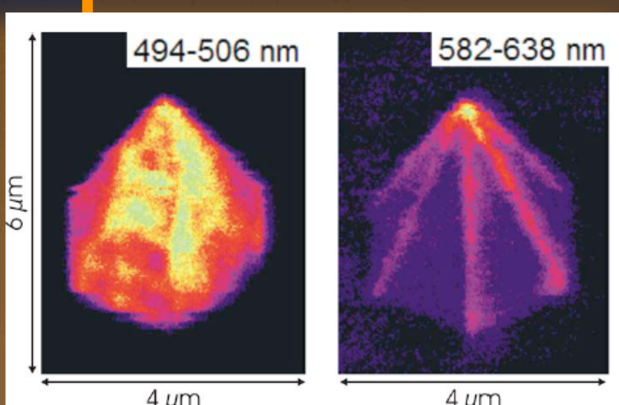
rechargeable batteries



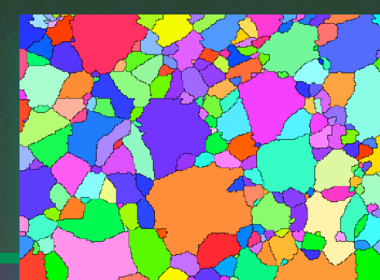
Energy Materials

piezoelectrics and electrostrictors





light emitting devices



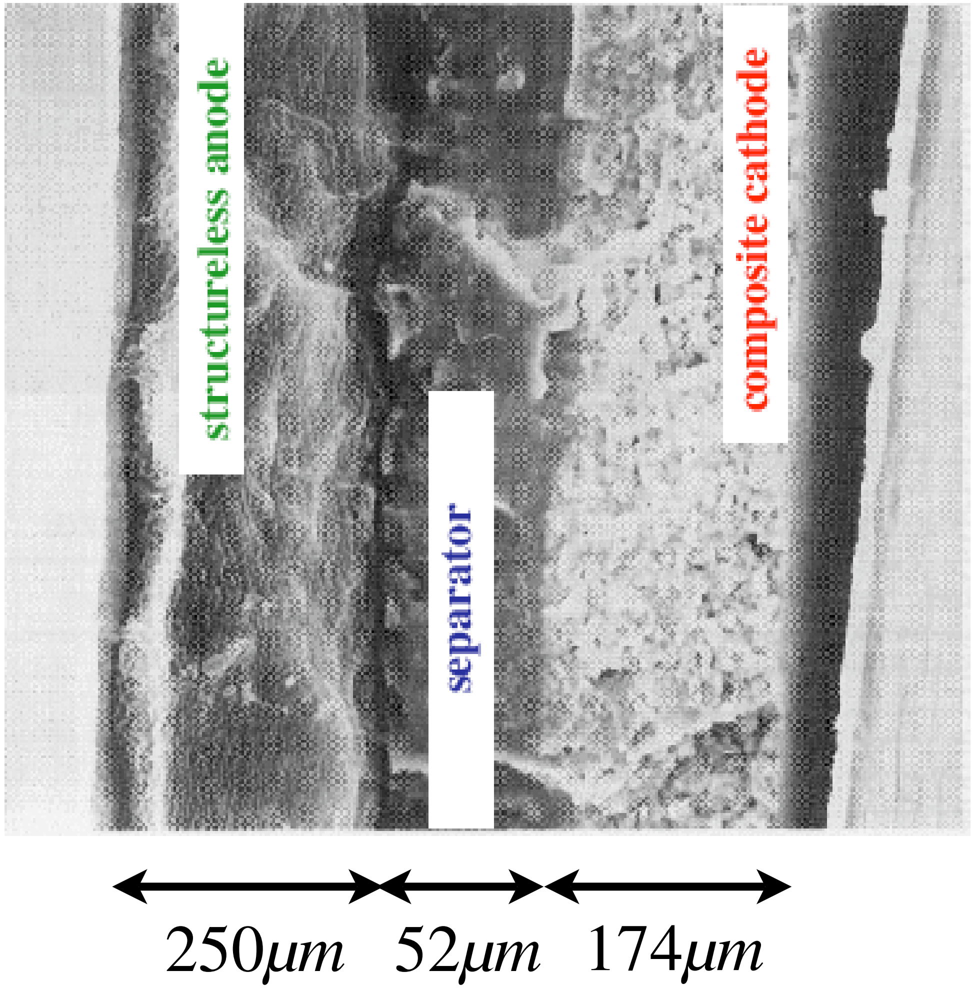
ferroelectrics

Current Research

Actuator Materials

Rechargeable Lithium-Ion Batteries

Yet-Ming Chiang, W. Craig Carter



C. A. Vincent and B. Scrosati "Modern Batteries: An Introduction to Electrochemical Power Sources." 2nd Ed. Butterworth-Heinemann, 1997.

diffusion term

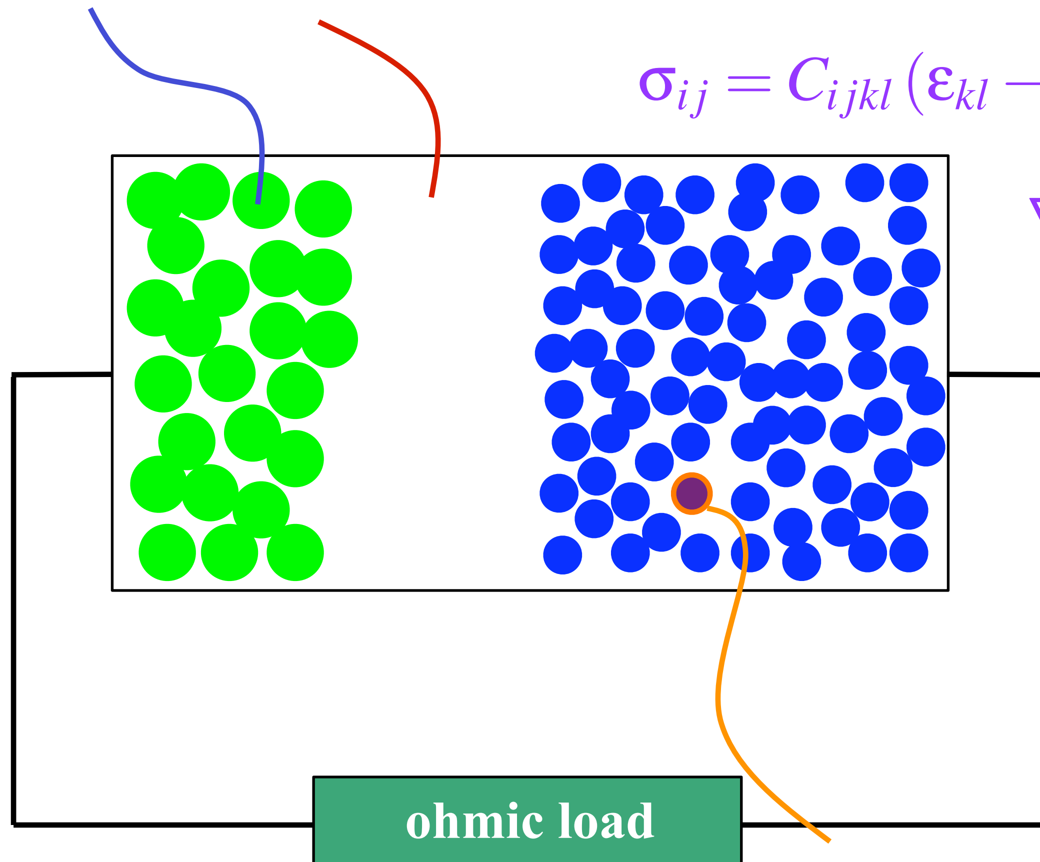
electromigration terms

$$\frac{\partial c}{\partial t} = \nabla \cdot (D_{Li} \nabla c) + \nabla \cdot (L \nabla \phi)$$

elastic fields

$$\sigma_{ij} = C_{ijkl} (\varepsilon_{kl} - \beta_{kl}(c - c_o))$$

$$\nabla \cdot \sigma = 0$$



$$0 = \nabla \cdot (\rho \nabla \phi) + \nabla \cdot (L \nabla c)$$

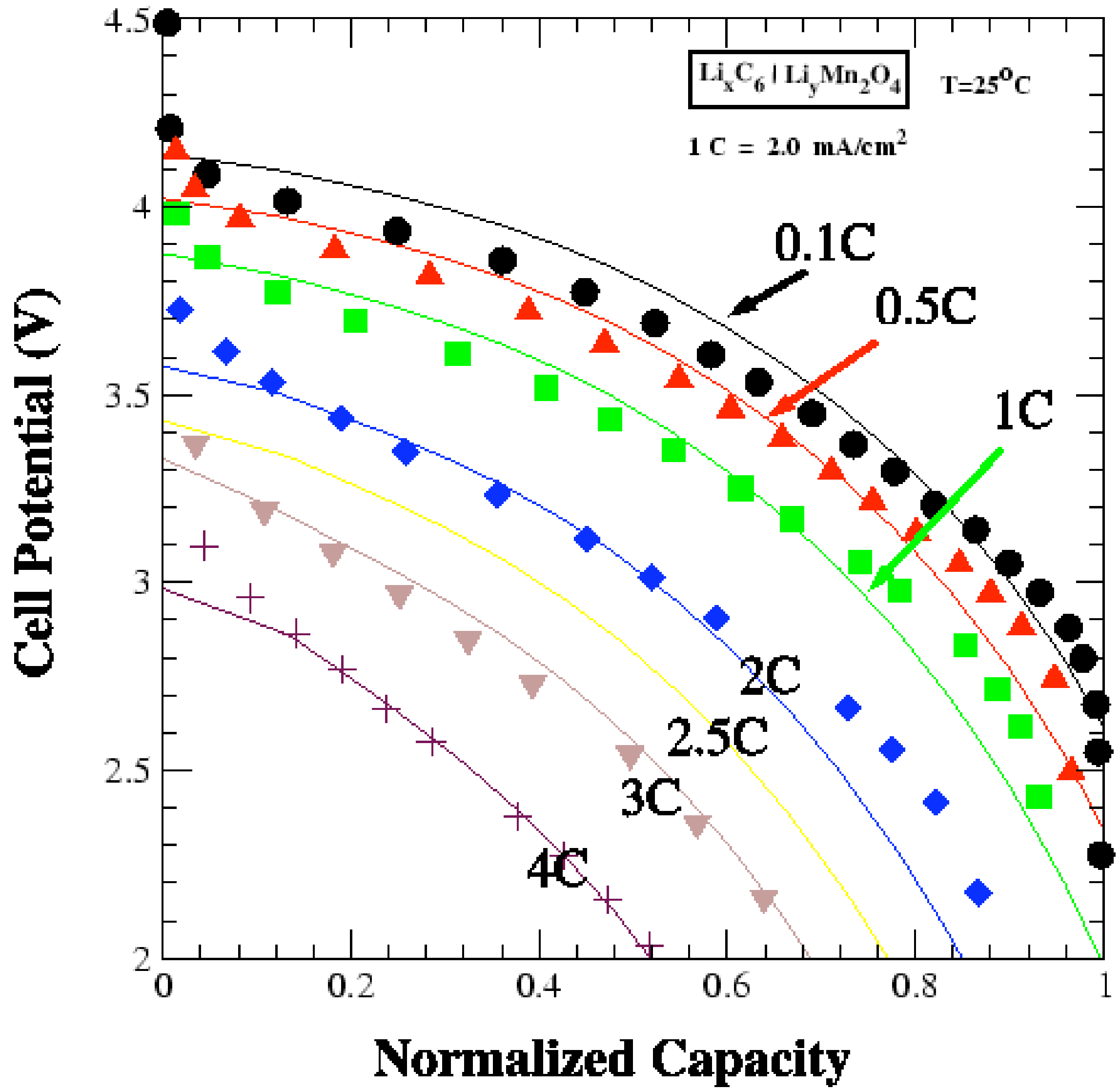
ohmic term

$$\vec{J} \cdot \hat{n} = J_o \left(e^{\frac{\alpha_a F \eta}{RT}} - e^{-\frac{\alpha_c F \eta}{RT}} \right)$$

surface reaction kinetics

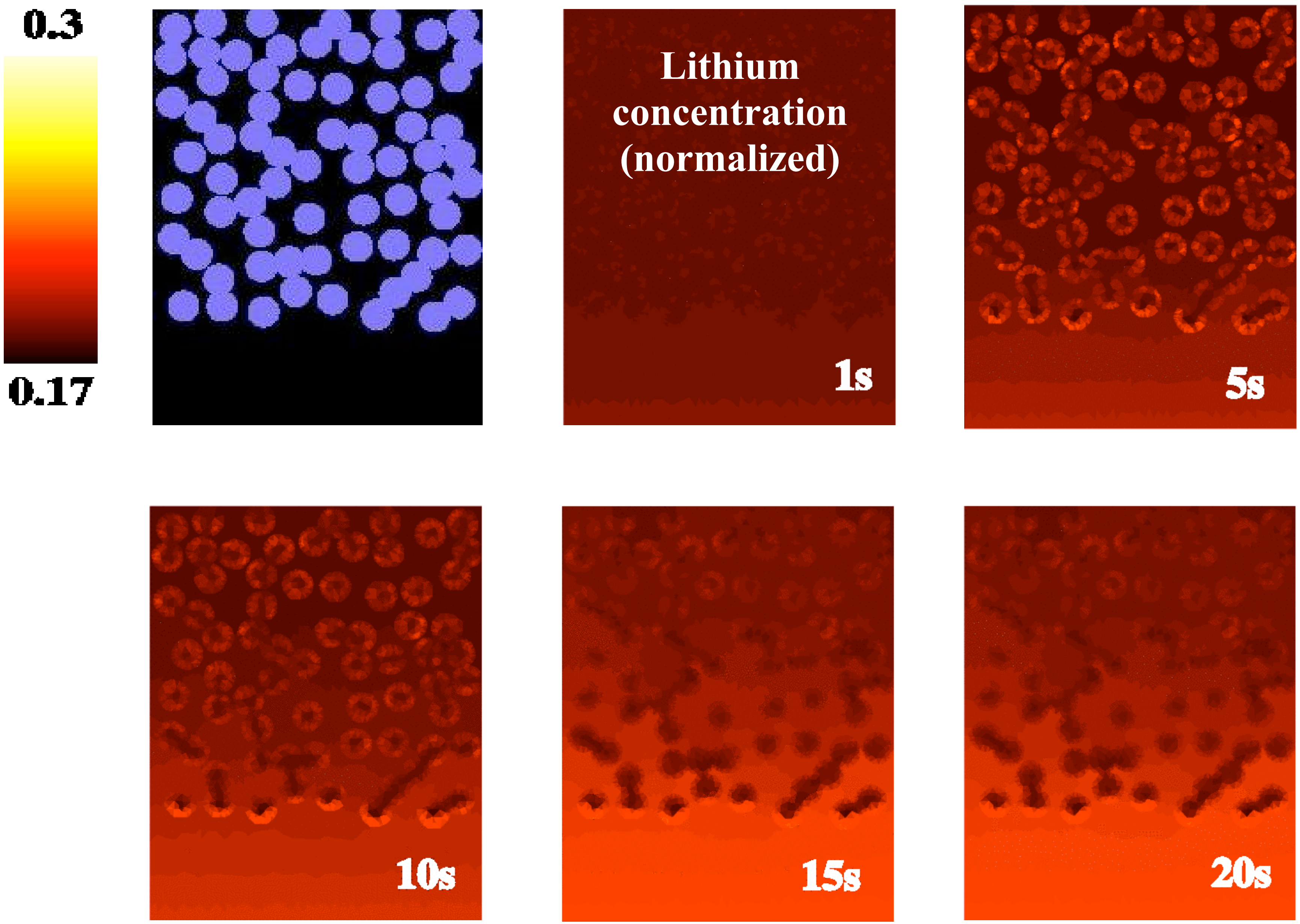
● graphite ● $LiMn_2O_4$

Model Validation: Comparison with Experiment

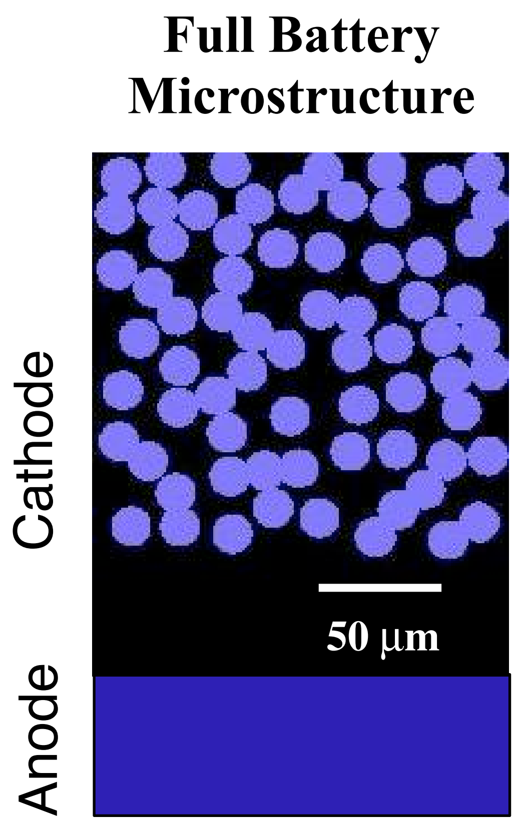


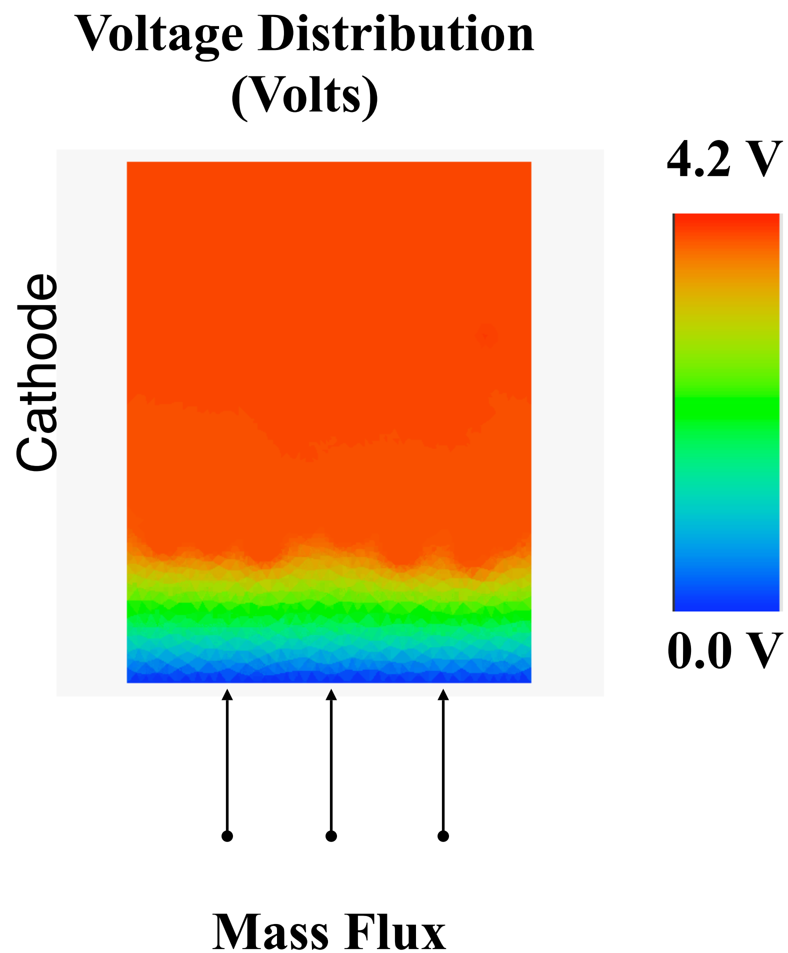
Experimental Data: Christopher Marc Doyle "Design and Simulation of Lithium Rechargeable Batteries." PhD thesis, Department of Chemical Engineering. University of California at Berkeley, 1995

Initial Stages of Battery Discharge



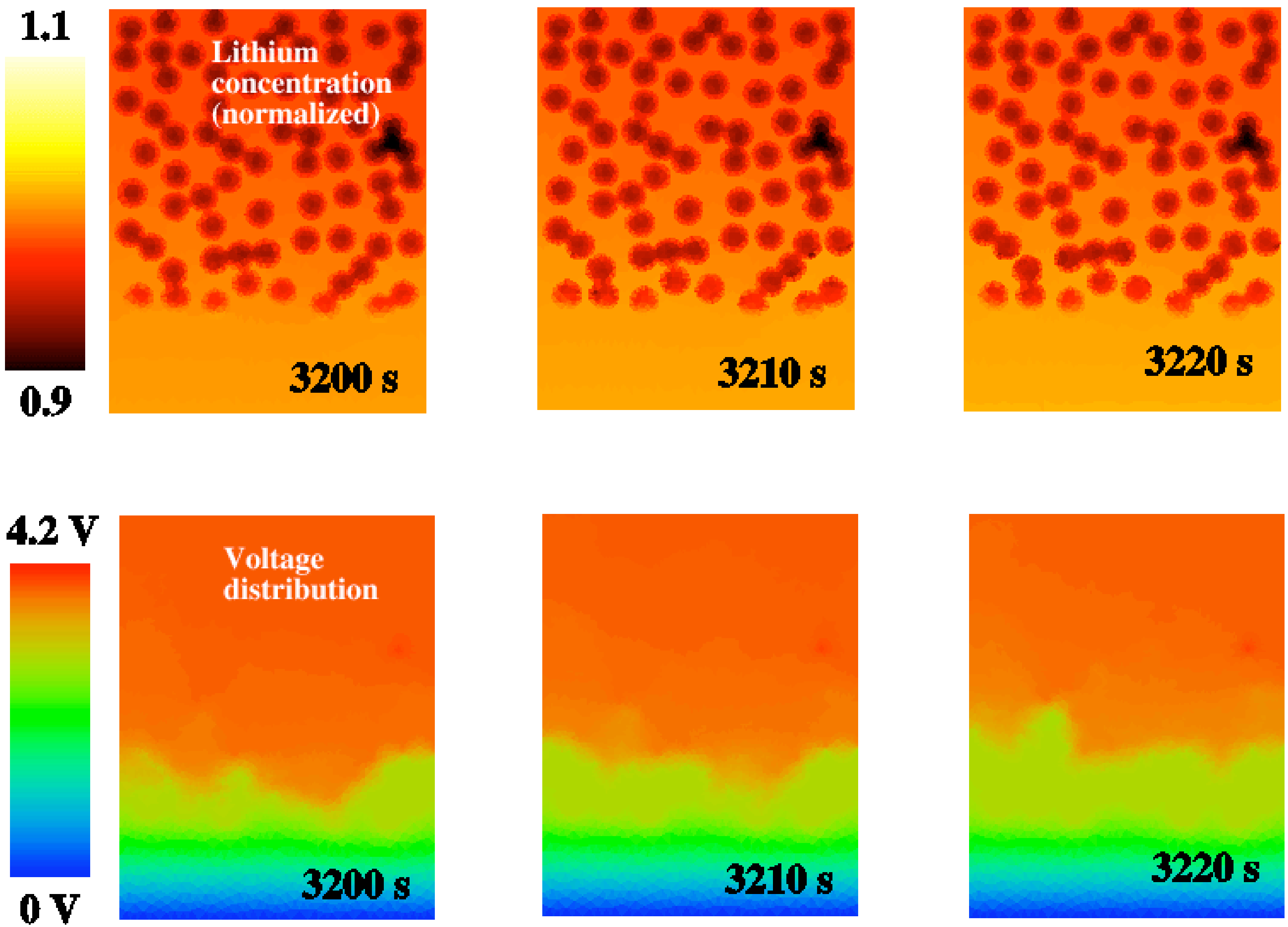
Late Stages of Voltage Distribution of Battery Discharge



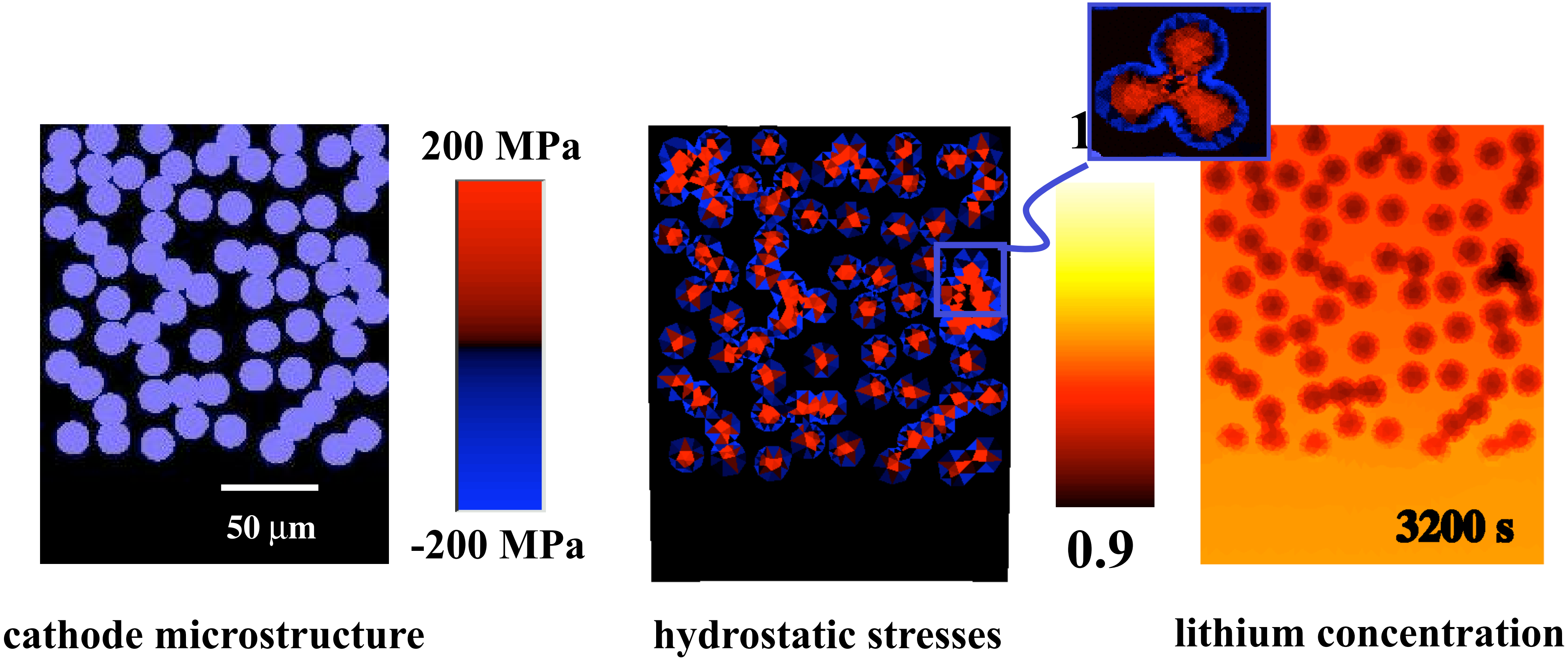


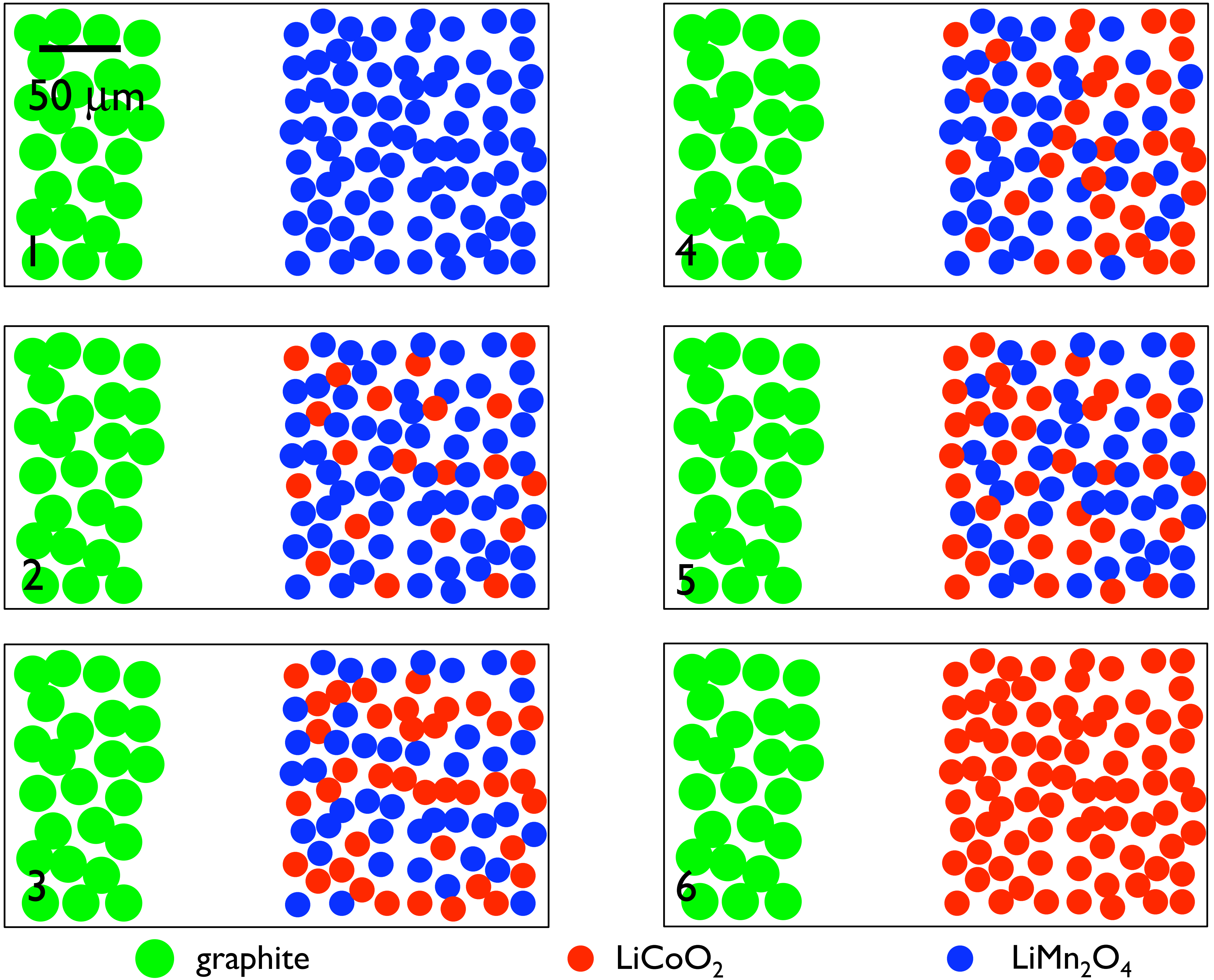
1C: 2.0 mA/cm^2

Late Stages of Battery Discharge

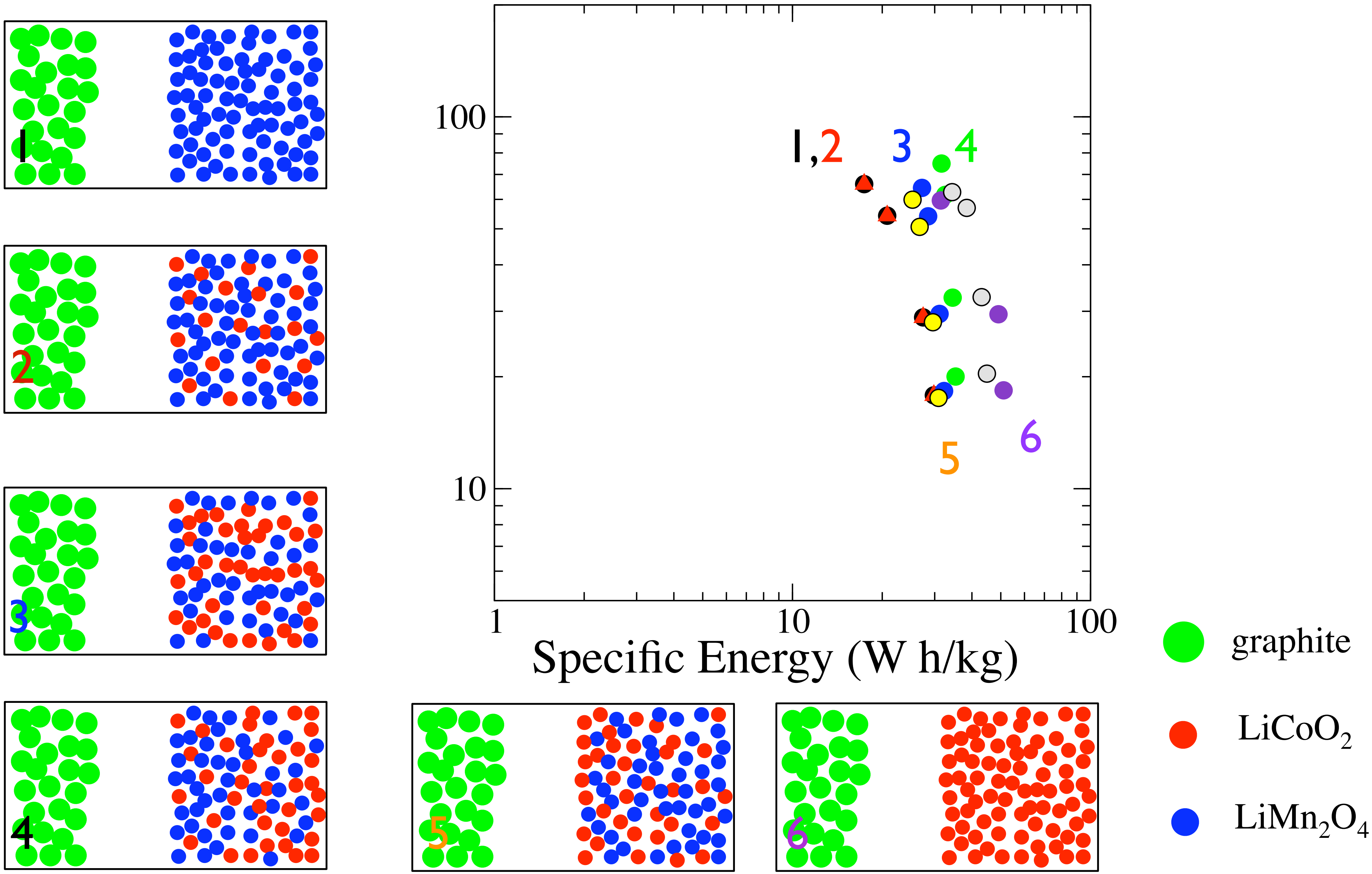


Galvanostatic Discharge Stresses

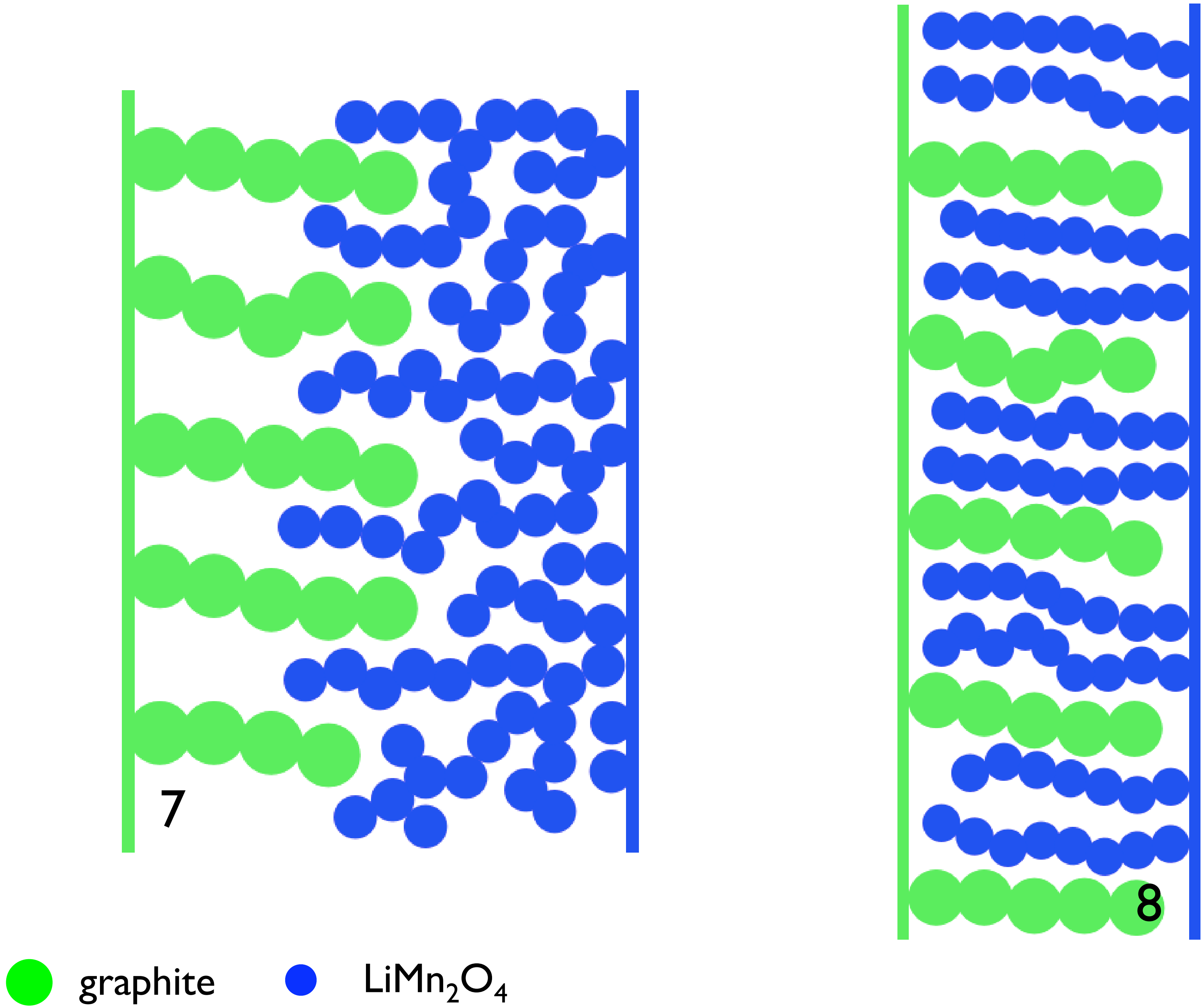


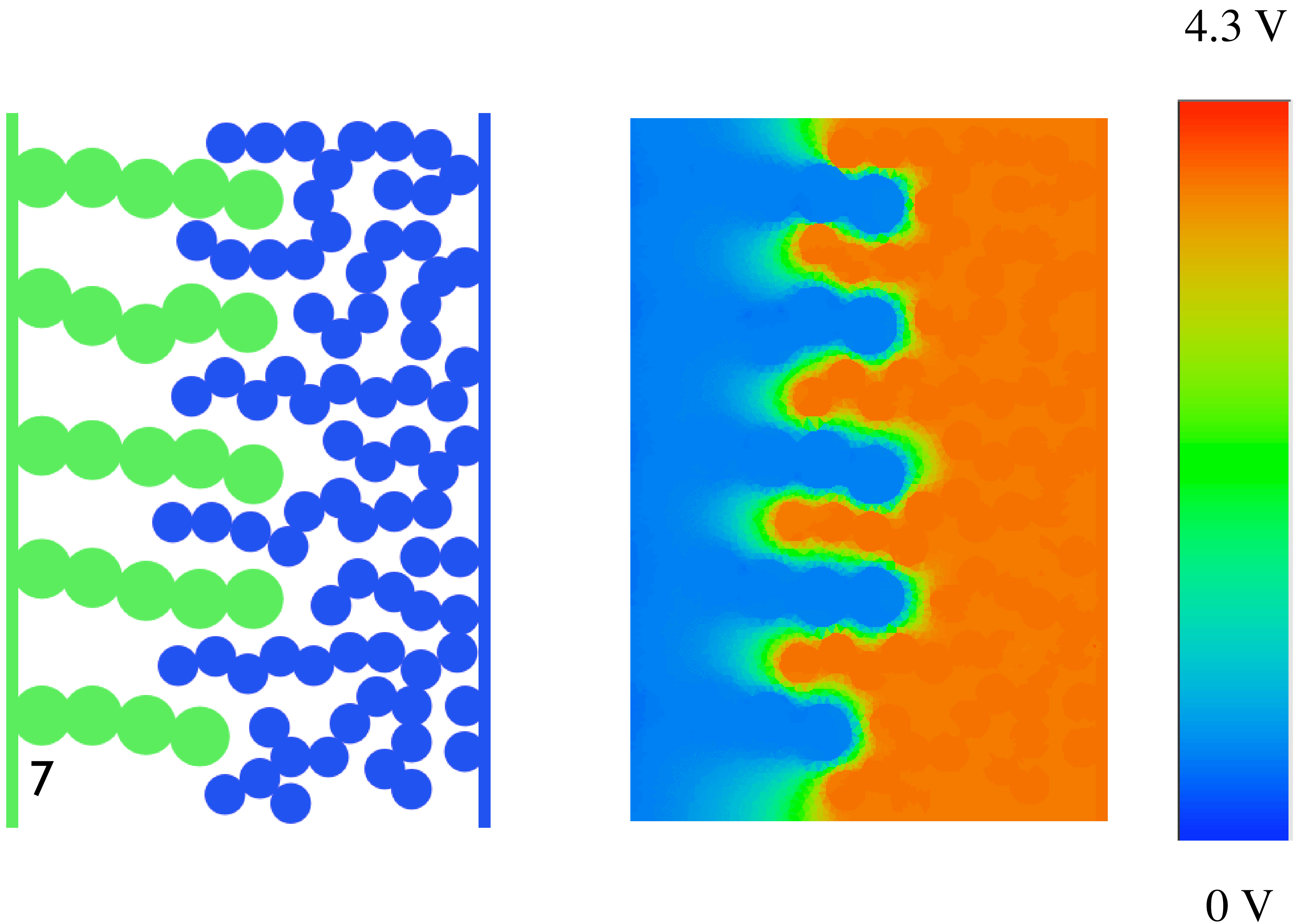

50 μm
1
2
3
4
5
6
graphite
LiCoO2
LiMn2O4

Summary Ragone Plot of Mixed Rocking Chair Batteries



Advanced Rechargeable Batteries

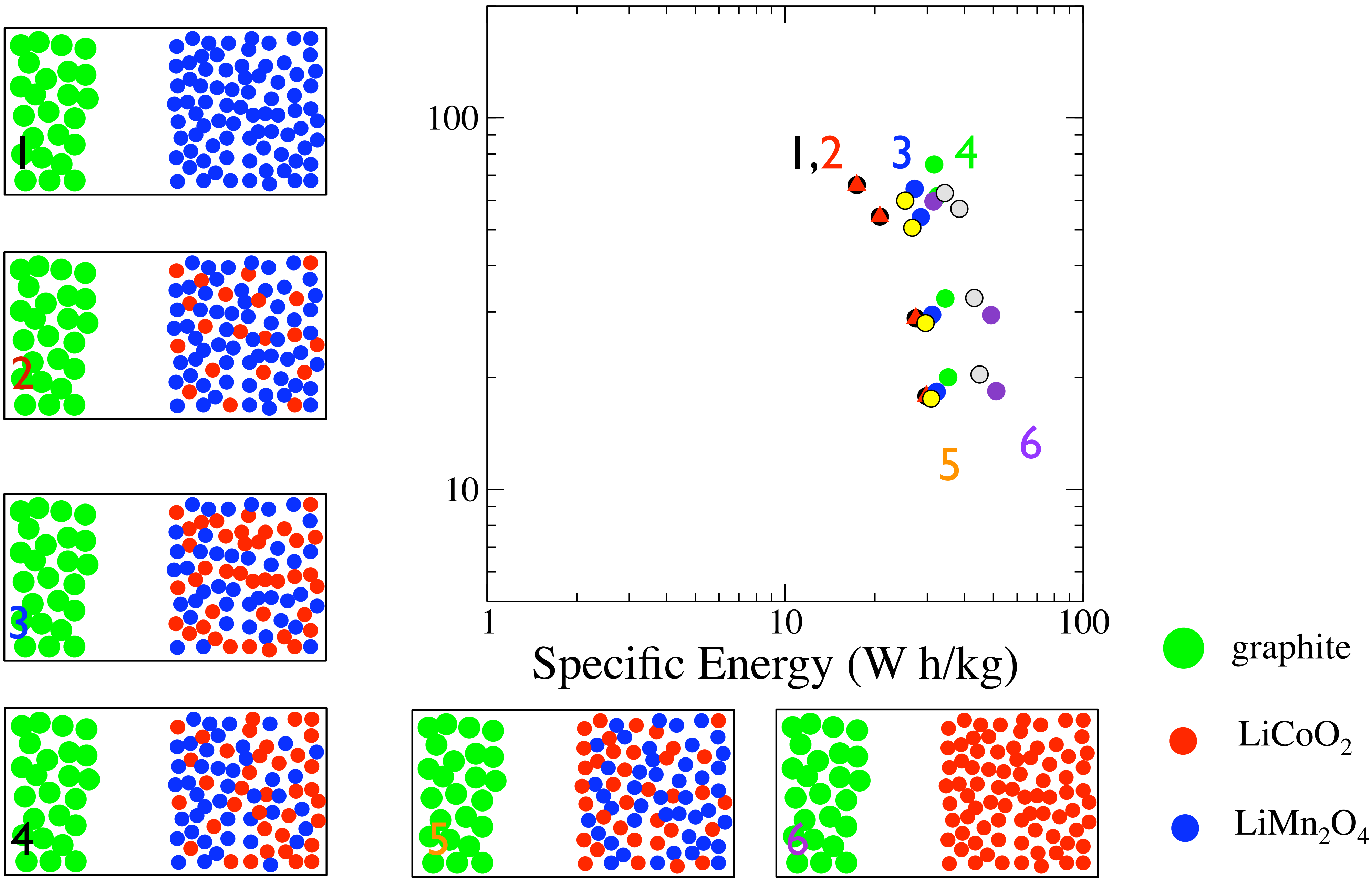




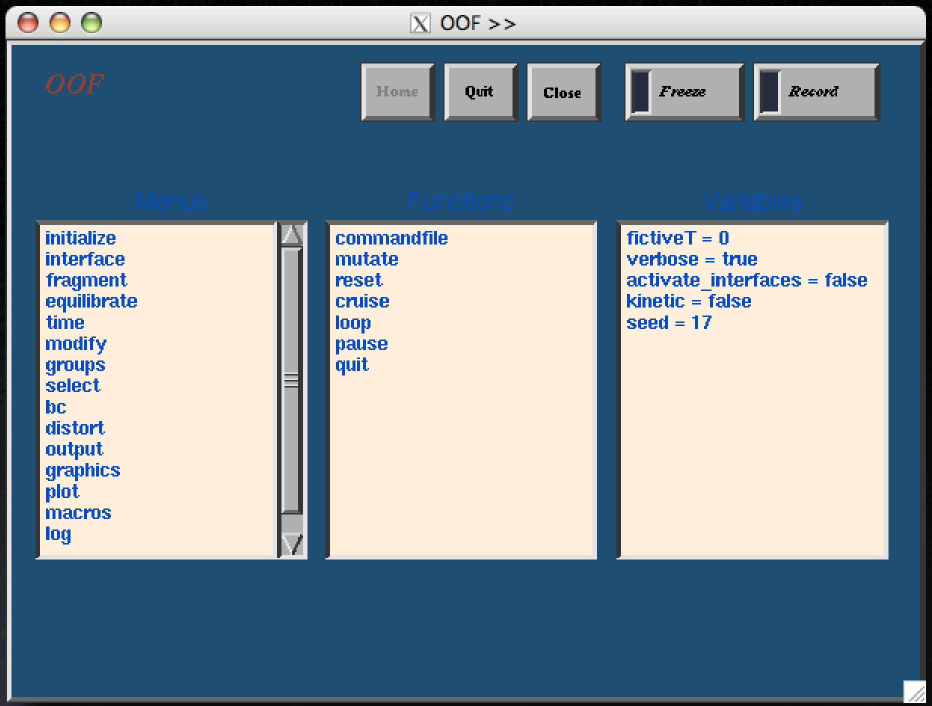
depleted after 250s

I=80 A/m²

Summary Ragone Plot of Rocking Chair Batteries

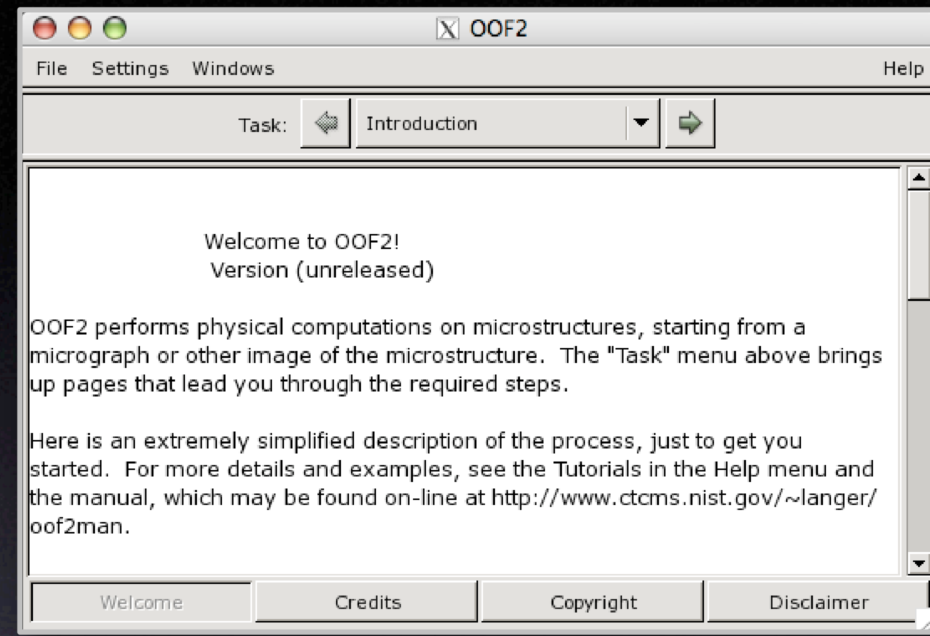


Electrochemical oof



- Mass Diffusion Equation
- Charge Continuity Equation
- Heat Diffusion Equation
- Electrochemical Couplings
- Time-Stepper Methods
- GMRES Solver
- Multimeshing Techniques
- Line (Interfacial) Elements

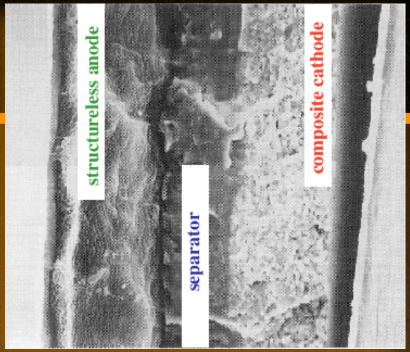
OOF2



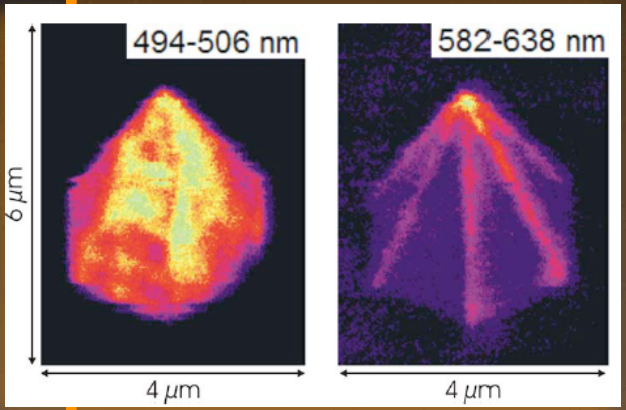
- Mass Diffusion Equation
- Charge Continuity Equation
- Heat Diffusion Equation
- Electrochemical Couplings
- Generalized Time-Stepper Methods
- Multiple Solvers and Preconditioners
- Multimeshing Techniques (in progress)
- Line (Interfacial) Elements

Outline

rechargeable
batteries



Energy Materials

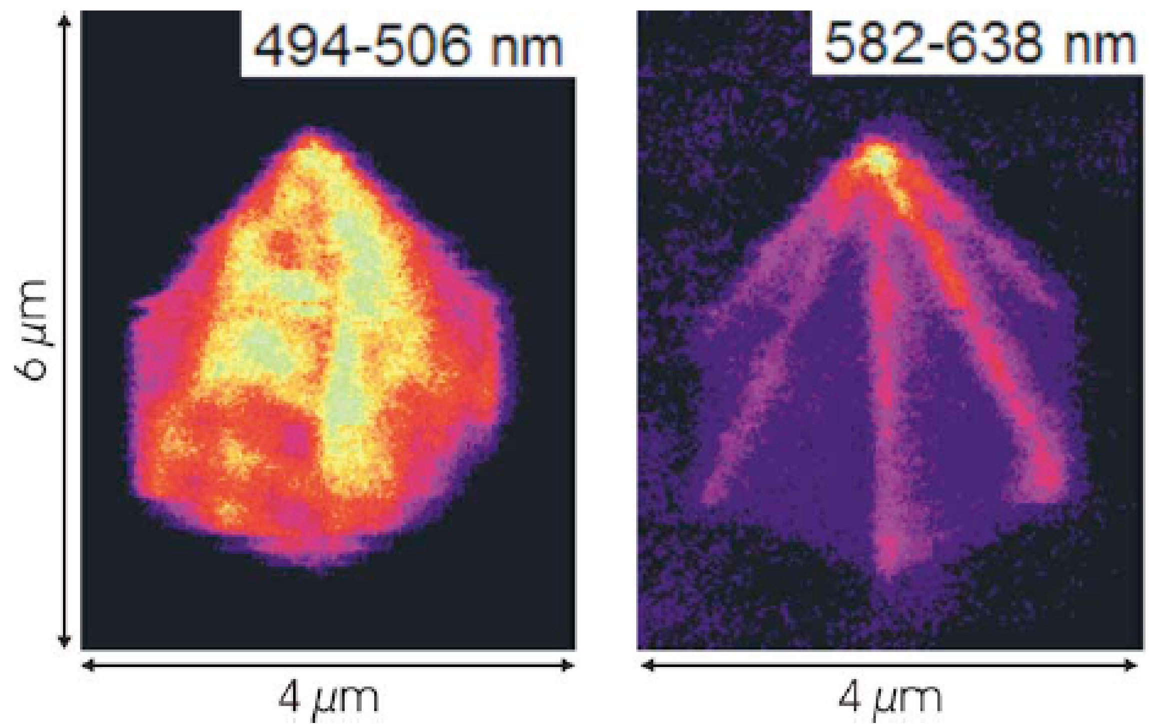


light emitting
devices

Actuator Materials

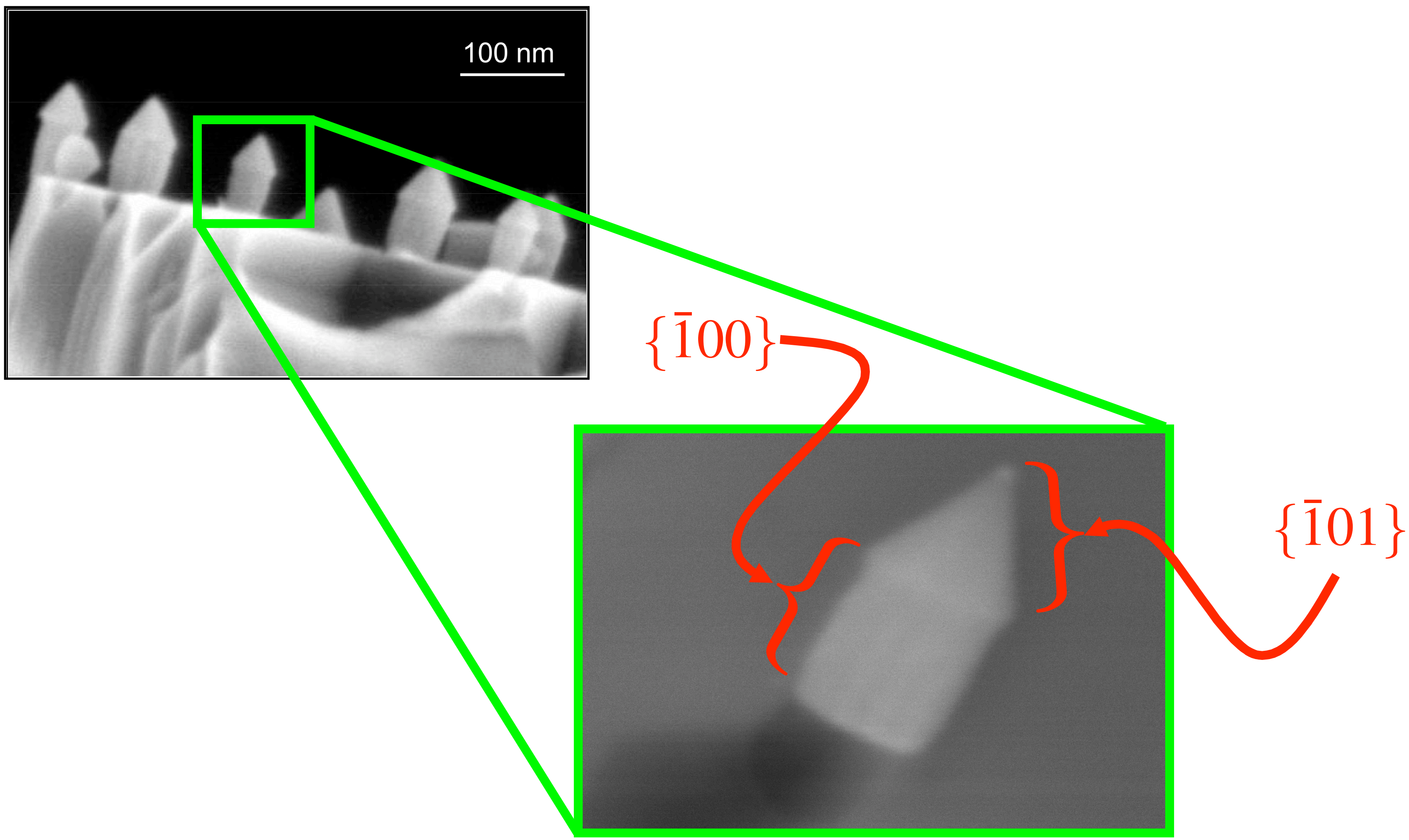
Stress Engineering of Light Emitting Devices

(Parijat Deb, Tim Sands)

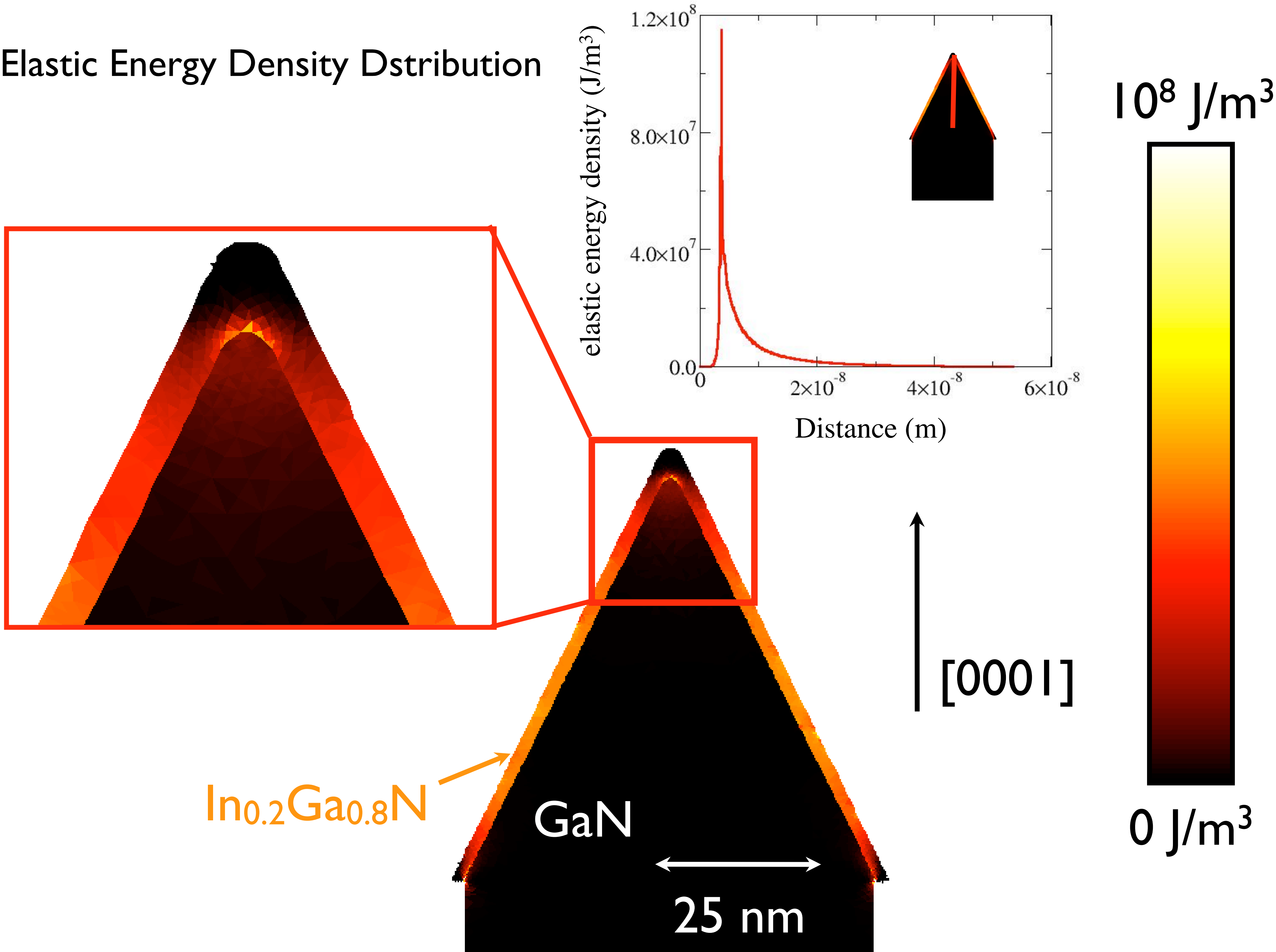


Solorzano et al. "Near-red emission from site-controlled pyramidal InGaN quantum dots" Applied Physics Letters 87, 163121 (2005)

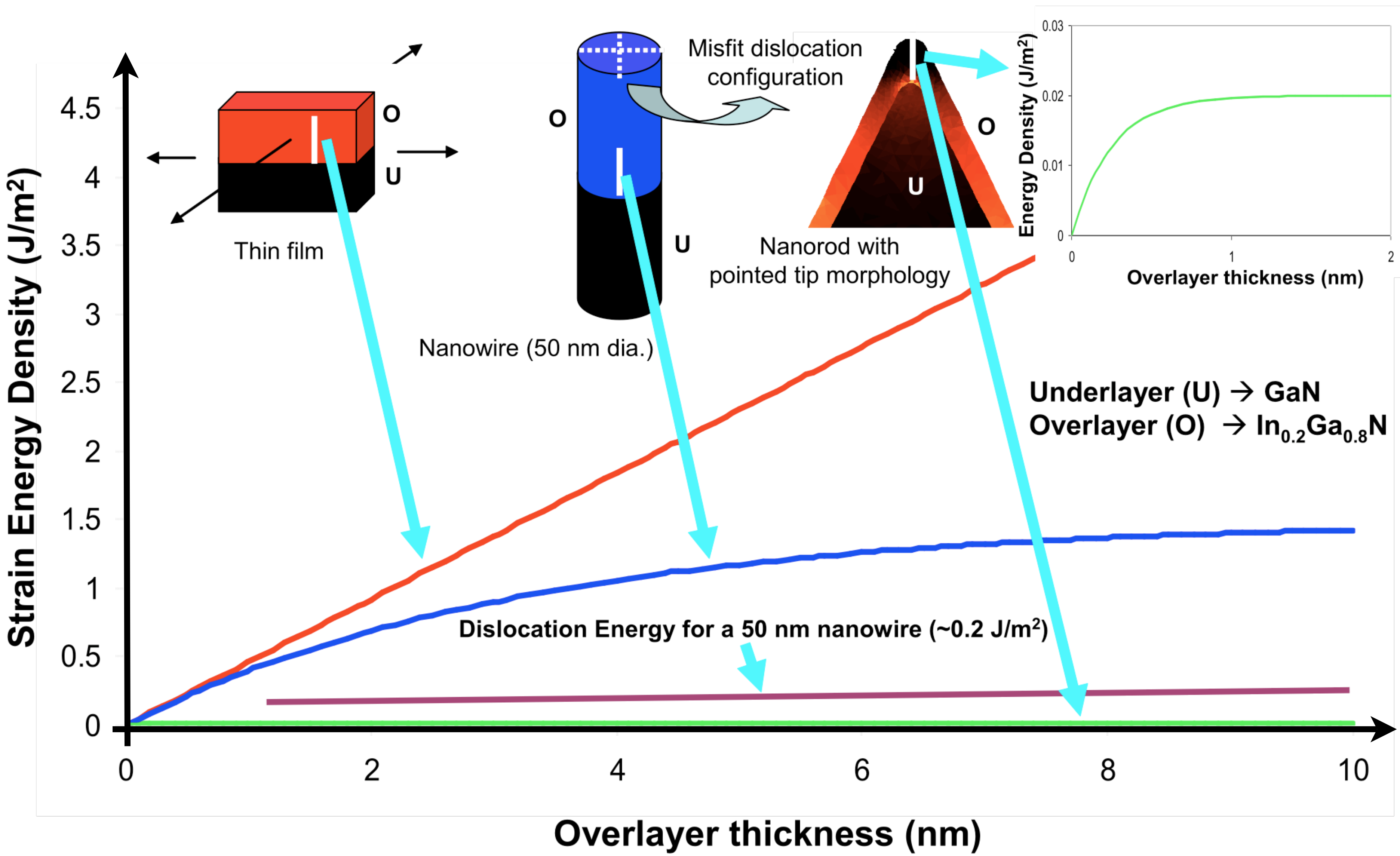
Crystallography of GaN Pyramids



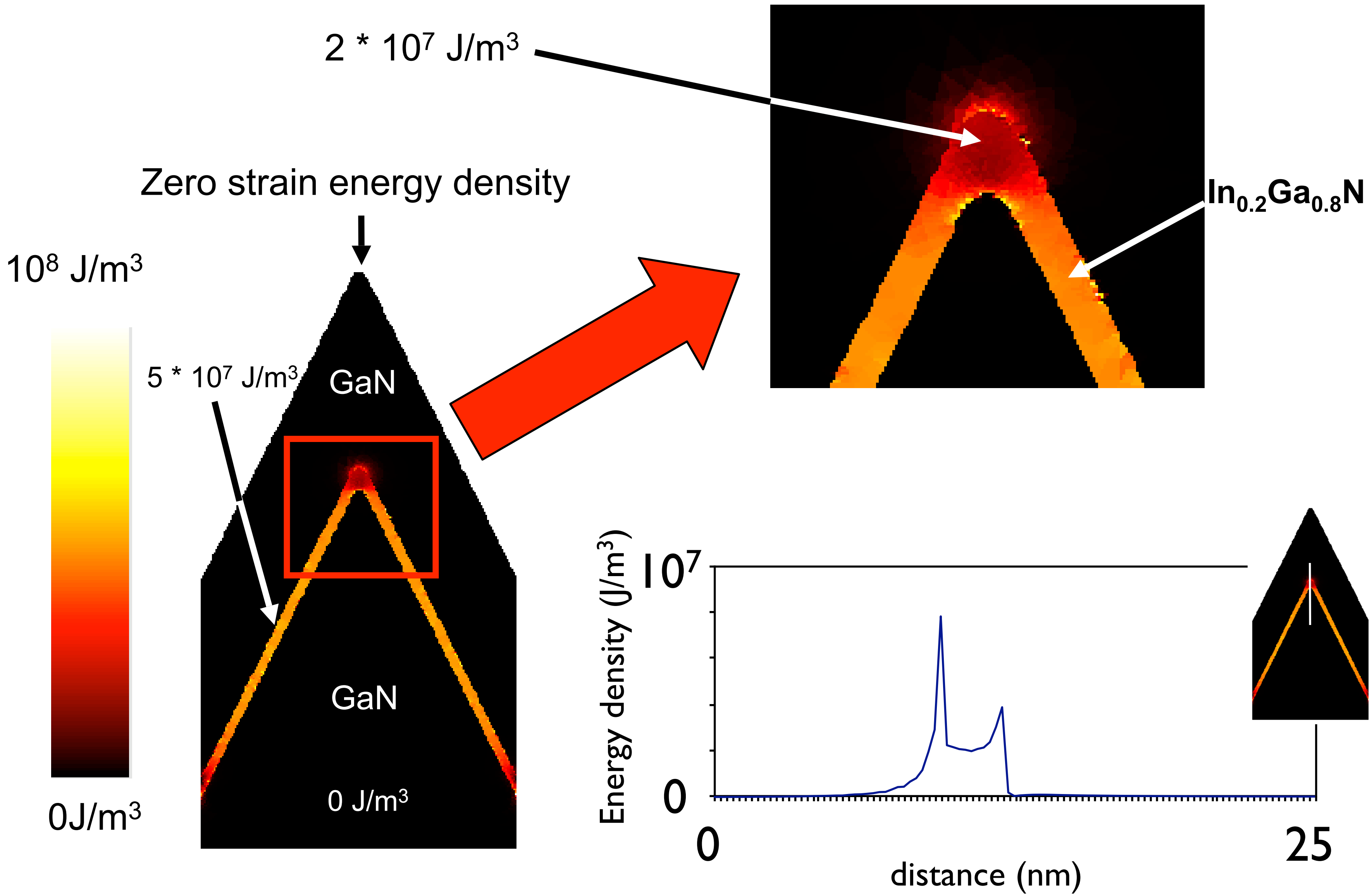
Elastic Energy Density Dstribution



Strain Energy Density

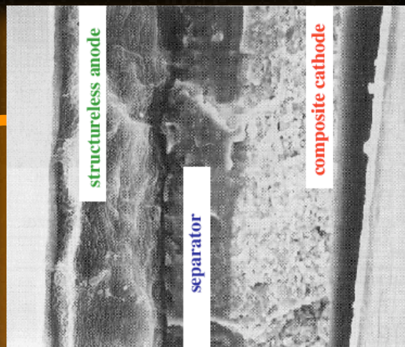


Embedded Quantum Well Heterostructure



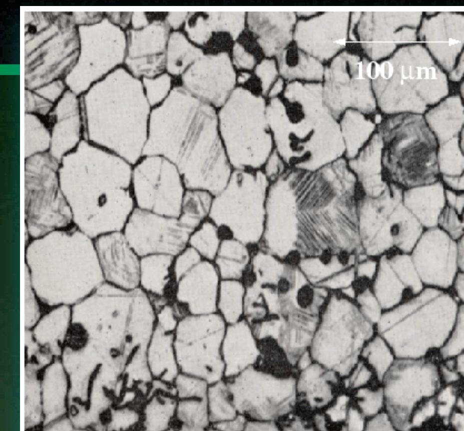
Outline

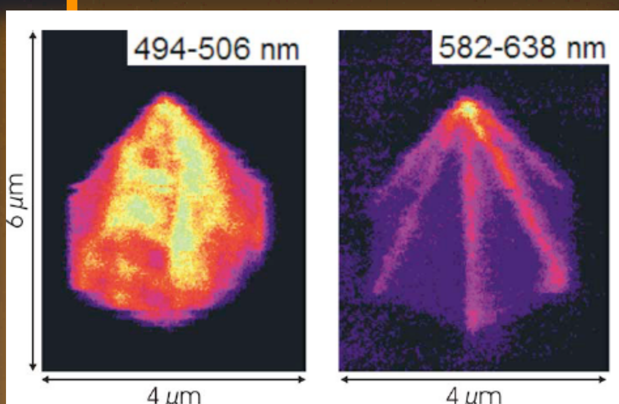
rechargeable batteries



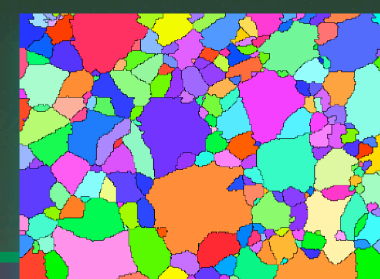
Energy Materials

piezoelectrics and electrostrictors





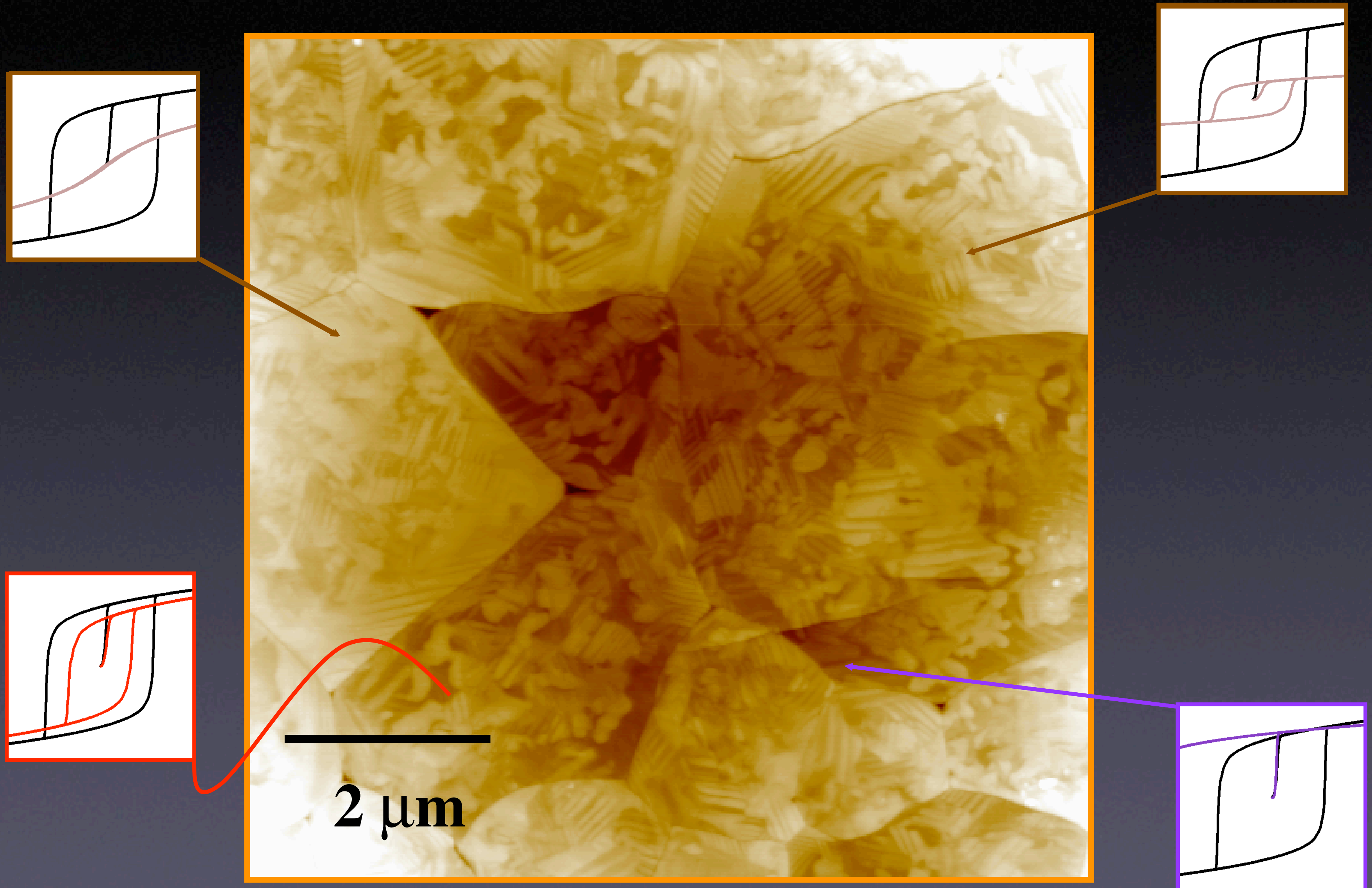
light emitting devices

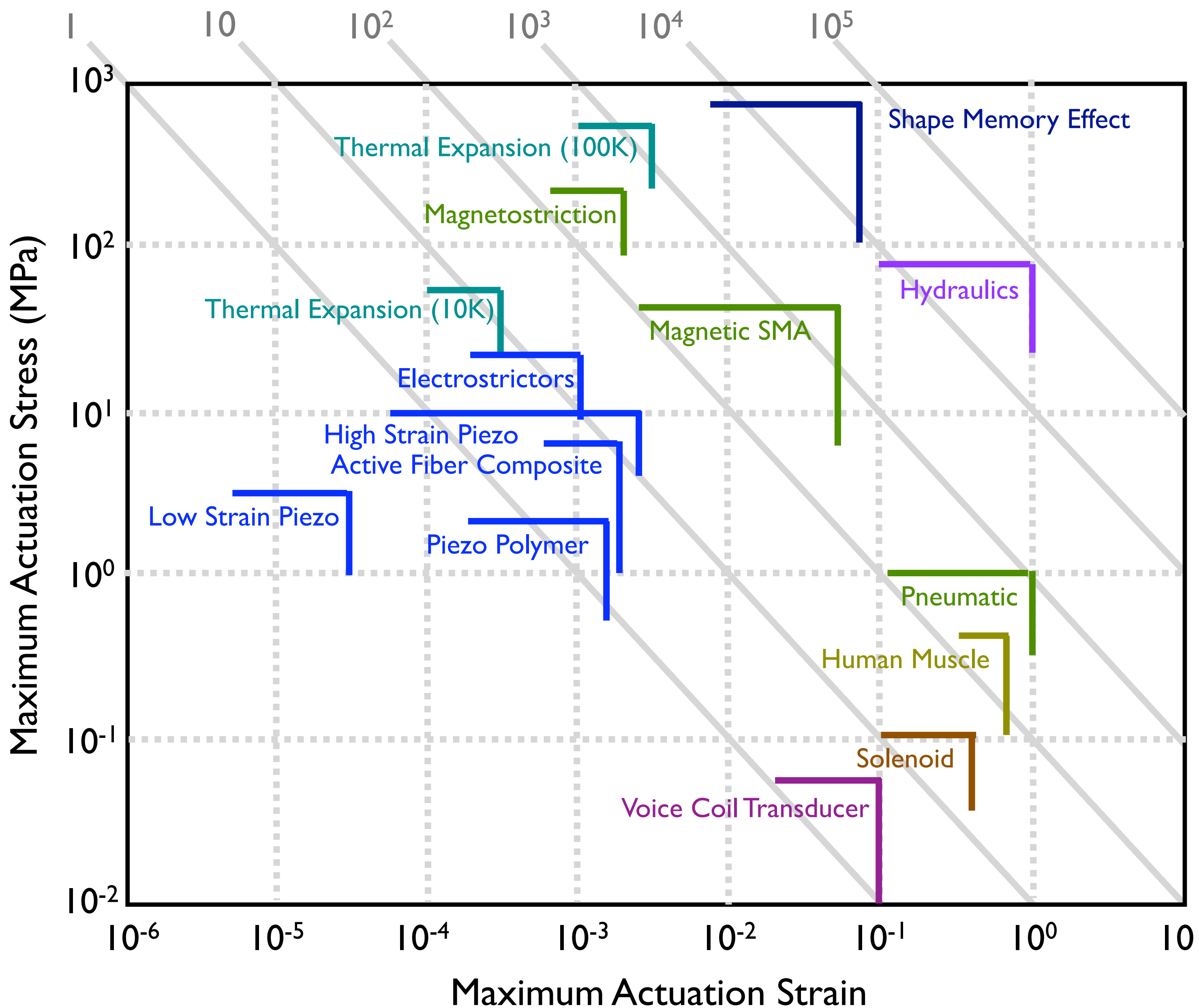


ferroelectrics

Actuator Materials

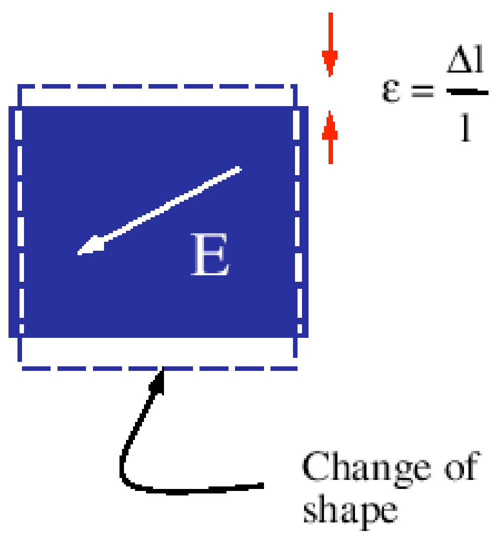
Polycrystalline PZT Film



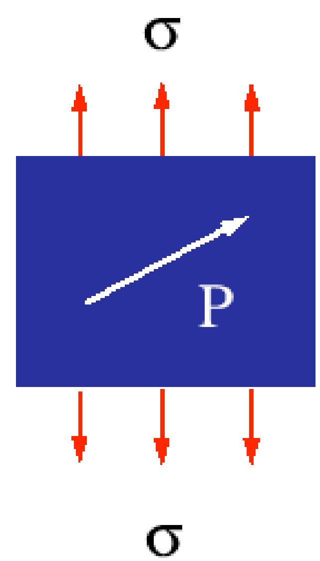


J. E. Huber, N. A. Fleck, and M. F. Ashby "The Selection of Mechanical Actuators Based on Performance Indices" *Proc. R. Soc. Lond. A*, **453**, 2185-2205 (1997).

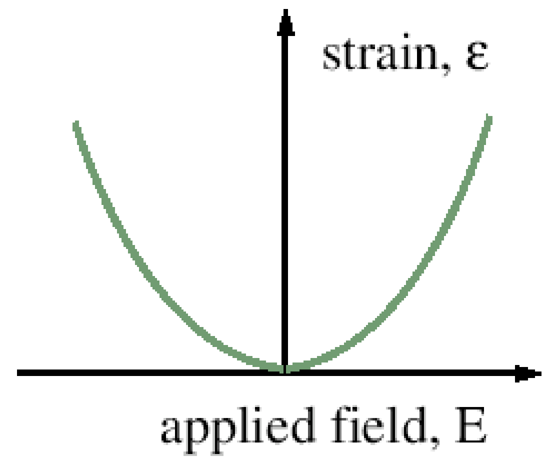
The Piezoelectric Solid



Converse piezoelectric effect



Direct piezoelectric effect



Higher order piezoelectric response

Electromechanical Helmholtz free energy

$$f = u - \vec{D} \cdot \vec{E}$$

$$f = \frac{1}{2}\sigma \cdot \varepsilon - \frac{1}{2}\vec{D} \cdot \vec{E}$$

$$\nabla \cdot \vec{D} = 0$$

$$\nabla \cdot \sigma = 0$$

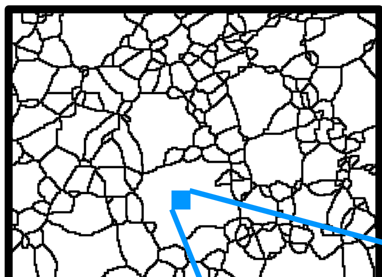
Simulation of Polycrystalline PZT Films

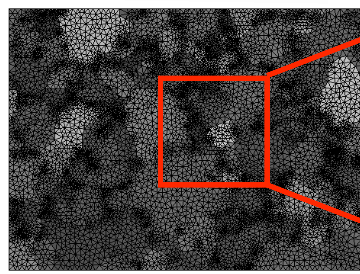
$$D_i = \epsilon_{ij} E_j + d_{ikl} \sigma_{kl}$$

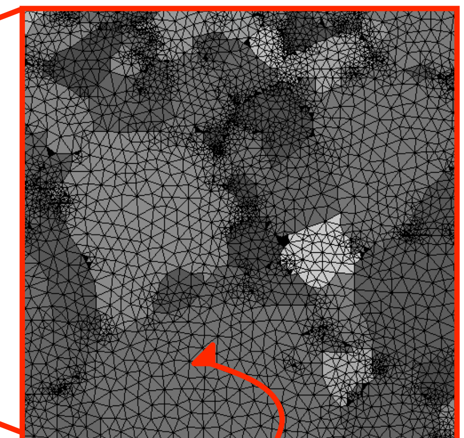
$$\nabla \cdot \vec{D} = 0$$

$$\sigma_{ij} = C_{ijkl} \left(\varepsilon^T_{kl} - d_{ikl} E_i - \alpha_{kl} \Delta T \right)$$

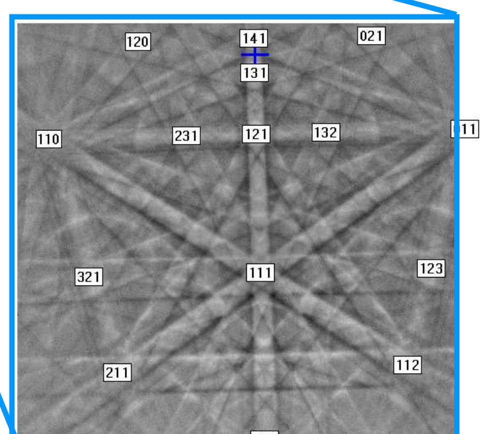
$$\nabla \cdot \sigma = \vec{0}$$

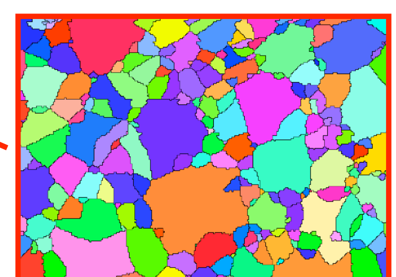






50 μm

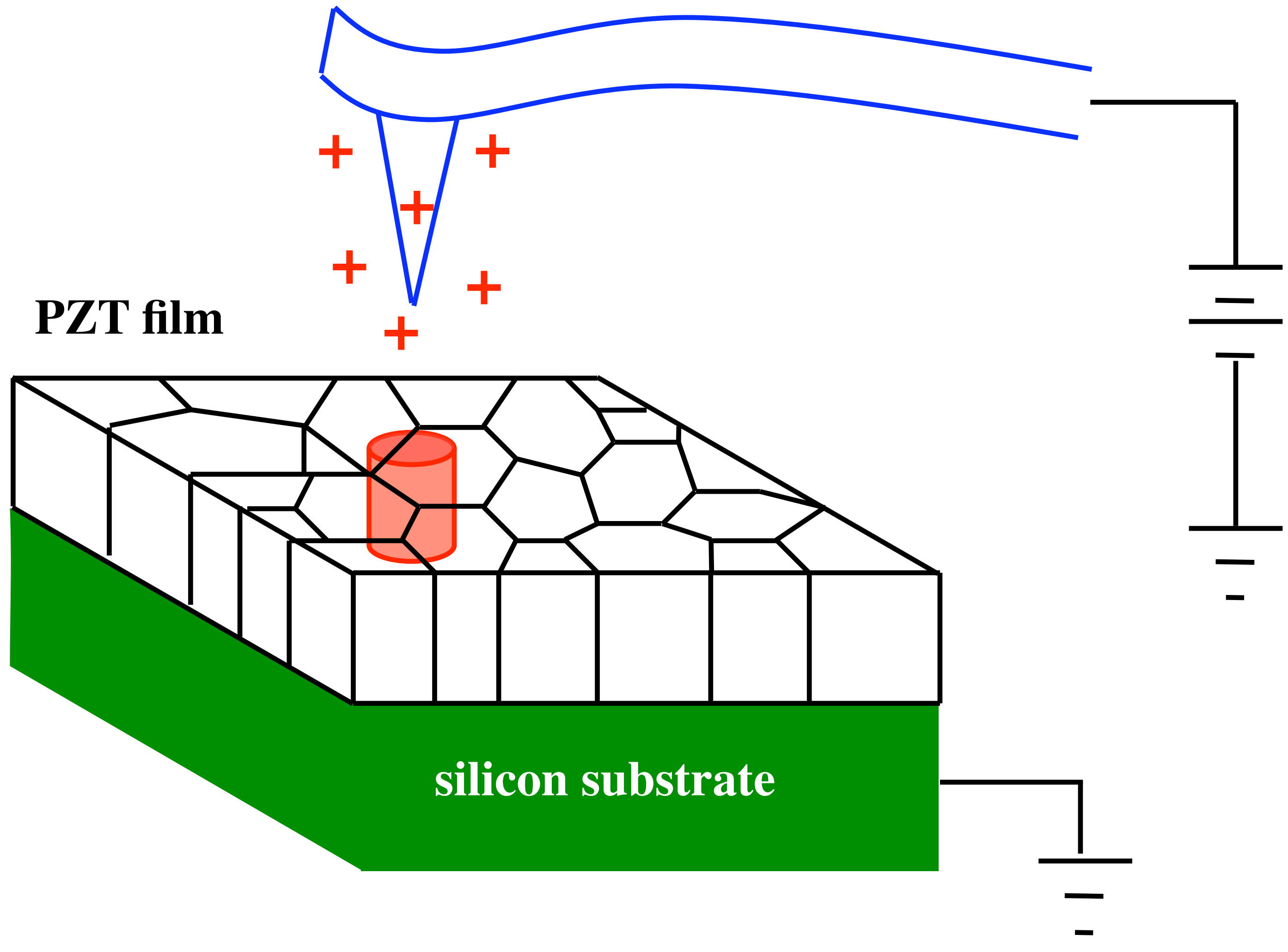




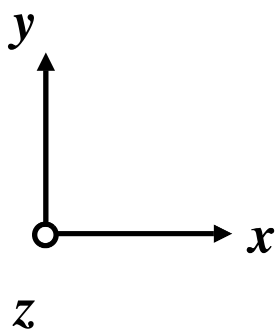
$$\frac{\partial P}{\partial t} = -M \frac{\delta F}{\delta P}$$

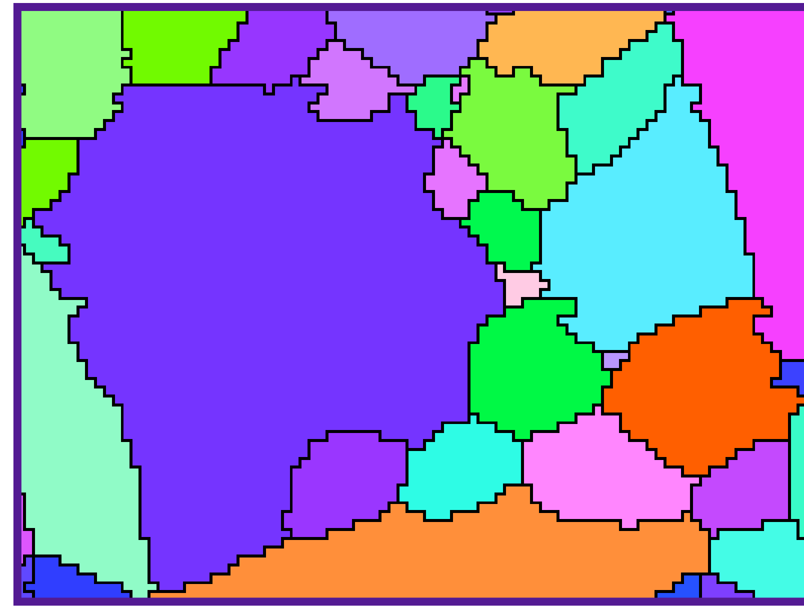
PZT microstructure courtesy of Samsung

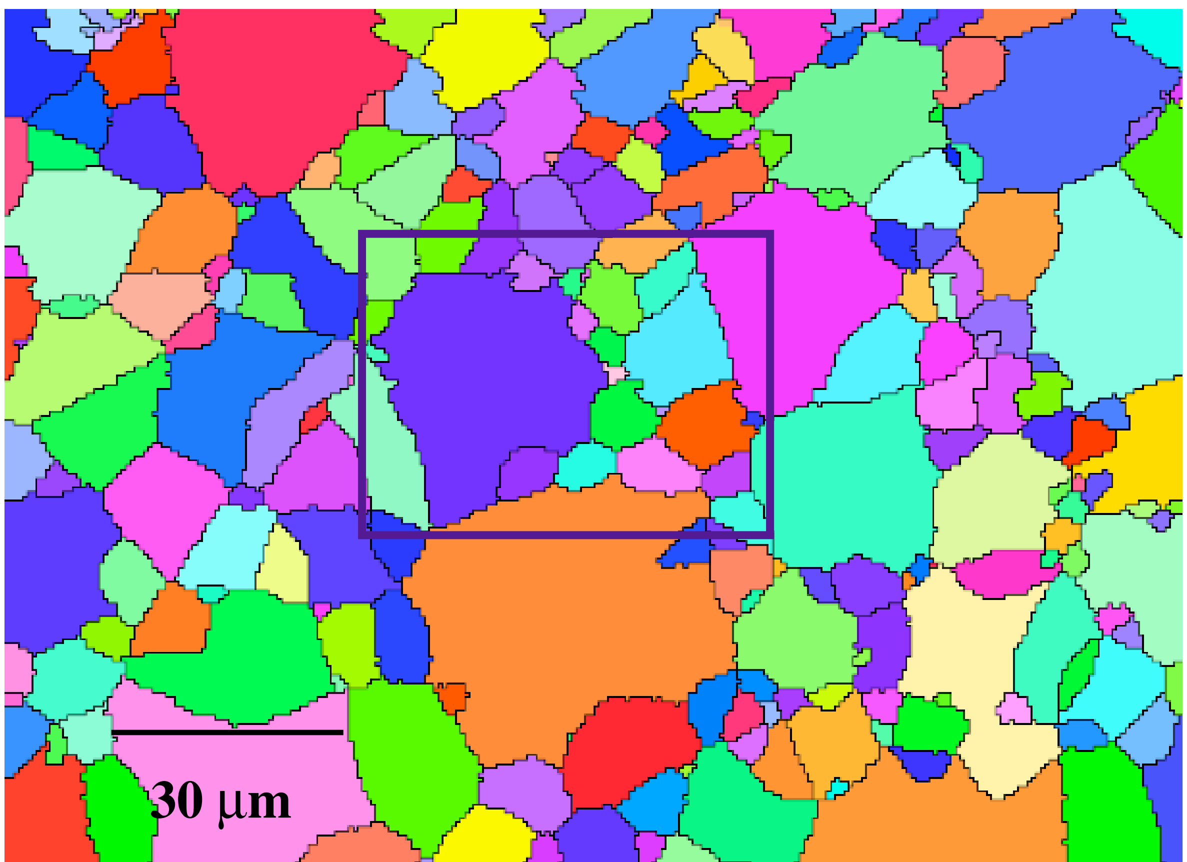
Piezoelectric Force Microscopy of Ferroelectric Films

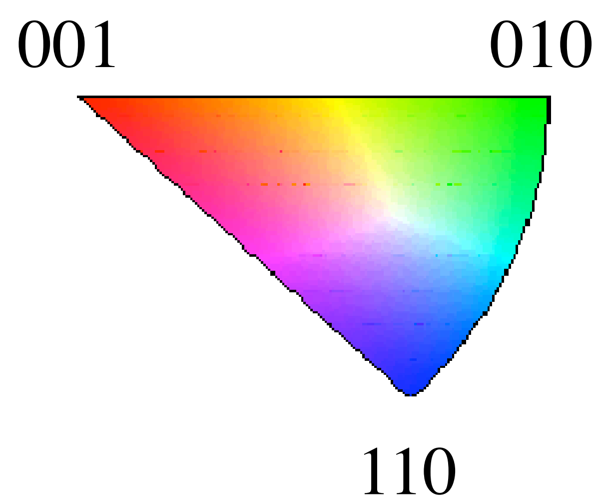


Virtual Piezoelectric Force Microscopy of Ferroelectric Films

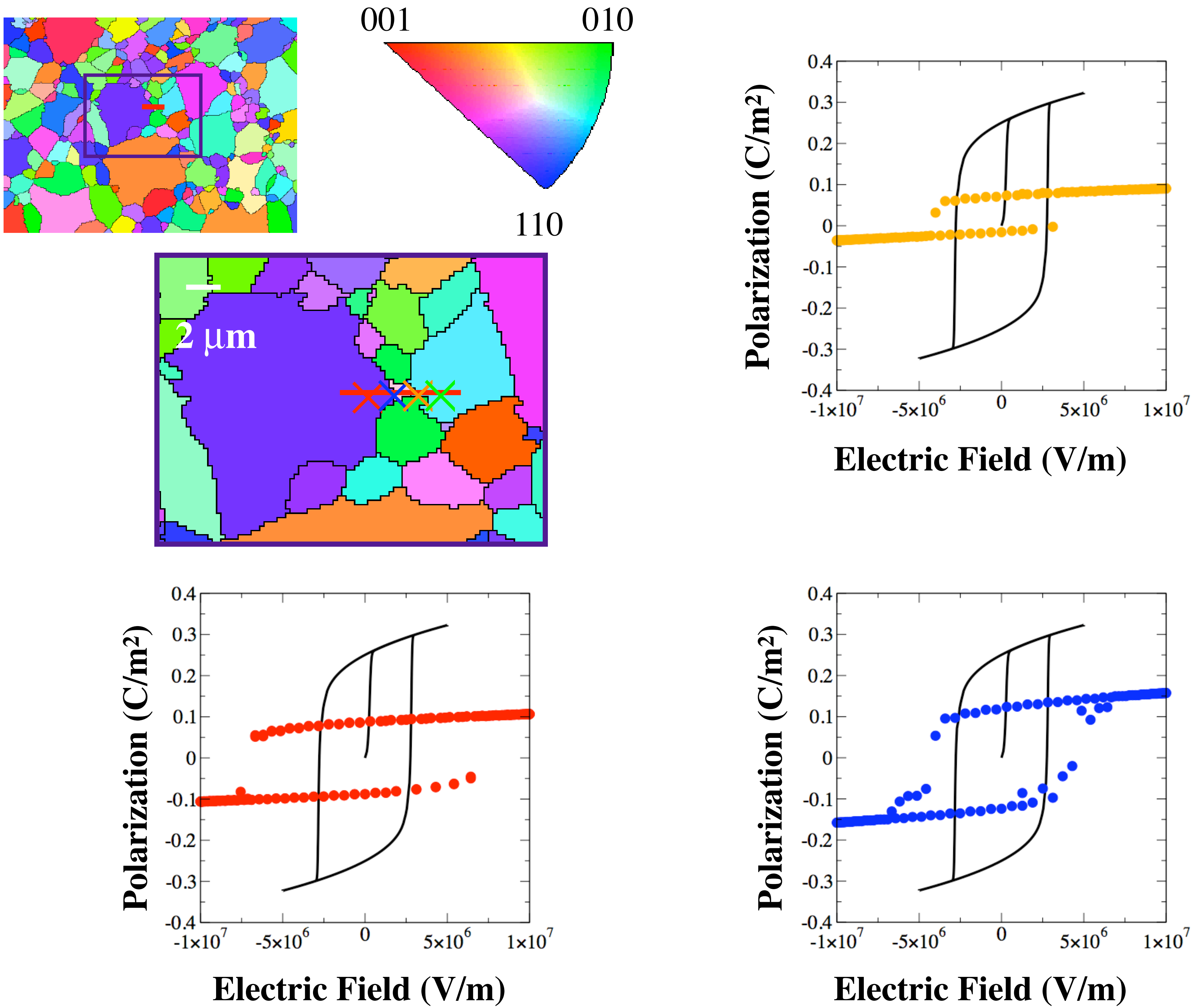


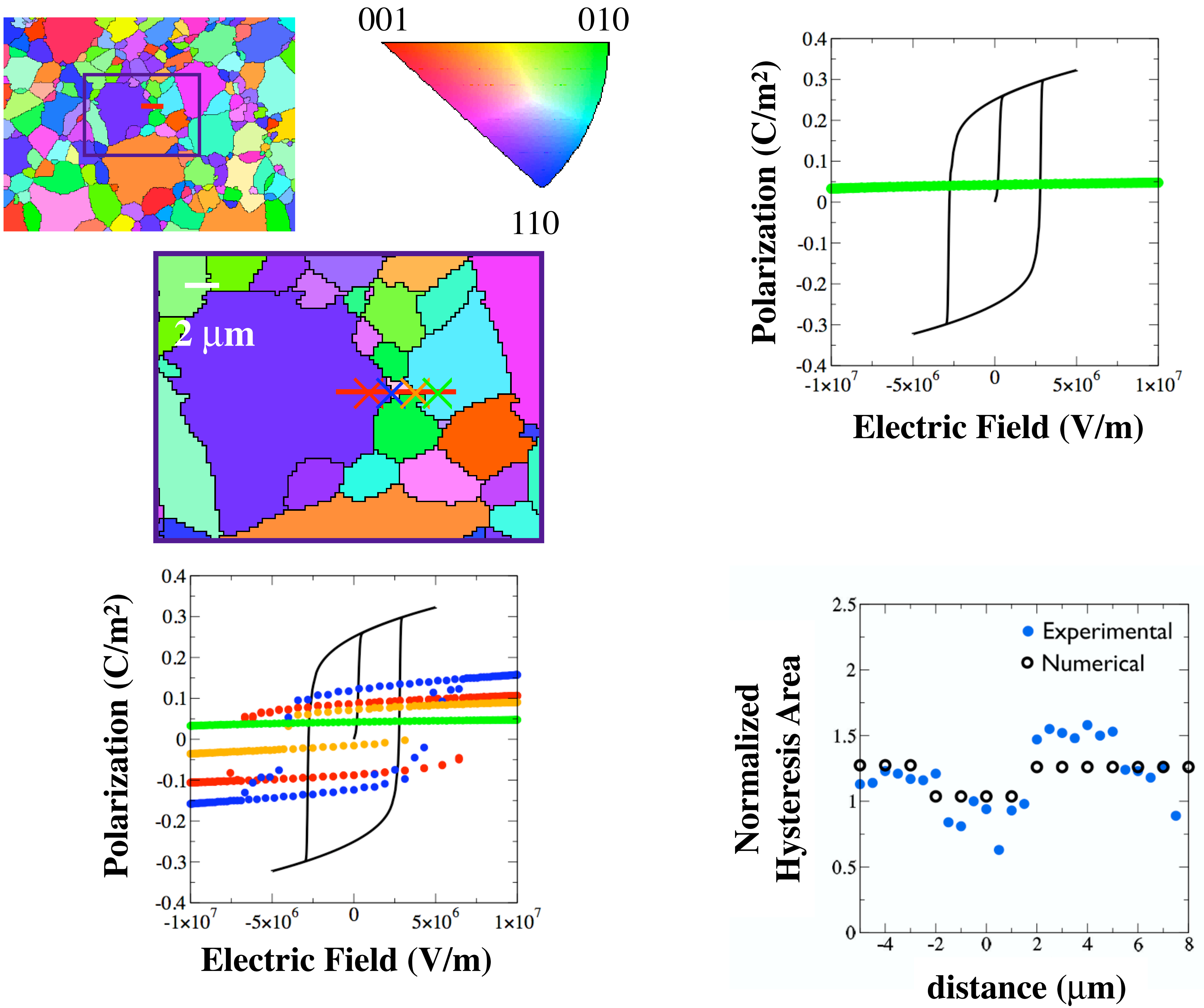




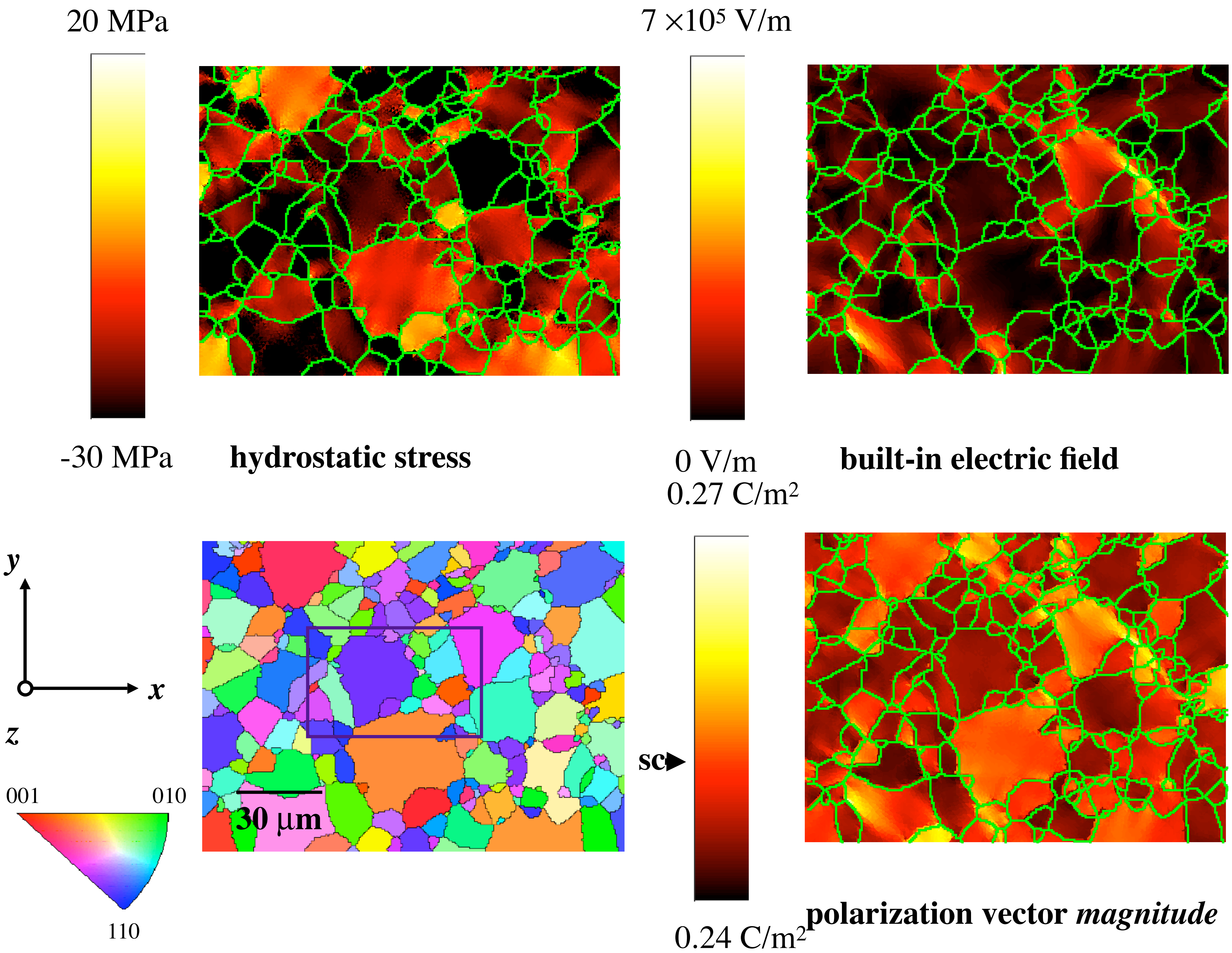


2 μm diameter probed area

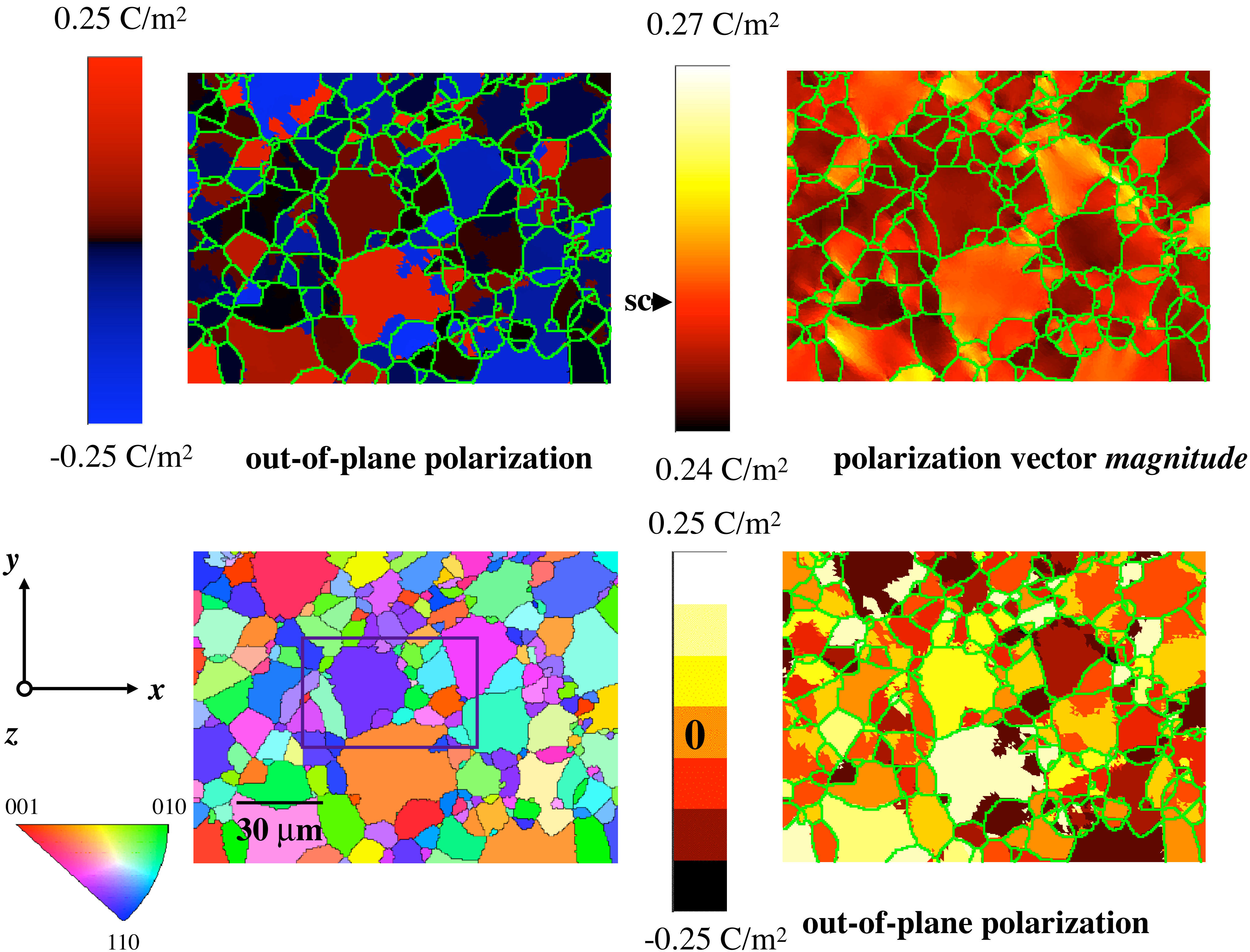

001
010
110
2 μm
Polarization (C/m²)
Electric Field (V/m)
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-1x10^7
-5x10^6
0
5x10^6
1x10^7
Polarization (C/m²)
Electric Field (V/m)
Polarization (C/m²)
Electric Field (V/m)



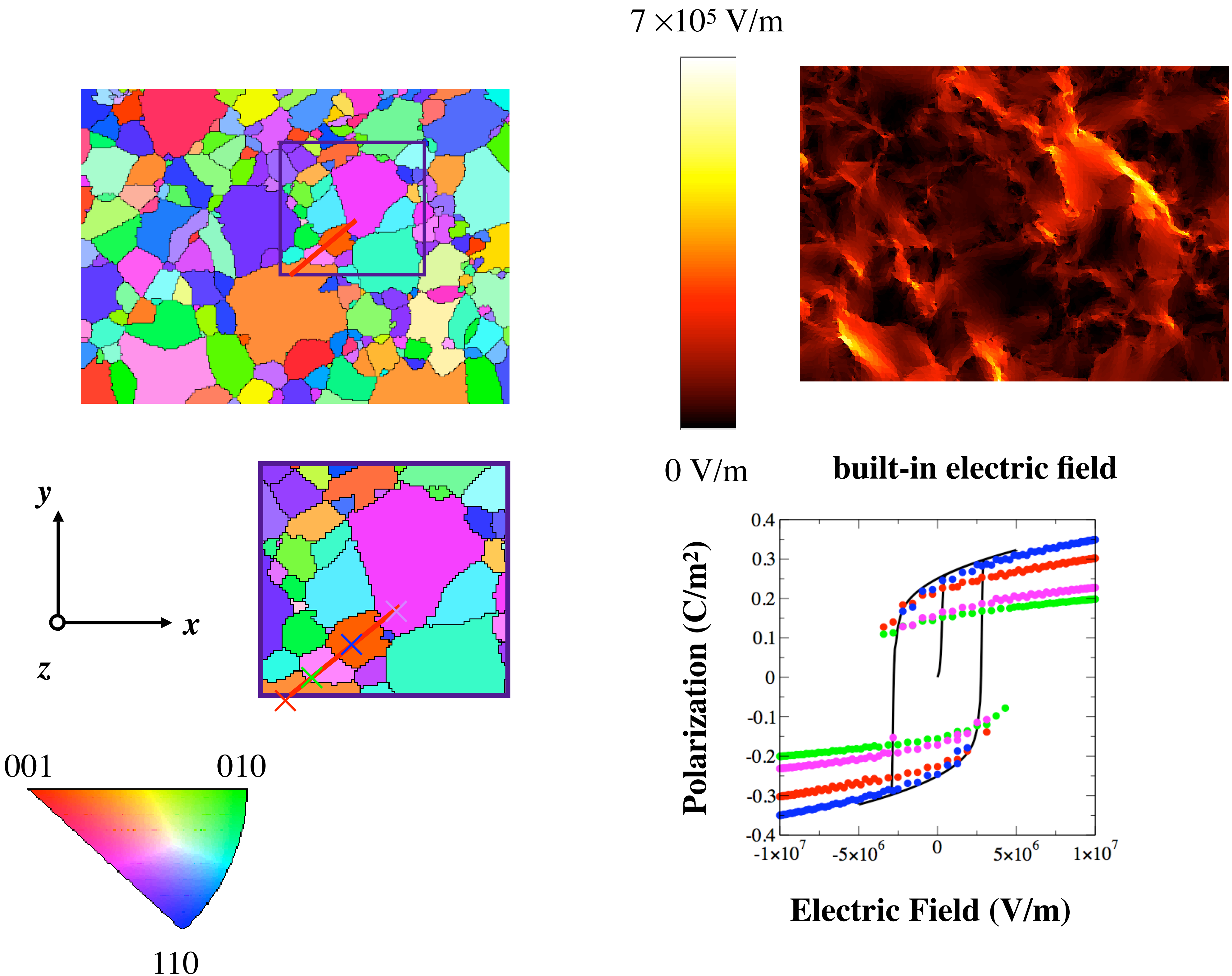
001
010
110
2 μm
Polarization (C/m²)
Electric Field (V/m)
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-1x10^7
-5x10^6
0
5x10^6
1x10^7
Polarization (C/m²)
Electric Field (V/m)
Experimental
Numerical
Normalized Hysteresis Area
distance (μm)
2.5
2
1.5
1
0.5
0
-4
-2
0
2
4
6
8



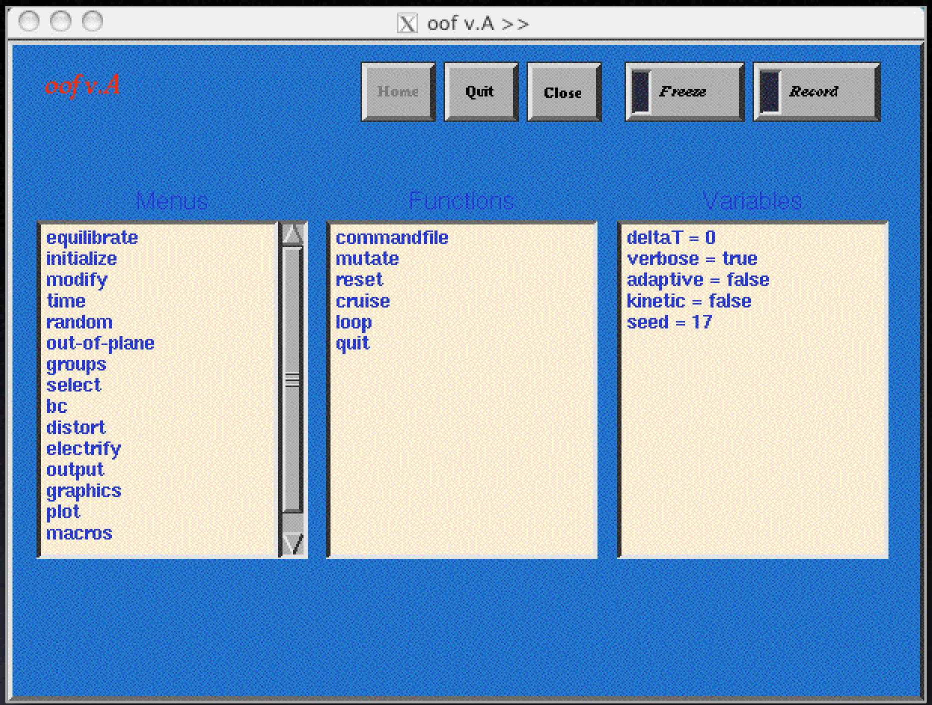
20 MPa
-30 MPa
hydrostatic stress
7 ×10⁵ V/m
0 V/m
built-in electric field
0.27 C/m²
0.24 C/m²
sc
polarization vector *magnitude*
y
x
z
30 µm
001
010
110



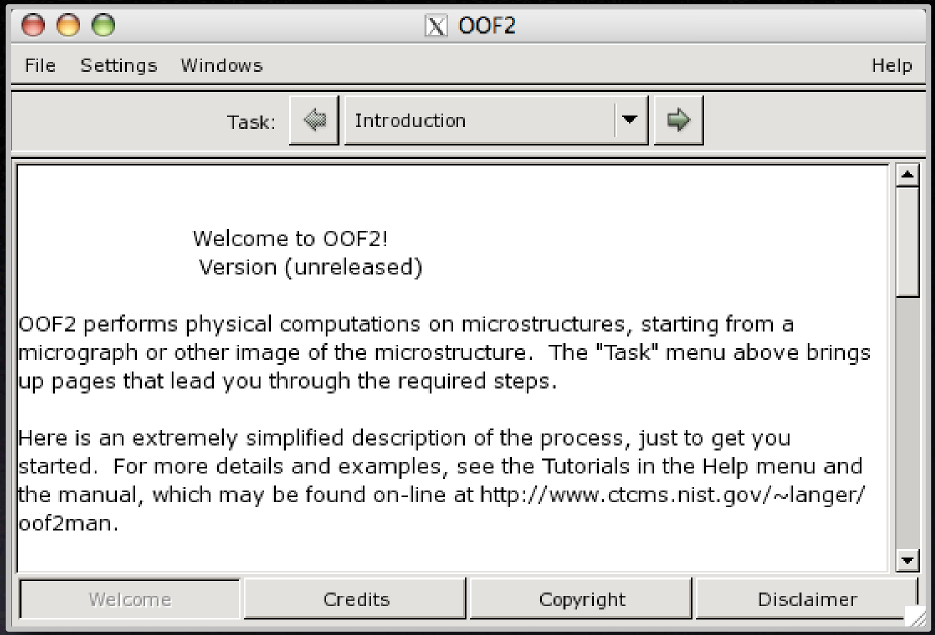
0.25 C/m^2
-0.25 C/m^2
out-of-plane polarization
0.27 C/m^2
sc
0.24 C/m^2
polarization vector *magnitude*
0.25 C/m^2
0
-0.25 C/m^2
out-of-plane polarization
y
x
z
001
010
110
30 µm


7 ×10^5 V/m
0 V/m
built-in electric field
y
x
z
001
010
110
Polarization (C/m²)
Electric Field (V/m)
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-1×10^7
-5×10^6
0
5×10^6
1×10^7

Ferroelectric oof



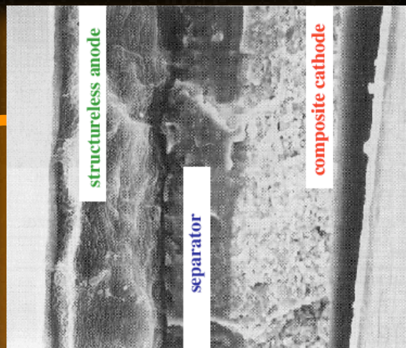
OOF2



Ferroelectric oof	OOF2
Coulomb's Equation	Coulomb's Equation
Piezoelectric Couplings	Generalized Piezoelectric Couplings
Non-Linear Solvers	Improved Non-Linear Solvers
Elementary Adaptive Meshing Tools	Advanced Adaptive Meshing Tools
Ferroelectricity	
Runge-Kutta Solvers	
Predictor-Corrector Method	

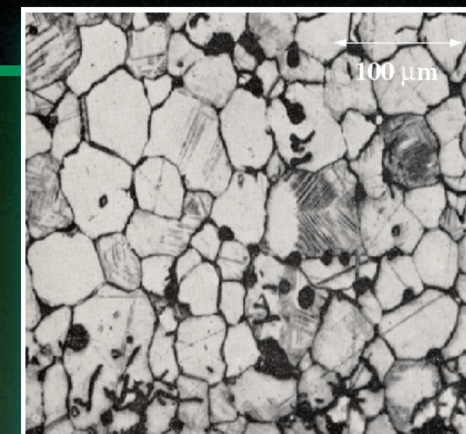
Outline

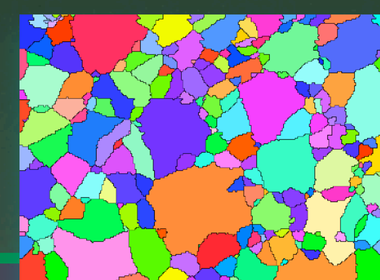
rechargeable batteries



Energy Materials

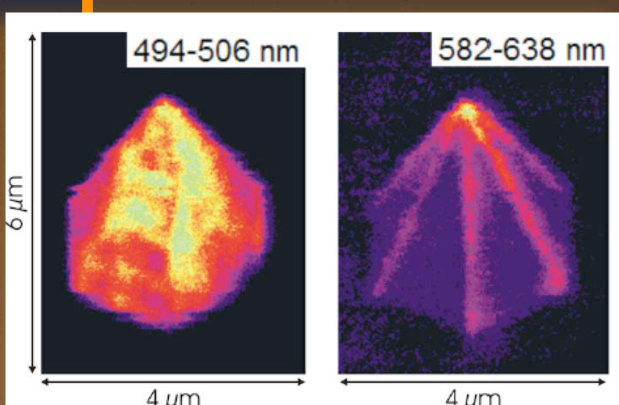
piezoelectrics and electrostrictors



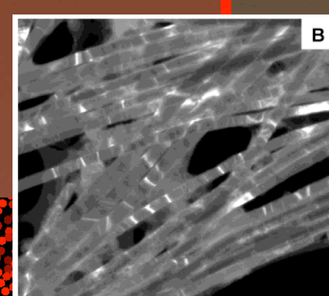


ferroelectrics

Actuator Materials

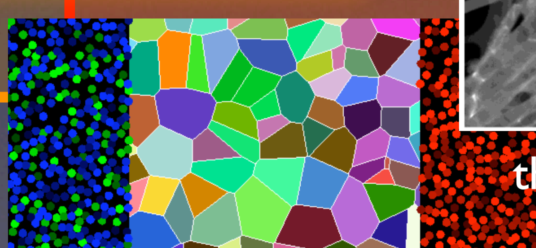


light emitting devices



Research

thermoelectric generators



solid oxide fuel cells

Credits

Ferroelectric Materials	Bryan Huey	UConn
	John E. Blendell	Purdue University
	W. Craig Carter	MIT
Rechargeable Batteries	Yet-Ming Chiang, W. Craig Carter	MIT
InGaN Light Emmiting Devices	Parijat Deb, Tim Sands	Purdue University
Electrochemical Actuators	Yet-Ming Chiang, Yukinori Koyama	MIT