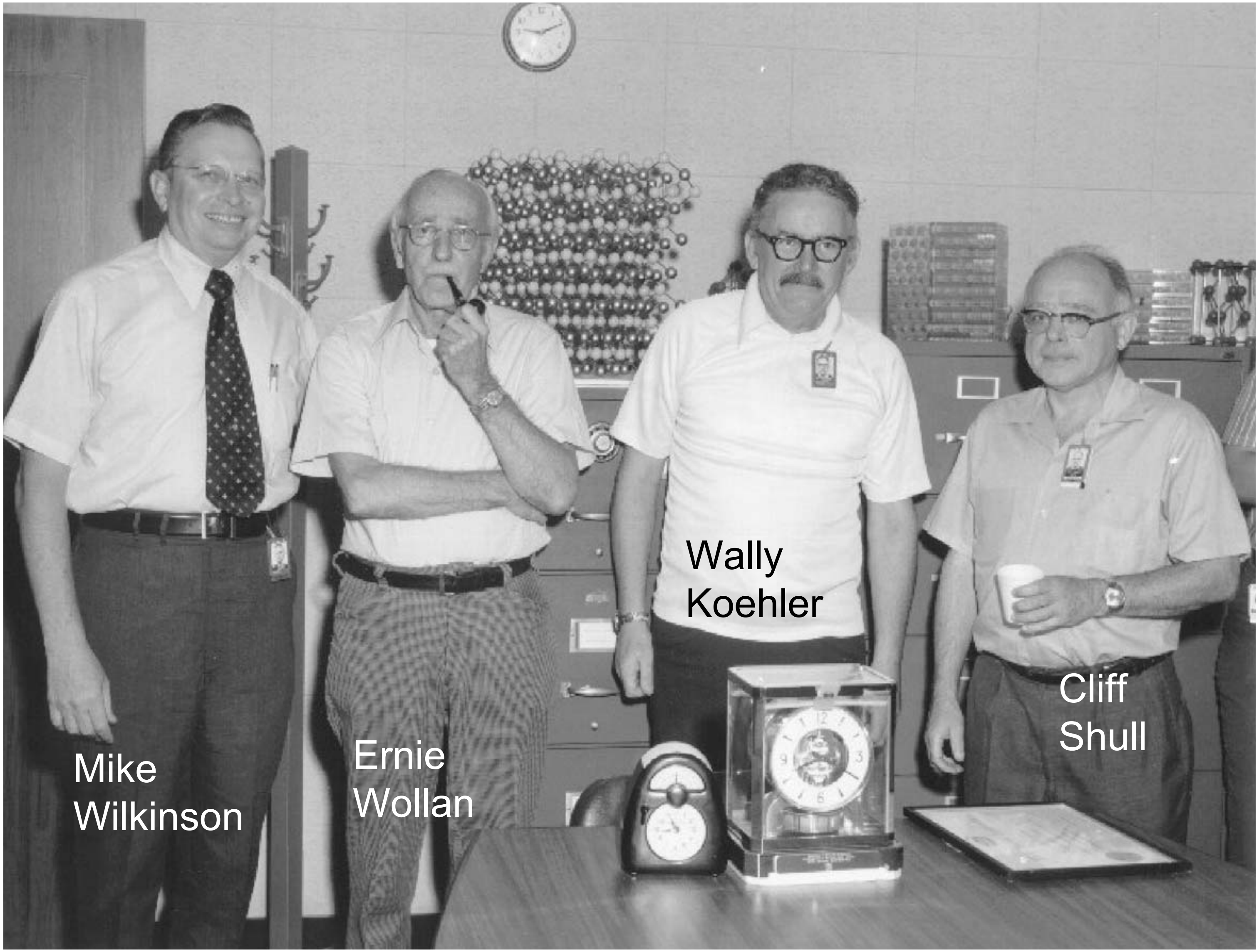
The Clifford G. Shull Prize

J. Michael Rowe

ACNS, June 7, 2004

Early Oak Ridge Team



Ralph Moon

Inveterate Committee Member

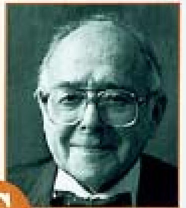
- By a rough count, I have served on over 50 in the last 30 years, excluding workshops, Temple and Lehman reviews
- Many for existing neutron sources – IPNS, LANSCE, HFIR, SNS, RRR
- Some unfortunately less successful – ANS, HFBR, INER
- Contrary to abstract, last mention…

The Nobel Prize in Physics 1994

The Royal Swedish Academy of Sciences has awarded the 1994 Nobel Prize in Physics for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter.

Neutrons reveal structure and *dynamics*

Clifford G. Shull, MIT, Cambridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.

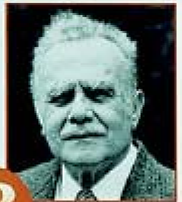


Shull made use of **elastic scattering** i.e. of neutrons which change direction without losing energy when they collide with atoms.

Because of the wave nature of neutrons, a diffraction pattern can be recorded which indicates where in the sample the atoms are situated. Even the placing of light elements such as hydrogen in metallic hydrides, or hydrogen, carbon and oxygen in organic substances can be determined.

The pattern also shows how atomic dipoles are oriented in magnetic materials, since neutrons are affected by magnetic forces. Shull also made use of this phenomenon in his neutron diffraction technique.

Bertram N. Brockhouse, McMaster University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.

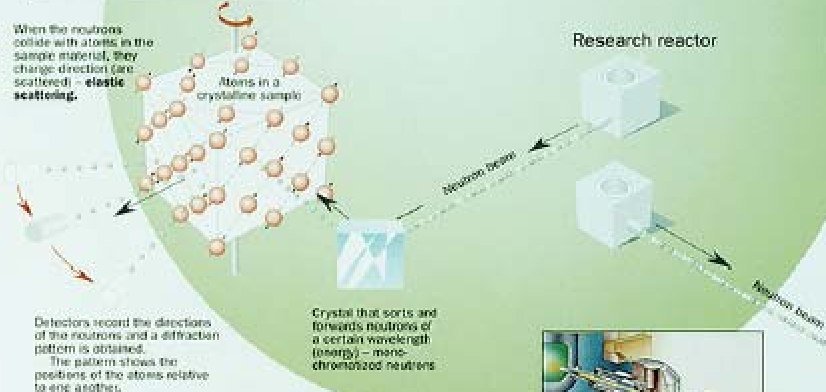


Brockhouse made use of **inelastic scattering** i.e. of neutrons, which change both direction and energy when they collide with atoms. They then start or cancel atomic oscillations in crystals and record movements in liquids and melts. Neutrons can also interact with spin waves in magnets.

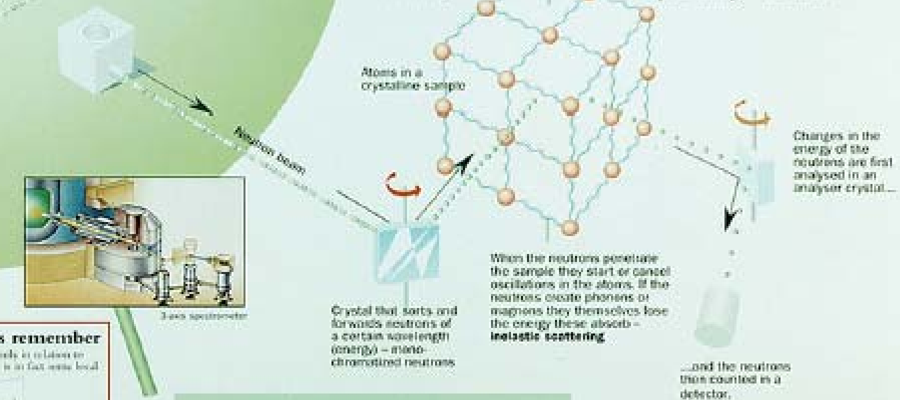
With his 3-axis spectrometer Brockhouse measured energies of phonons (atomic vibrations) and magnons (magnetic waves). He also studied how atomic structures in liquids change with time.

Neutrons bounce against atomic nuclei. They also react to the magnetism of the atoms.

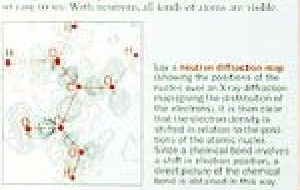
Neutrons show where atoms are



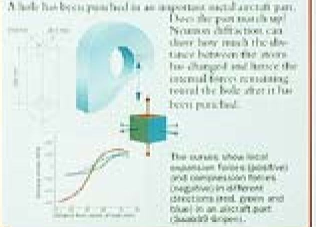
Neutrons show what atoms do



Neutrons see more than X-rays



Neutrons reveal inner stresses



Neutrons show what atoms remember

How it started

Brockhouse and Shull made their pioneering contributions at the first nuclear reactors in the USA and Canada back in the 1940s and 1950s. It was then that the resources of the reactors became available for peacetime research.

... how it continues

Thousands of researchers are now working at the many neutron research centers throughout the world. New and very advanced neutron scattering installations have been built and more are planned in Europe, the USA and Asia. At these super-installations the researchers are studying the structure of new ceramic superconductors, molecular movements on surfaces of interest for catalytic exhaust cleaning, virus structures and the connection between the structure and the elastic properties of polymers.

KUNGL. VETENSKAPSAKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

Further reading:

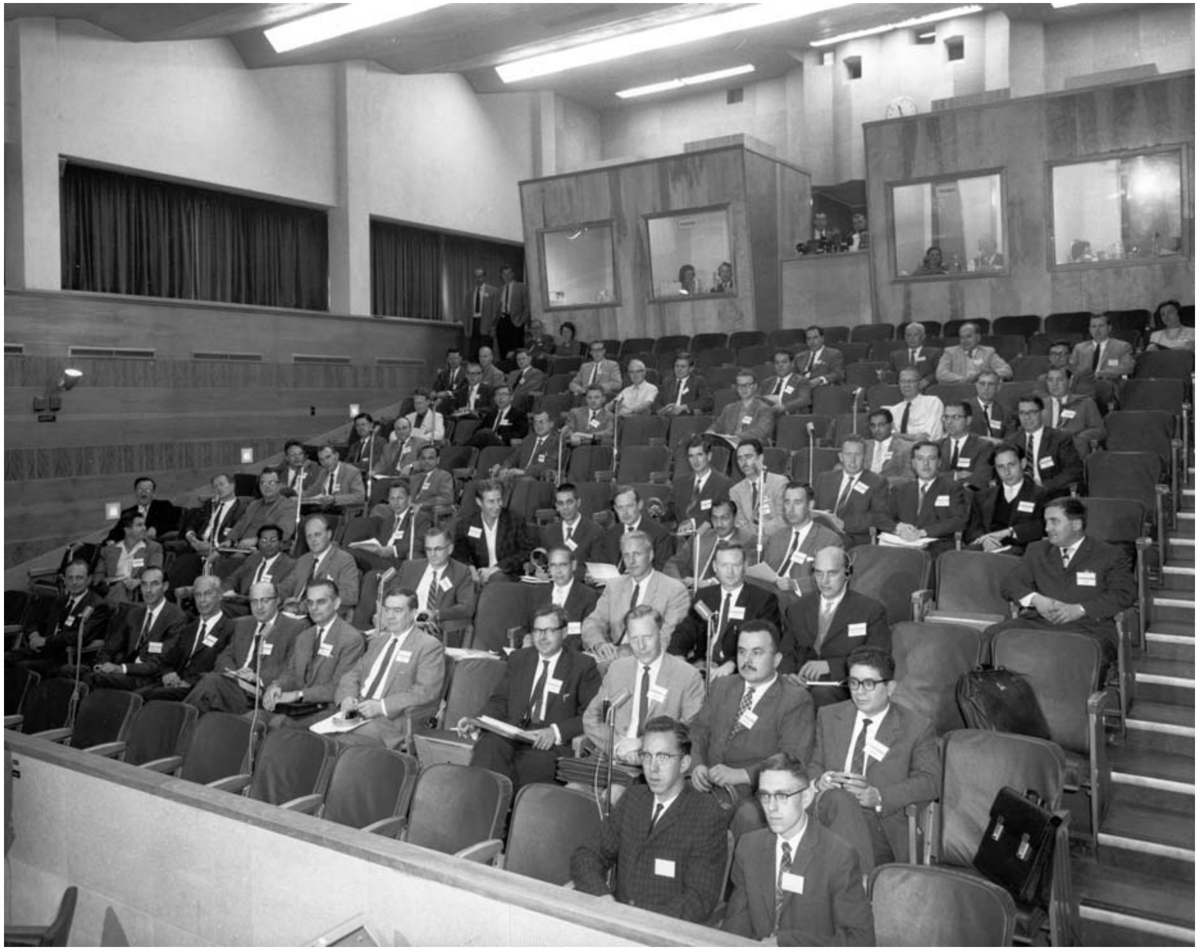
- D.J. Hughes *The Nuclear Reactor as a Research Instrument.* SCIENTIFIC AMERICAN, VOL. 189, AUGUST 1953, P. 23.
- H. Lengeler and J.L. Finney *The European Spallation Source,* EUROPHYSICS NEWS, VOL. 25, P. 77, 1994.
- *Information about the Nobel Prize in Physics 1994 (press release),* THE ROYAL SWEDISH ACADEMY OF SCIENCES.

B. N. Brockhouse & 3-Axis

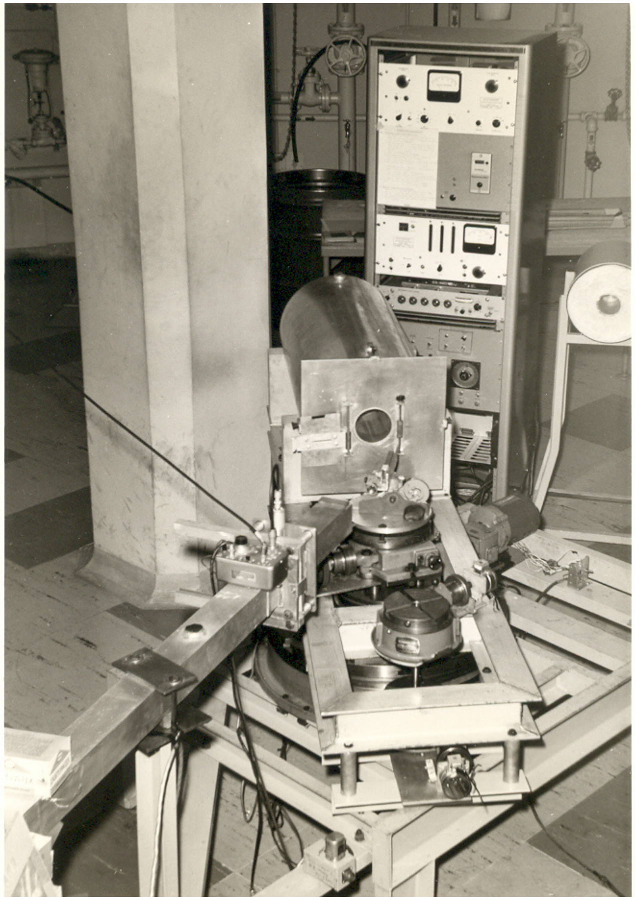
1962-1966

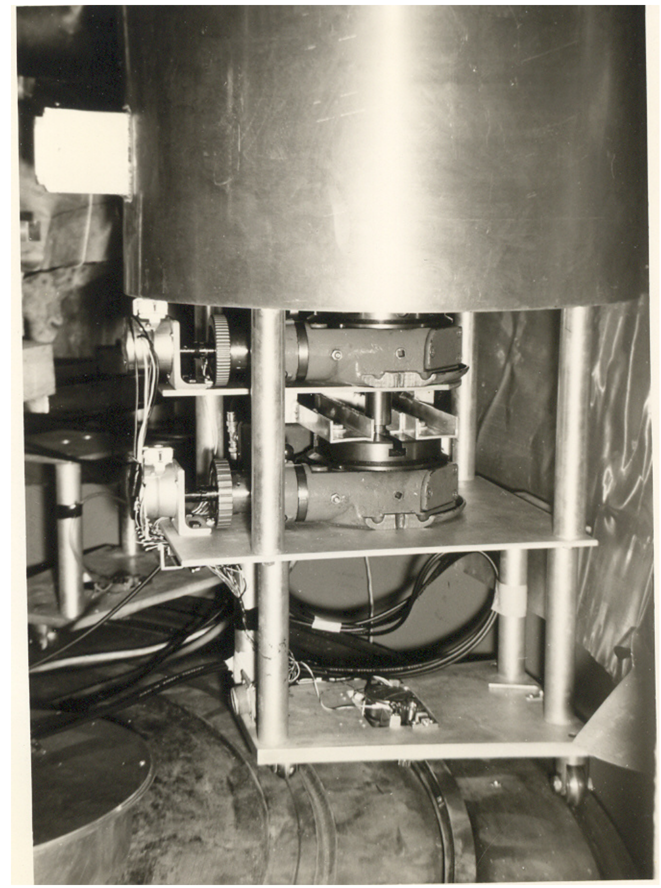
- One of Bertram Brockhouse’s first three PhD students along with Eric Svensson and Sow Hsin Chen
- PhD Theses were simpler then
  - Design and construction of 3-axis spectrometer
  - Measure lattice dynamics of a metal – ß-Sn

Inelastic Scattering 1962



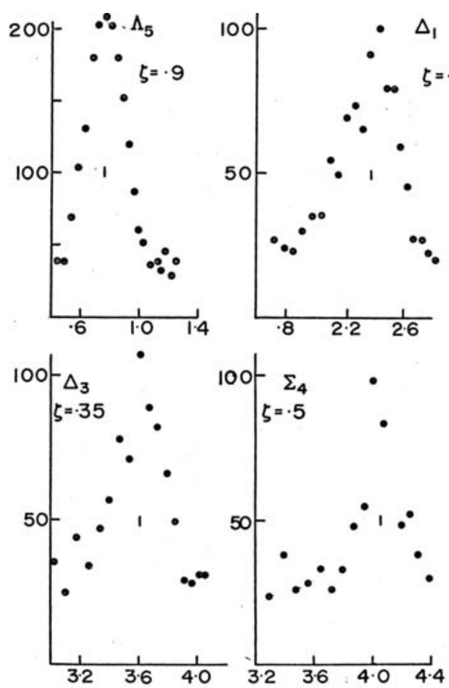
McMaster 2 and 3-axis

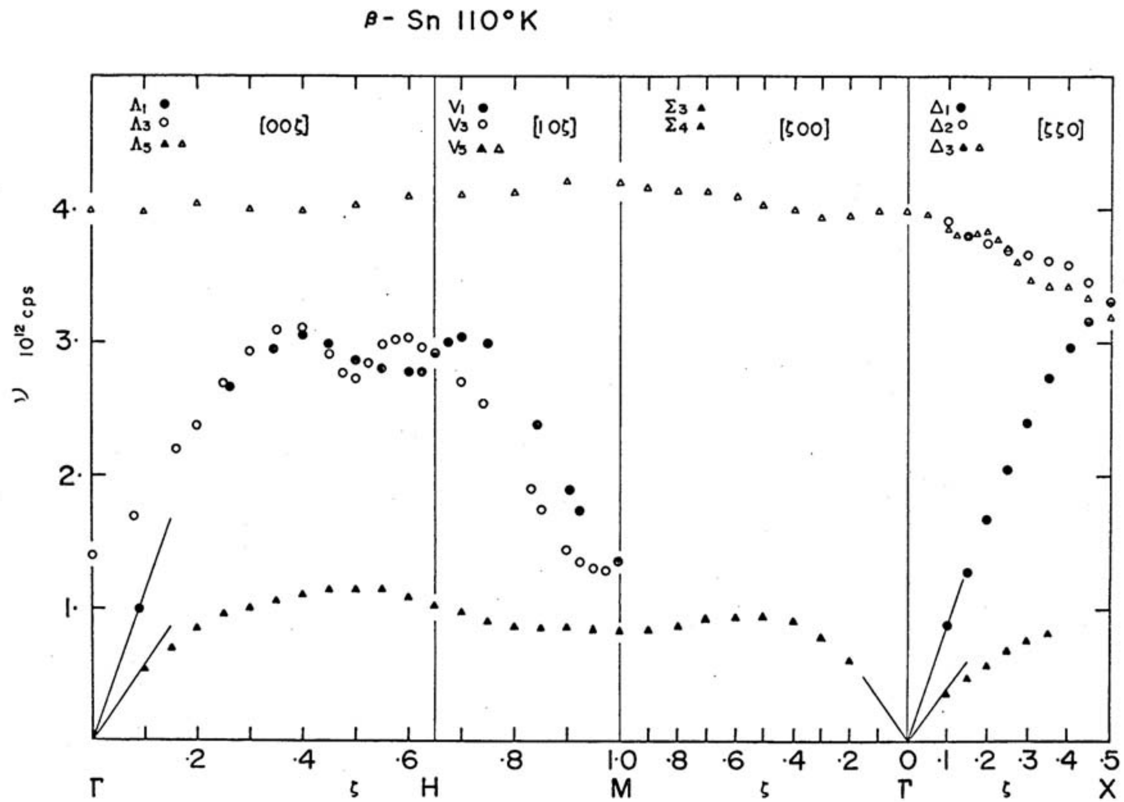




1960’s Automation!

Lattice Dynamics of ß-Sn





Argonne National Laboratory

- Post doctoral appointment in 1966, after meeting Jack Rush & Don Connor at HFBR criticality meeting
  - My first cold source (operate, not design), D_2O ice
  - First TOF spectrometer (4 chopper system)
  - David Price joined ANL, and we began a series of measurements on α-Sn, InSb & CdTe at HFIR, working with Harold Smith and Bob Nicklow

Argonne National Laboratory II

- David, Bob Kleb, George Ostrowski, & I built TNTOFS (LRMECS flight path) as part of CP-5 complex with Selmer Peterson & Jack Williams
- Lot’s of fun with science
  - Liquid Ar (Kurt Sköld, Pete Randolph at MTR)
  - Many molecular reorientations with Jack Rush
  - Hydrides (Pd, Nb, Ta…)
  - Cyanides (Susman, Hinks KCN, NaCN)
  - Aneesur Rahman

Assorted Results

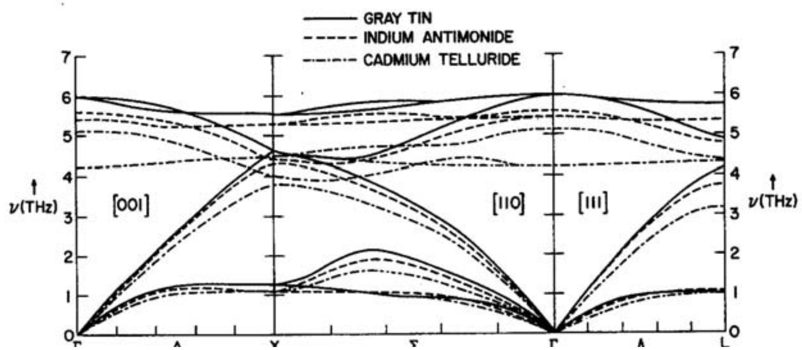
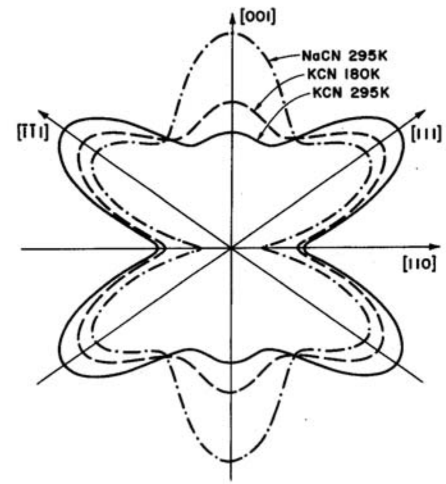


FIG. 2. Dispersion relations for α-Sn (solid lines), InSb (dashed lines), and CdTe (chain lines) derived from shell-model calculations using the parameters of Table III.



Inelastic Neutron Scattering from a Liquid ^3He-^4He Mixture*

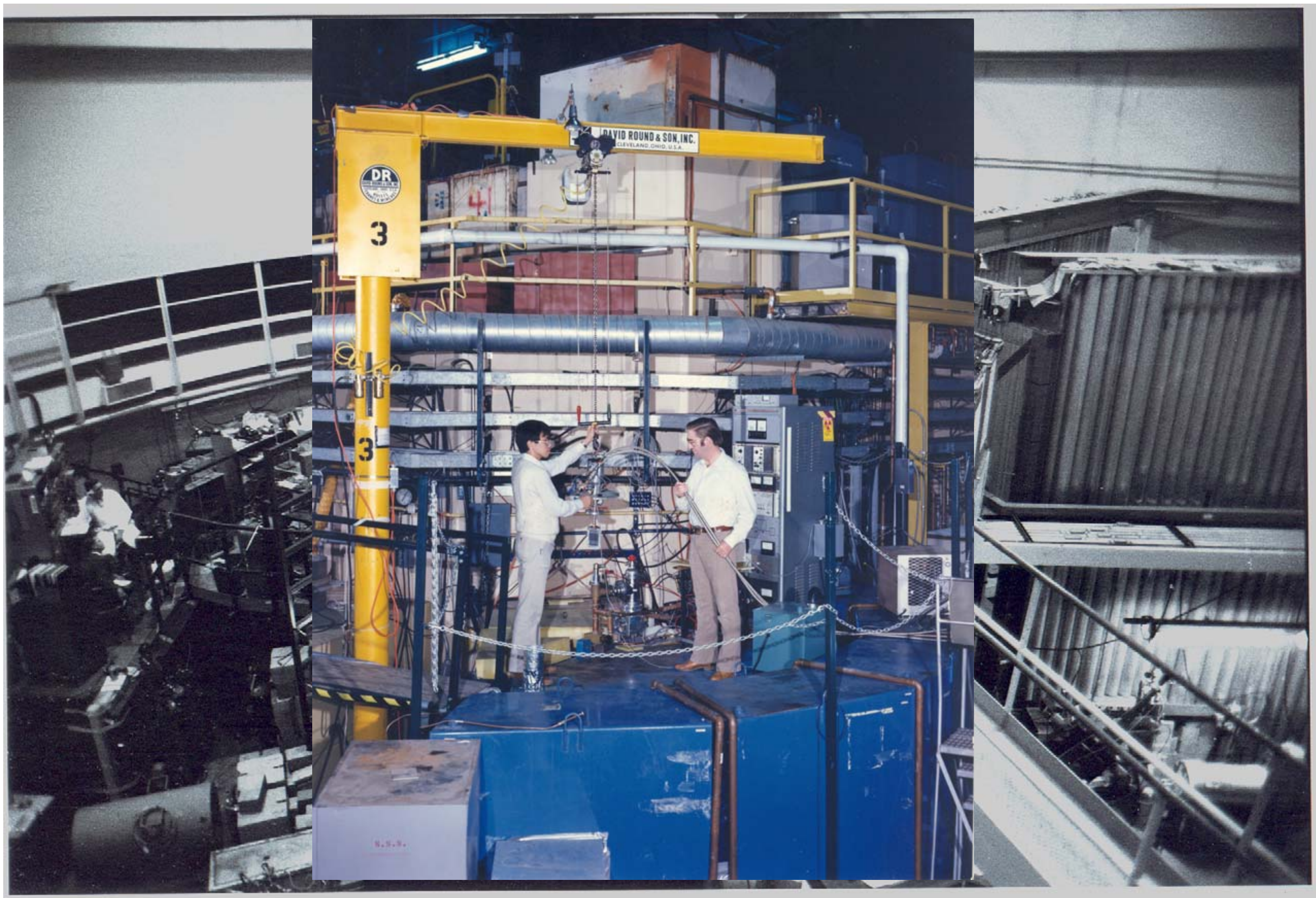
J. M. Rowe
Solid State Science Division, Argonne National Laboratory, Argonne, Illinois 60439, and Institute for Materials Research, National Bureau of Standards, Washington, D. C. 20234

and

D. L. Price and G. E. Ostrowski
Solid State Science Division, Argonne National Laboratory, Argonne, Illinois 60439

(Received 18 June 1973)

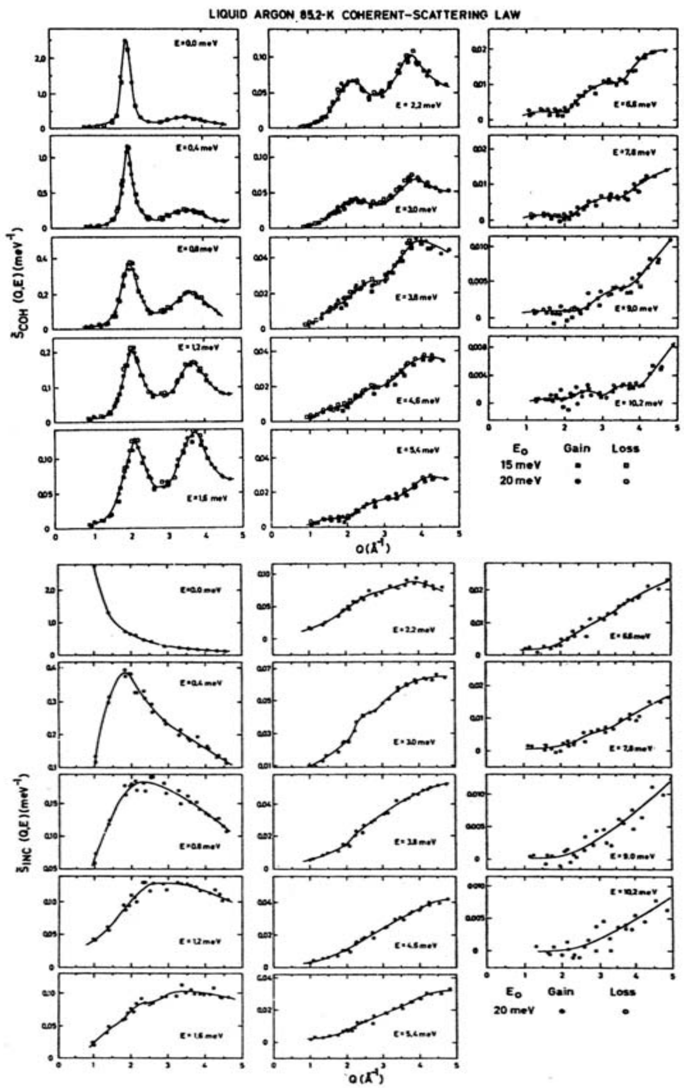
TNTOFS

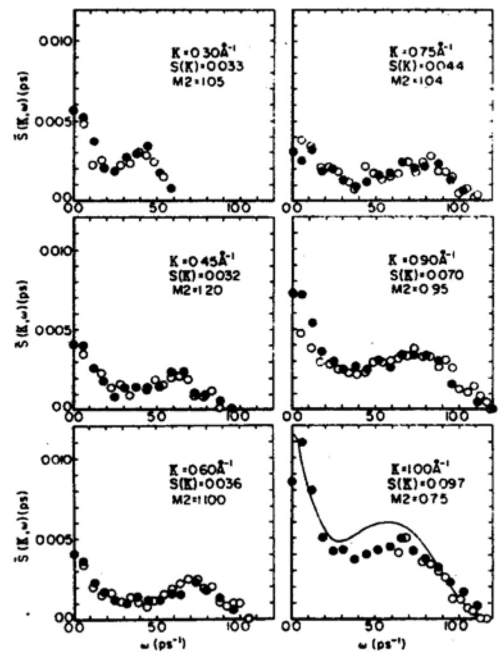


Serendipity & Liquids

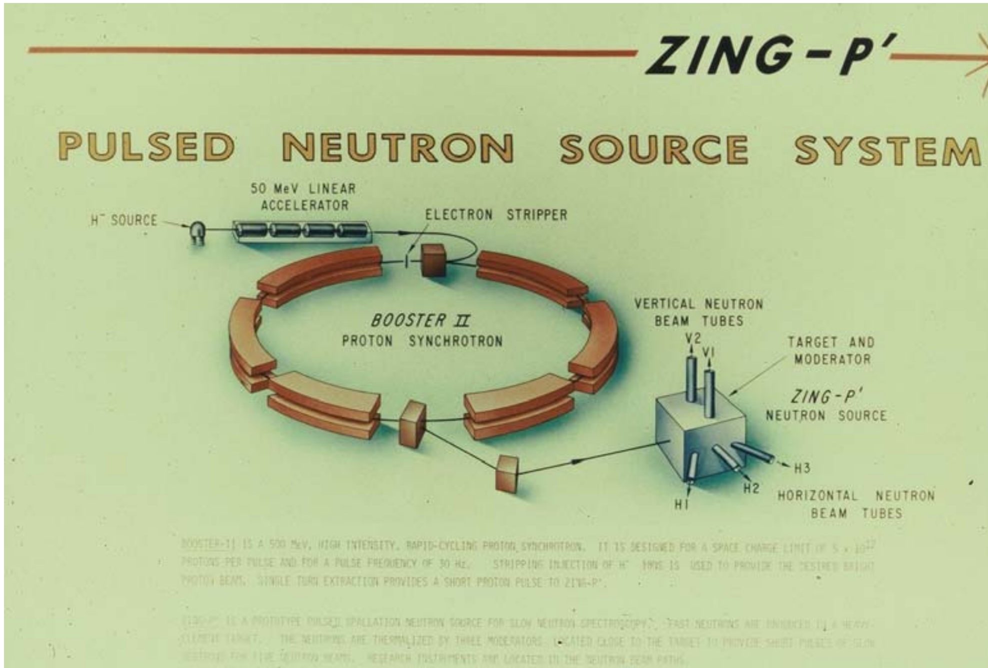
- Kurt Sköld was post-doc
  - Liquid argon Coherent & Incoherent (MTR)
- Aneesur Rahman
  - “RAD Terminal” across from my office
  - Anees & I got to know each other
  - Liquid Rb MD & Experiment (John Copley)
    - MD predicted collective excitations at low Q
    - We measured them at TNTOFS (after I left)

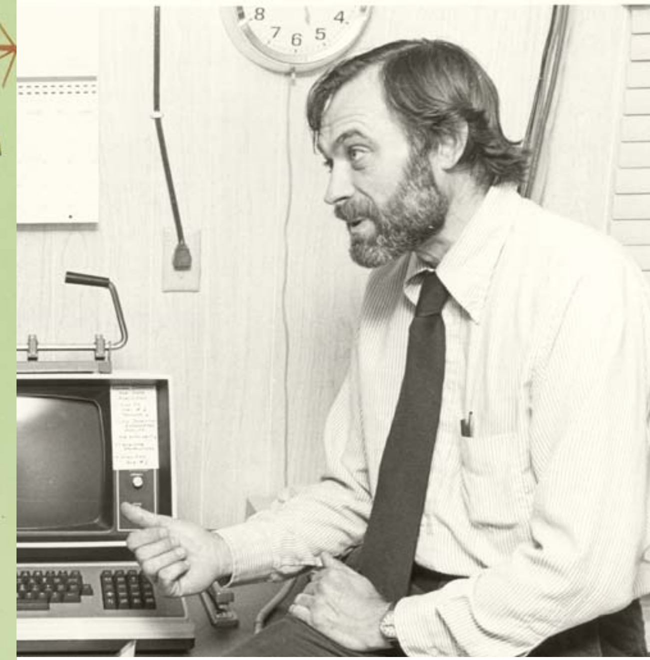
Liquids

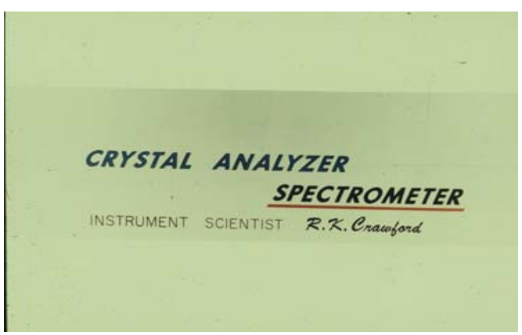

LIQUID ARGON 85.2-K COHERENT-SCATTERING LAW
E = 0.0 meV
E = 0.4 meV
E = 0.8 meV
E = 1.2 meV
E = 1.6 meV
E = 2.2 meV
E = 3.0 meV
E = 3.8 meV
E = 4.6 meV
E = 5.4 meV
E = 6.6 meV
E = 7.8 meV
E = 9.0 meV
E = 10.2 meV
E0 Gain Loss
15 meV
20 meV
Q (Å-1)


K = 0.30 Å-1
S(K) = 0.033
M2 = 1.05
K = 0.75 Å-1
S(K) = 0.044
M2 = 1.04
K = 0.45 Å-1
S(K) = 0.032
M2 = 1.20
K = 0.90 Å-1
S(K) = 0.070
M2 = 0.95
K = 0.60 Å-1
S(K) = 0.036
M2 = 1.00
K = 1.00 Å-1
S(K) = 0.097
M2 = 0.75
S̃(K, ω) (ps)
ω (ps-1)

ZING-P Building


ZING-P'
PULSED NEUTRON SOURCE SYSTEM
50 MeV LINEAR ACCELERATOR
H⁻ SOURCE
ELECTRON STRIPPER
BOOSTER II
PROTON SYNCHROTRON
VERTICAL NEUTRON BEAM TUBES
V2
V1
TARGET AND MODERATOR
ZING-P'
NEUTRON SOURCE
H1
H2
H3
HORIZONTAL NEUTRON BEAM TUBES




CRYSTAL ANALYZER SPECTROMETER
INSTRUMENT SCIENTIST R.K. Crawford

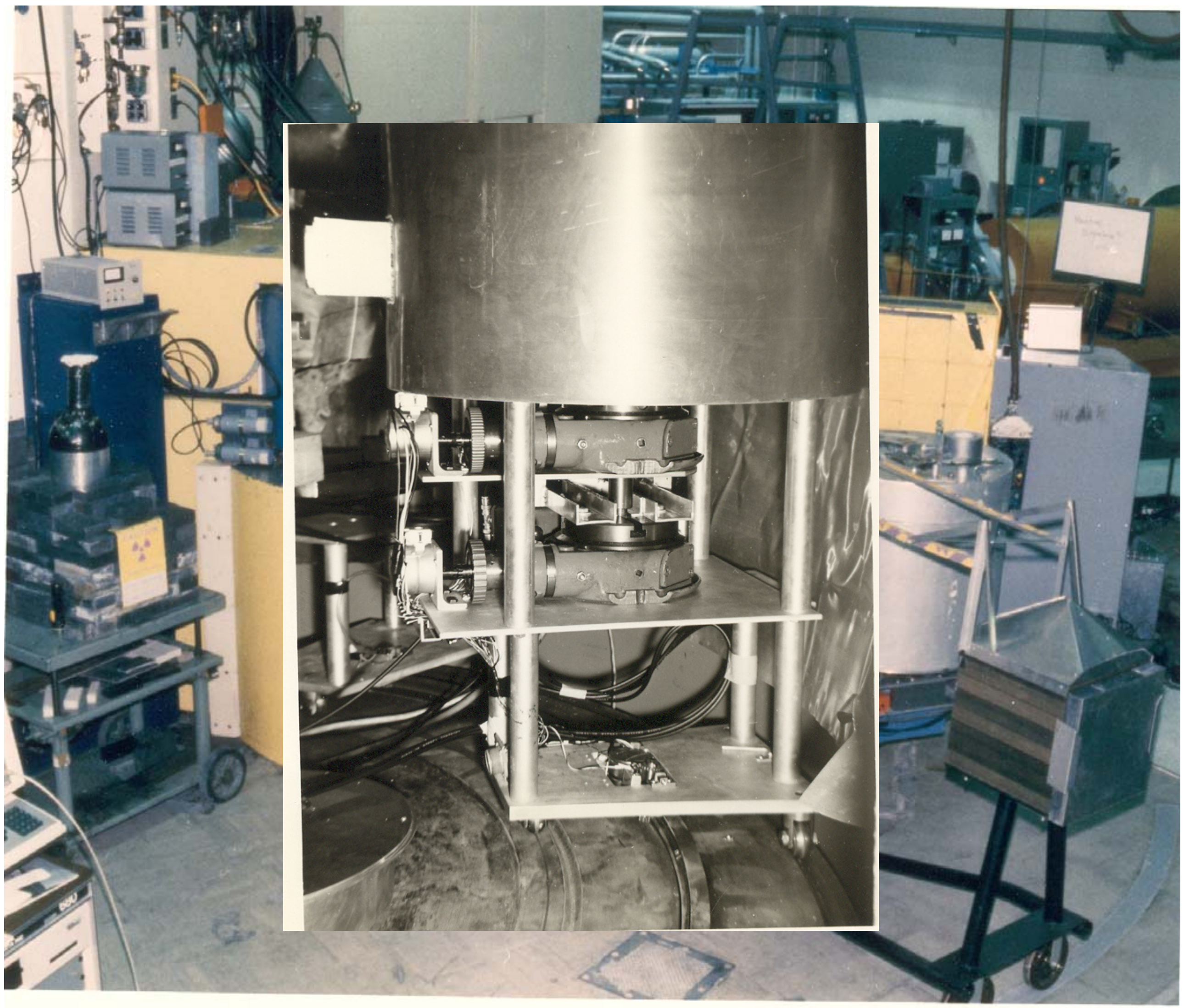

HIGH RESOLUTION POWDER DIFFRACTOMETER
INSTRUMENT SCIENTIST J.D. Jorgensen


CHOPPER SPECTROMETER
INSTRUMENT SCIENTIST C.A. Pelizzari

NBS 1973-1979

- Came to NBS in 1973, with promise from Jack Rush – **NO MANAGEMENT**
- Began design of BT-4 triple-axis with Jack Rush, Sam Trevino and Hank Prask in 1972
- Decided on Ames design, went to inspect, and met Nancy Chesser (m 1/1/75)
- Bought drum from Ames, and installed at NBSR 1973-1975

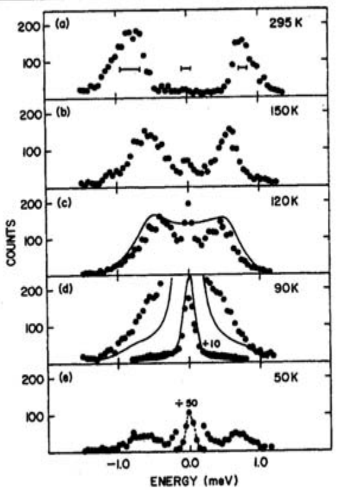
BT-4 Triple Axis

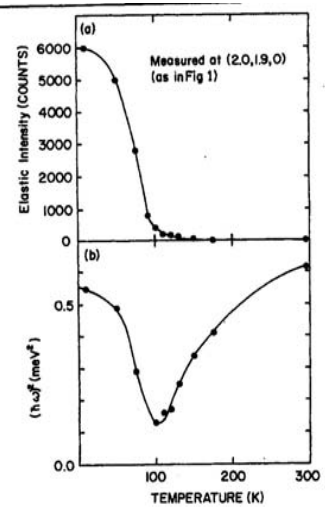


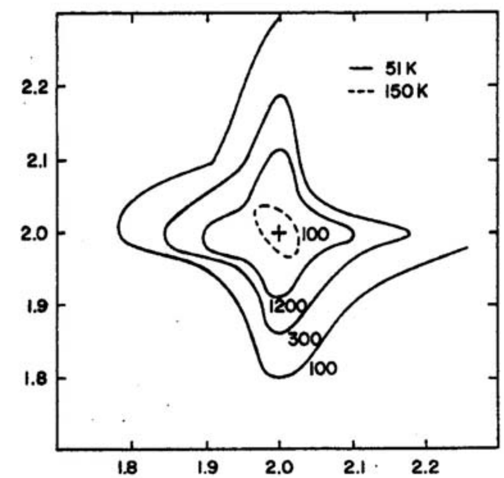
NBS 1973-1979

- **Mostly science after BT-4**
  - **Structure and dynamics KCN, NaCN, RbCN, CsCN**
    - **Soft TA mode**
    - **Quadrupolar, dipolar phase transitions**
    - **Steric hindrance, strain scattering**
  - **Mixed alkali halide/alkali cyanides, quadrupole glass state**
- **Metal hydrides**
  - **PdH, PdD, PdT dynamics (old high T_c days)**
  - **Ta, Nb, $CeD_{2.12}$, trapping, storage hydrides…**

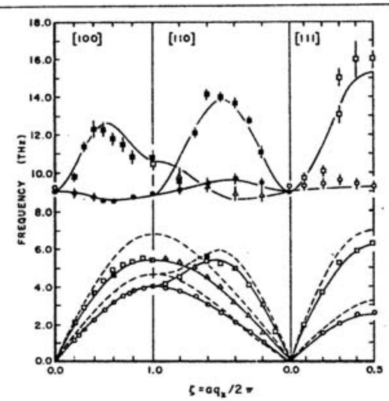
Science Results



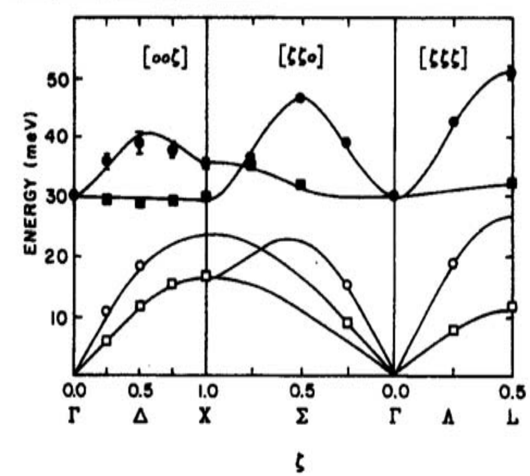




PdD$_{0.6}$



PdT$_{0.6}$



NBS 1980-87

- First NBS “Competence Project” in 1979
  - Built 8m SANS (Charlie Glinka on staff)
  - Started our first real visualization effort & first fast network (Norm Berk, “Roger Ramjet”)
- IMSE crosscut circa 1983, CNRF proposal
- Seitz-Eastman 1984
- First \$1.5 M in FY1985
- D_2O ice cold source installed 1987
- Construction funding FY1987

CNRF Estimate

Original Estimate

~$3K/m² – LANL 1M

Building, penetration, safety analysis, neutron guides, $15.0
½M
new cold source plug

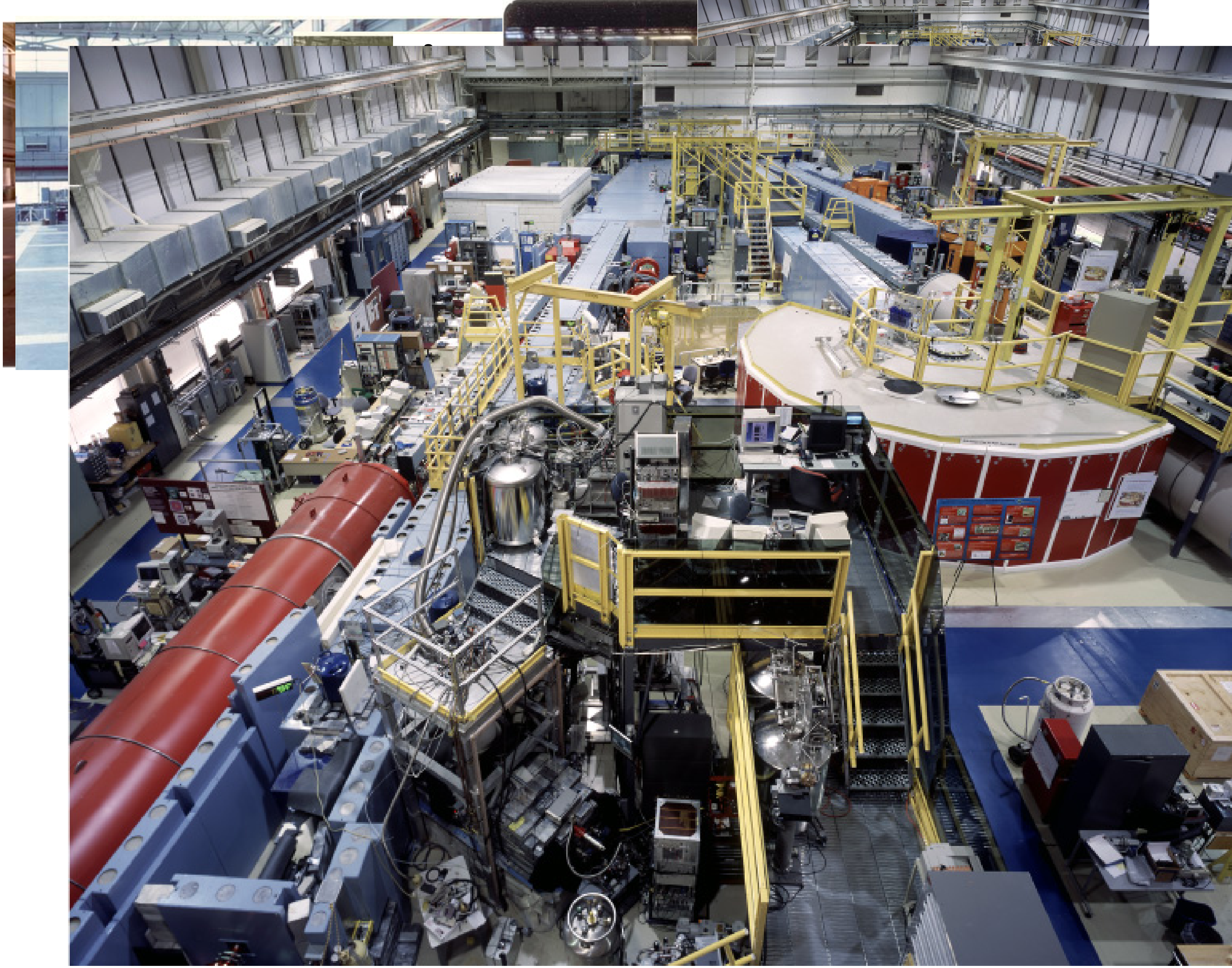
Instruments (initial complement) 6/8 new, 2 upgraded 8.00
Includes data acquisition.

Contingency 3

$ 26.0M

Management Days 1987-2004

- Began construction of guide hall in fall of 1987
  - Ivan Schroder & I became construction managers
- Dedicated guide hall January 1989
- CHRNS partnership with NSF started 1989
  - Originally 30m SANS, ½ SPINS
  - Now includes 7 instruments in shared program



Management Days 1987-2004

- **All planned instruments operating, time to start recycling, replacing…**
- **Installed 2nd Generation hydrogen source in 2000 (Bob Williams and Paul Kopetka were my partners in both sources)**
  - Factor of two gain for most wavelengths
  - 100% reliability last year
- **Submitted license renewal application 4/9/2004**
- **Division Chief 1989; Center Director 1997; Retired March 2004**

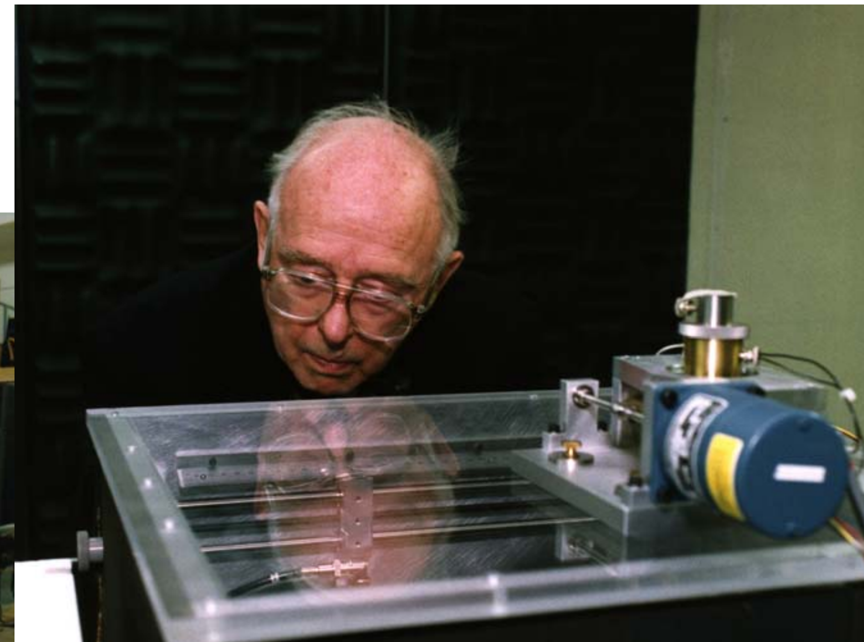
Three Who Made it Possible

Bob Carter

Carl Muehlhause

Harry Landon

Cliff Visits the NCNR



Triple Axis Developments

Lessons?

- Be lucky!
  - Thesis advisor (the world came to BNB)
  - Room assignment (A. Rahman)
  - Choose instruments well (meet spouse)
  - Work with outstanding people at great places (far too many to mention)
- All decisions are temporary (“no management”)

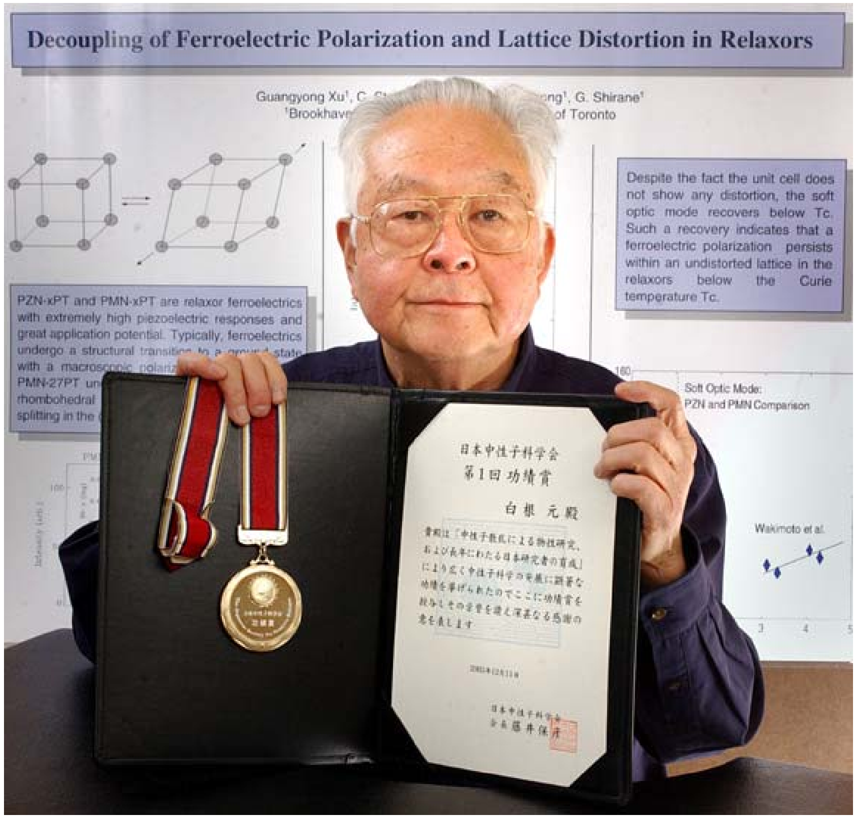
Conclusions?

- Bert always said that an experimentalist has to get the data right, and should err in interpretation if anywhere.
- Therefore, I want to spend a little time on my thoughts and predictions for the future.
- These are personal, and subject to Bert’s dictum.

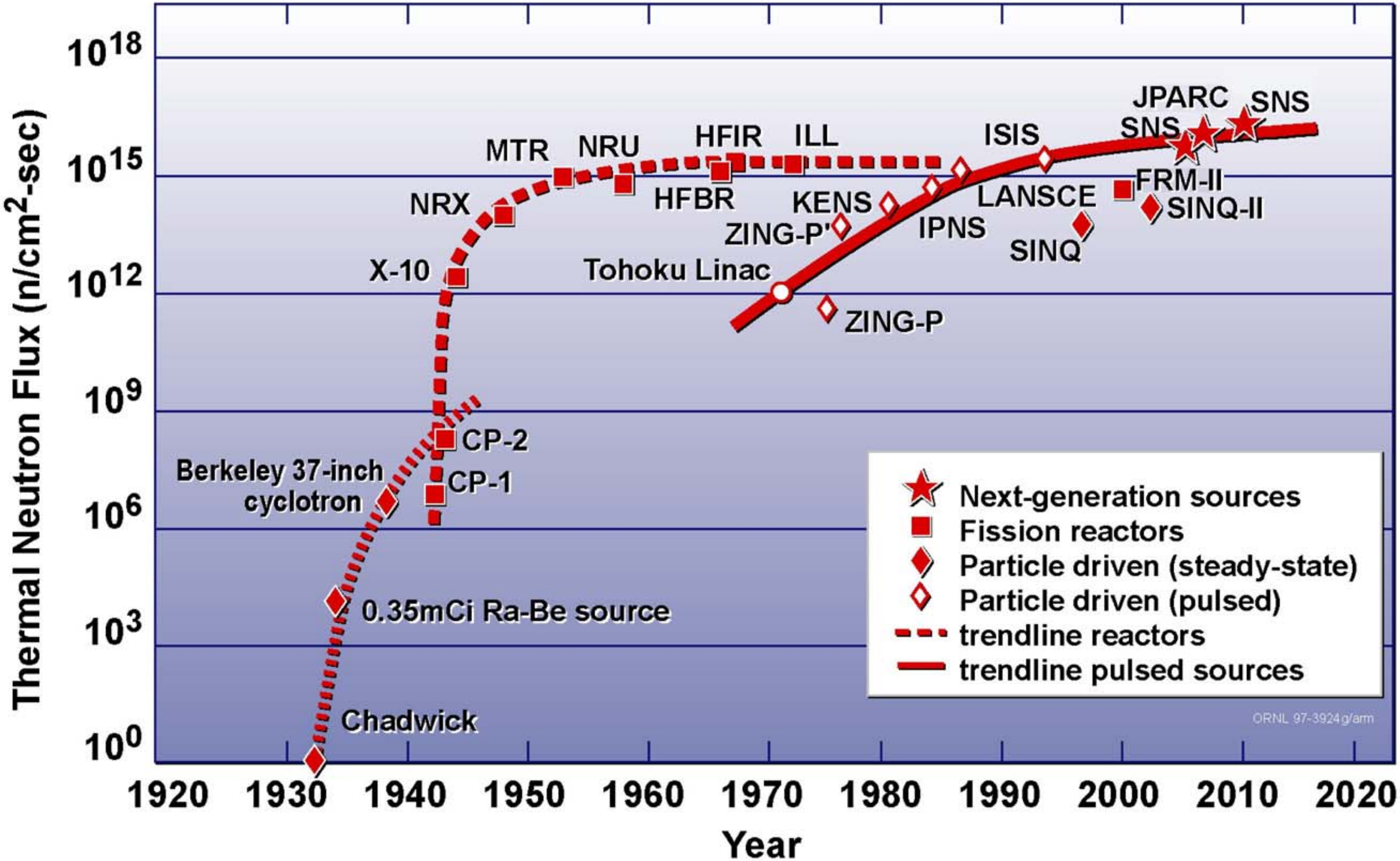
Trends

- In my 42 years, sources only increased in flux by approximately x10 (NRU to HFBR, HFR, HFIR)
- Capabilities increased by x100 to x1000
  - Detectors (number, solid angle)
  - Instrument designs (Spin echo, HFBS…)
  - Monochromator design (PG, bent crystals, horizontal and vertical focussing)
  - Neutron guides (regular, ^{58}Ni, supermirror, ballistic…)
  - Sample Environment (Stress, P,T,H…)
- Pulsed sources (ZING-P $\rightarrow$ IPNS $\rightarrow$ ISIS $\rightarrow$ SNS)
  - $\cong 3 \times 10^4$ allowing *qualitative* changes in techniques
- Facility use evolved from 95% professional NS $\rightarrow$ 20%; community has grown

Gen Shirane 80 Birthday
July 15, 2004



Source Development



(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)

Future

- **Techniques will continue to improve**.
  – Existing sources not fully exploited
  – SNS opens new opportunities
- **IT will transform the user experience**
  – 1966 PDP-8; 1973 PDP-11; 1980 VAX; 2000 Beowulf clusters; 2010 ?
  – Facilities world-wide will agree on standard user interfaces
  – Data analysis will be real time (models, simulations…),allowing science to be the focus
  – Remote access will grow, in spite of firewalls and other security issues

Future II

- Budget situation in US is tight, and will get worse; it will then get better!
- Science drives everything
  - Funding of current sources (including SNS) depends on scientific and engineering output
  - Current users must help make case
  - Any new source will only be considered when the science REQUIRES it
- Personally, I intend to participate, because it will be fun.