Thermal Neutron Scattering Research – Bettis Perspective

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History

- Thermal neutron scattering was active area of applied physics research in 1950s-1960s
- AEC Reactor Development Division sponsored a sizable thermal neutron scattering research program at General Atomics from 1960-1970
  - Integral (analytical) research program to develop theoretical TSL evaluations and processing tools (evaluations & analytical methods tightly coupled)
    - Central Force Models fit to experimental material structural, mechanical, thermodynamic properties
  - Differential research program to validate theoretical evaluations
    - Measurements used GA LINAC (best available facility at the time)
    - Experimental TSL evaluations not pursued by GA - inferior approach & impractical
- GA research program/strategy very **successful** and **productive**
  - Produced all ENDF TSLs until the adoption of modified Mattes & Keinert H-H_2O TSL in ENDF/B-VII.0
- No significant technical improvements to analytical methods over intervening 55 years

Recent History

- In early 2000s Bettis and NCSU independently recognized computational material science tools have matured and can be used to develop theoretical TSLs from first principles
- Bettis funded integration of VASP (density functional theory) and PHONON (lattice dynamics) codes into MedeA computational material science framework
  - Bettis developed theoretical TSLs for metal hydrides for internal use in classified applications
- NCSU first organization outside NR Program to use VASP/PHONON to generate theoretical TSLs from first principles
  - 2011 NCSU graphite differential scattering measurements at SNS
- NR/NCSP collaboration begun in FY2014-FY2015
  - NCSU theoretical TSL development (Bettis matching funding)
  - RPI MD simulations and SNS measurements (NR pass through)

Lessons Learned

- Theoretically developed TSLs preferred evaluation strategy
  - DFT/lattice dynamics (VASP/PHONON) approach suitable for solid moderators for which incoherent approximation is appropriate
    - Metal hydrides, ice, …
  - MD simulations suitable for liquid and amorphous moderators
    - H_2O, Lucite, CH_2, …
    - Available force fields sufficient for organic and inorganic material evaluated to date
  - Relaxation of incoherent approximation will extend DFT/lattice dynamics approach to include solid moderators exhibiting interference effects
    - Polycrystalline materials (Be, BeO, Graphite, UO_2, …)
    - Bettis independently pursuing modifications to PHONON to support coherent interference calculations

- Validation strategy
  - Validation using SNS differential neutron scattering measurements are practical
    - Can be used directly for liquids and amorphous materials
    - Integrate over alpha for apples/apples comparison of TSLs using the incoherent approximation
    - Can be used directly once incoherent approximation is relaxed
  - Supplement using neutron transmission, thermophysical property measurements, and benchmark testing

Lessons Learned (Continued)

- Experimentally developed TSLs not practical
  - Cost/difficulty to adequately sample $S(\alpha,\beta)$ in α,β space needed for most applications
  - Concerns about ability to measure all relevant conditions
  - Concerns about experimental resolution

Bettis Recommended Strategy

- Follow **proven GA development strategy**
- Develop TSL evaluations based on theory
  - DFT/lattice dynamics for polycrystalline materials
  - MD simulations for liquids and amorphous materials
- Validate theoretical TSL evaluations via measurements
  - Differential neutron scattering (SNS or similar facilities)
  - Neutron transmission (RPI or similar facilities)
  - Thermophysical properties (heat capacity, enthalpy, entropy, …)
  - Integral experiment benchmarks (when available)
- Improve analytical tools to remove unnecessary approximations
  - Generalize elastic scattering treatment to any crystal structure
  - Remove incoherent, cubic, and Gaussian approximations
  - Add support for natural input format from MD simulations
  - Covariance data support

When Are We Done

- Updated analytical methods to relax unnecessary approximations
  - Need to refresh after 55 years of inactivity
- Updated TSL evaluations in ENDF/B
  - Important to criticality safety
  - Important to reactor design
- Trained cadre of professionals who can continue progress in this area for another decade or two
- NCSP not in this alone, NR has **mutual interest**
- NR providing support
  - Matching funding for theoretical TSL and analytical methods work by NCSU (Bettis)
  - Facilitating MD simulation and SNS measurements by RPI (NR pass through)

Coming Attractions

- Bettis working to provide independently developed TSL evaluations to NNDC in FY2016
  - Yttrium Hydride (YH_2)
  - Hexagonal Ice
- Bettis considering independent development of additional TSLs in out years
  - ZrH_2 (gamma, delta, epsilon phases)
  - $H\text{-}UH_3$
  - $H\text{-}PuH_2$
- Critical mass and stability in TSL development community will provide long-term benefits to NCSP and NR