Technical Program Review
Nuclear Criticality Safety Program
March 15 – 16, 2016 • SNL, Albuquerque, NM, USA

Thermal Scattering Law Data Generation and Advanced Methods Development

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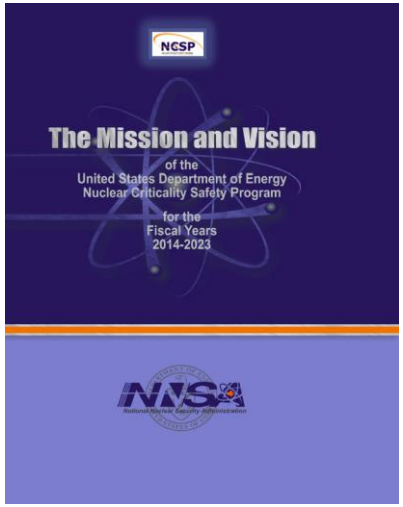
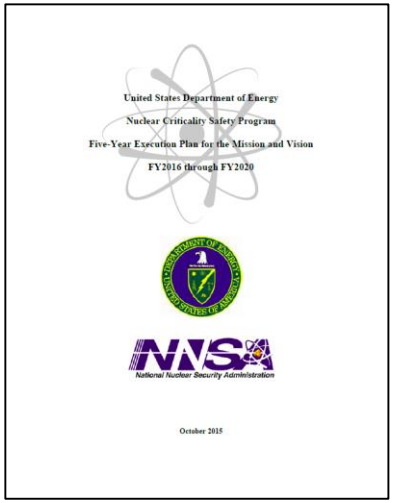
Acknowledgement

- Funding by the NCSP and NNPP programs
- Collaboration with LLNL and BAPL
- Undergraduate and graduate students and postdocs at North Carolina State University

Objectives

1. Generate TSL file 7 libraries (and related cross section files) for materials of interest to NCSP and NNPP
2. Develop the next generation tool for TSL data generation





Appendix B
Nuclear Data

Priority Needs */ **Additional Needs**	Thermal scattering (BeO, HF, D_2O, SiO_2, CH_2, C_2F_4, $C_5O_2H_8$, etc.), ^{239}Pu, Cr, ^{237}Np, Pb, ^{55}Mn, Ti, ^{240}Pu / ^{233}U, Th, Be, ^{51}V, Zr, F, K, Ca, Mo, Na, La

Progress to Date

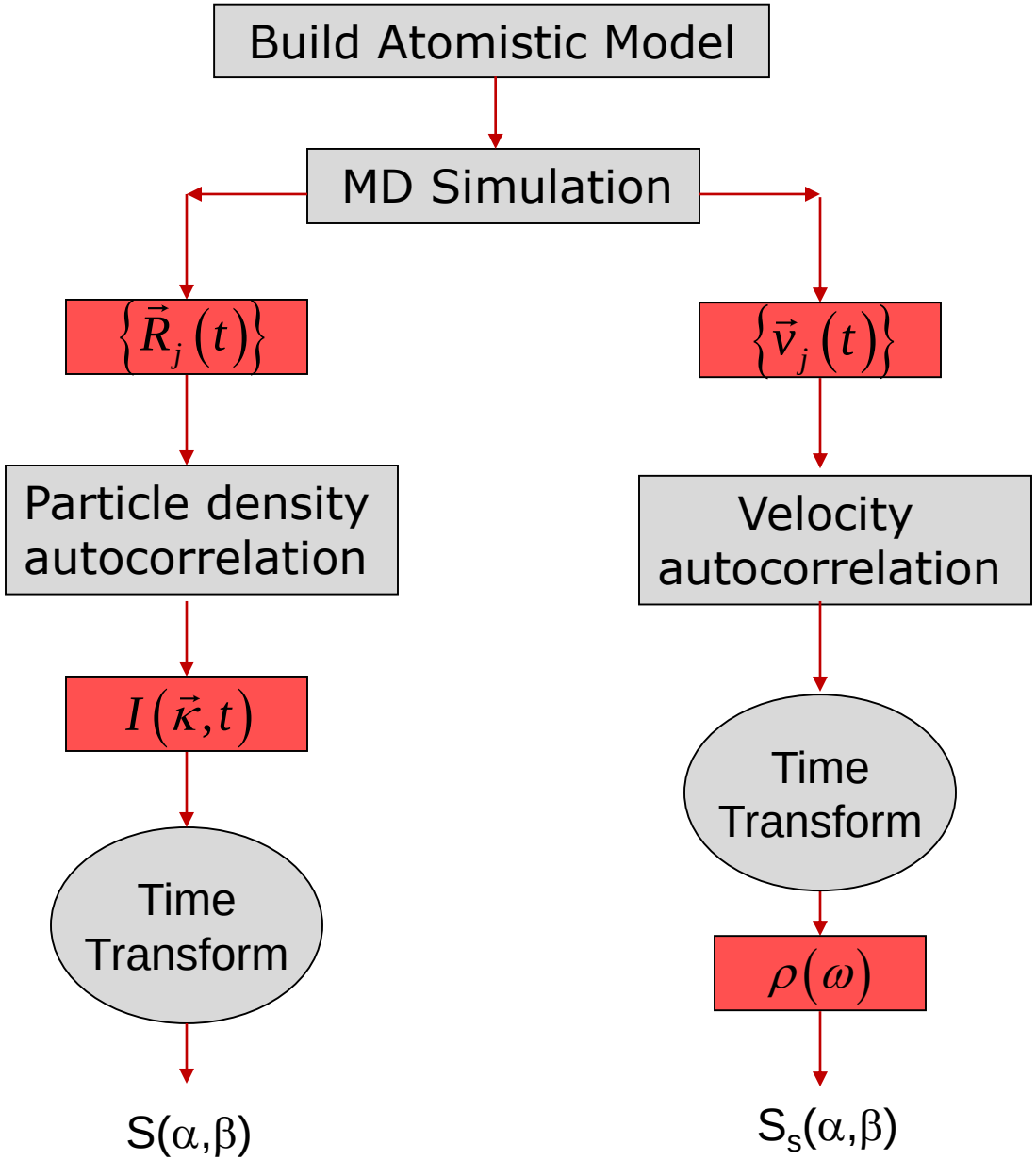
Task	Expected completion	Actual completion	Comments
SiO_2	FY'14	FY'14	Contributed to NNDC
SiC	FY'14	FY'14	Contributed to NNDC
$(C_5H_8O_2)_n$	FY'15	FY'15	Contributed to NNDC
$(CH_2)_n$	FY'16	FY'15	File 7 ready for NNDC
Lubricant Oil	FY'17		On going
TSL Code Development	FY'16		1) Code flow and structure 2) Generalized coherent elastic scattering module 3) Generalized coherent inelastic scattering module

Publications

1. Y. Zhu, A. I. Hawari, "Implementation of a Generalized Coherent Elastic Scattering Formulation for Thermal Neutron Scattering Analysis," Proceedings of International Conference on Nuclear Criticality Safety, Charlotte, NC, USA, 2015.

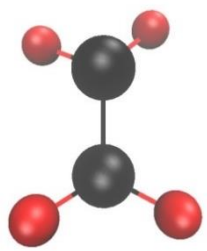
2. A. I. Hawari, A. Petersen, Y. Zhu, J. L. Wormald, D. P. Heinrichs, M. L. Zerkle, "Analysis of Thermal Neutron Scattering in Polymethyl Methacrylate (Lucite)," *Trans. American Nuclear Society*, 113, 2015.

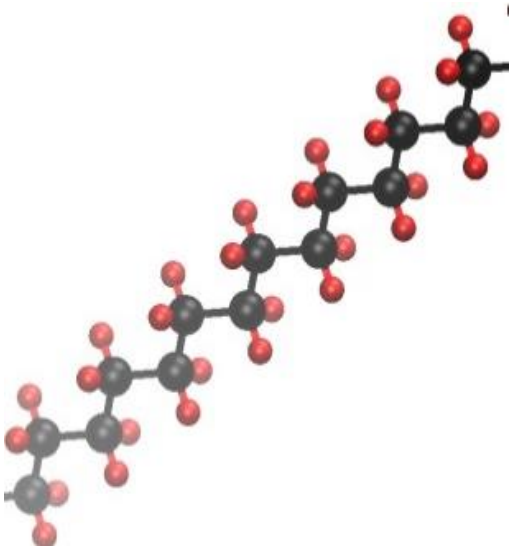
3. Several abstracts (eventually papers) have been submitted to ND 2016

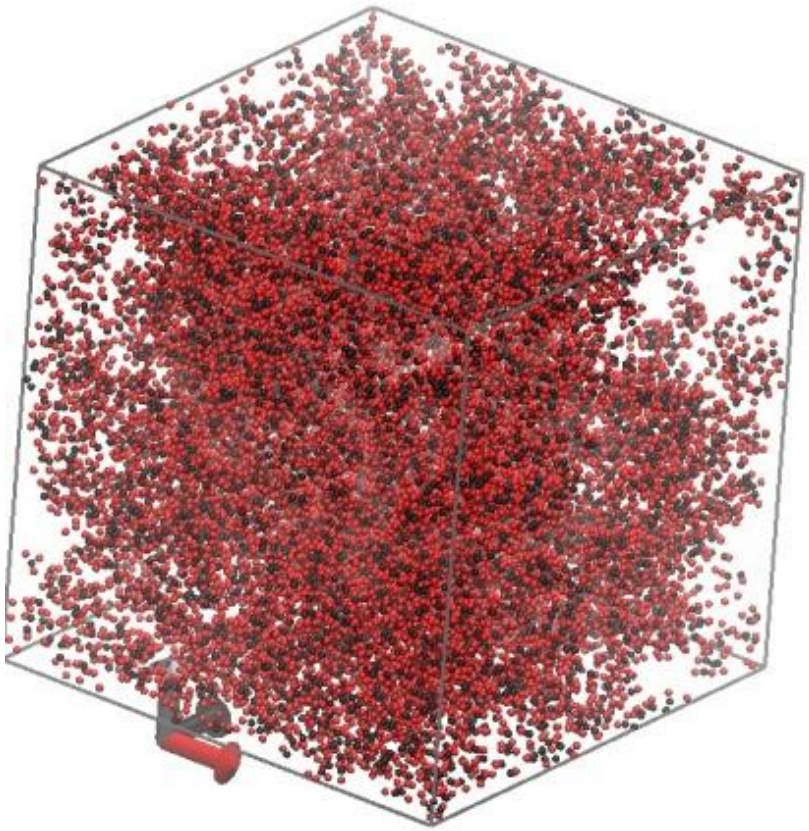

Build Atomistic Model
MD Simulation
$\{\vec{R}_j(t)\}$
$\{\vec{v}_j(t)\}$
Particle density autocorrelation
Velocity autocorrelation
$I(\vec{\kappa},t)$
Time Transform
Time Transform
$\rho(\omega)$
S(α,β)
$S_s(\alpha,\beta)$

Polyethylene MD Model

- Poly(ethylene) polymer
- 20 polymer chains
- 200 monomers (C_2H_4) long
- 24000 atoms







MD Potential Function

$$E = E_{vdw} + E_Q + E_B + E_A + E_T$$

$$E_{vdw} = AR^{-12} - BR^{-6}$$

$$E_Q = CQ_iQ_j/\epsilon R_{ij}$$

$$E_B = {}^1/_2\, k_0(R - R_0)^2$$

$$E_A = {}^1/_2\, K_{IJK}\left(cos\theta_{IJK} - cos\theta\right)^2$$

$$E_T = E_{IJKL} = {}^1/_2\, V_{JK}\{1 - cos[n_{JK}(\varphi - \varphi_{Jk}^0)]\}$$

Dreiding force field

L-J (VDW) term:

Fitted for the system to match the experimental density

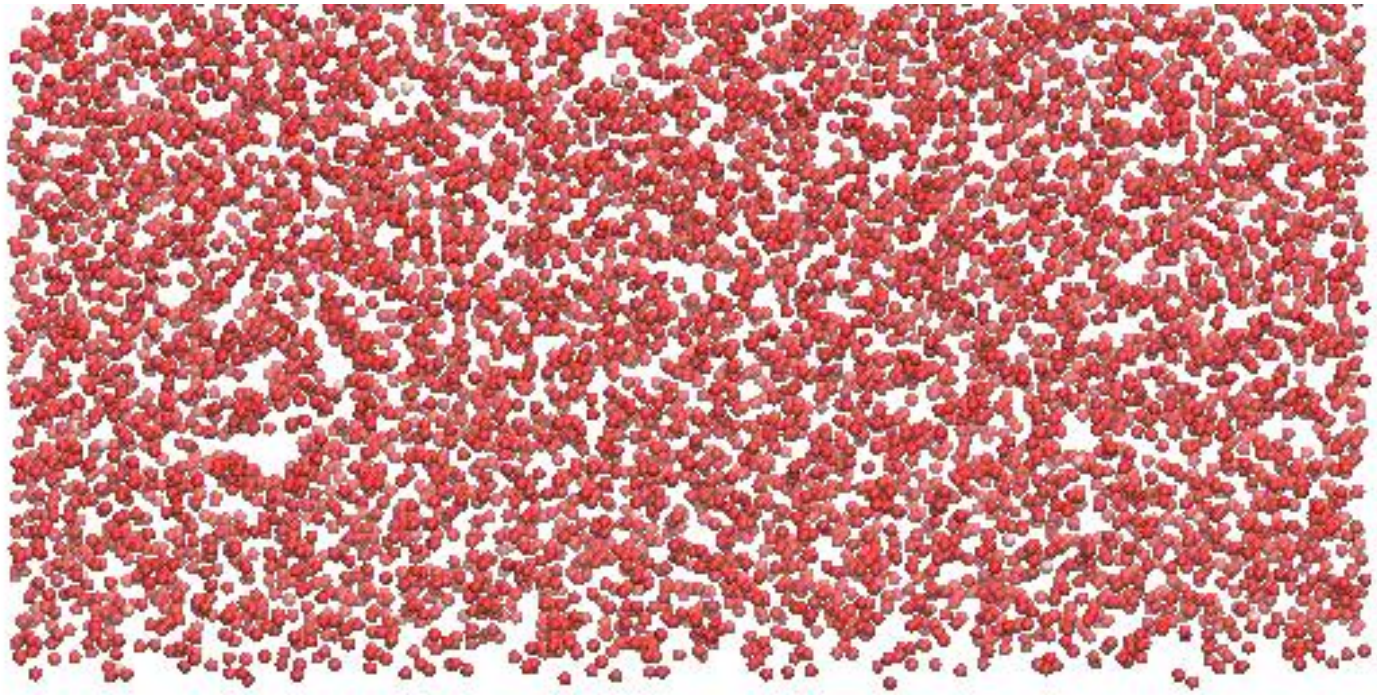
> 0.9 g/cm³

Dihedral barrier term:

Fitted for the system to match the experimental amorphous/crystal composition

~ 80% crystal fraction

MD Simulation



T = 300 K P = 1 atm

Iterate to achieve objectives

Computational Approach

$$C(t) = \left\langle \overrightarrow{v_j(0)} \cdot \overrightarrow{v_j(t)} \right\rangle = \frac{1}{N}\sum_{j-1}^{N} \overrightarrow{v_j(0)} \cdot \overrightarrow{v_j(t)}$$

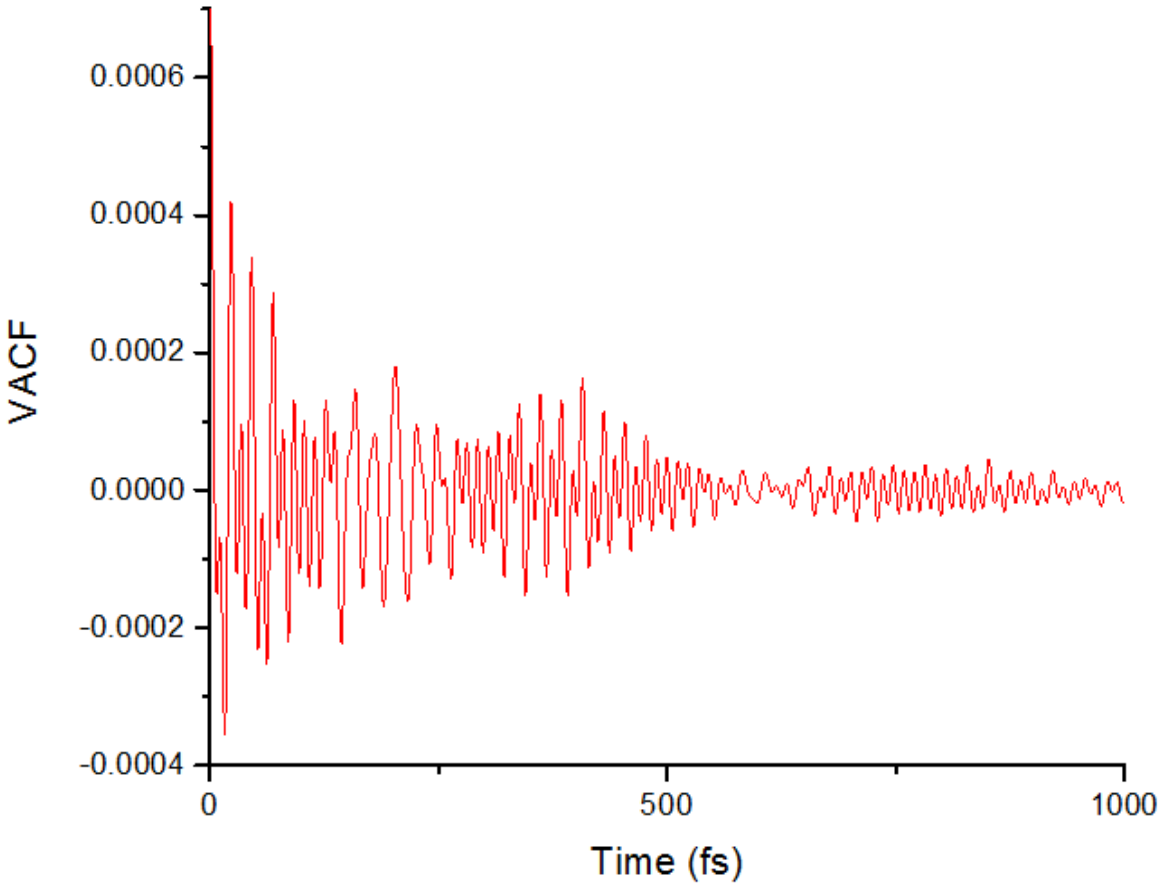
$$\rho(\omega) = \frac{M}{3\pi k_\beta T}\int_{-\infty}^{\infty} C(t)e^{-i\omega t}dt$$

Use NJOY/LEAPR

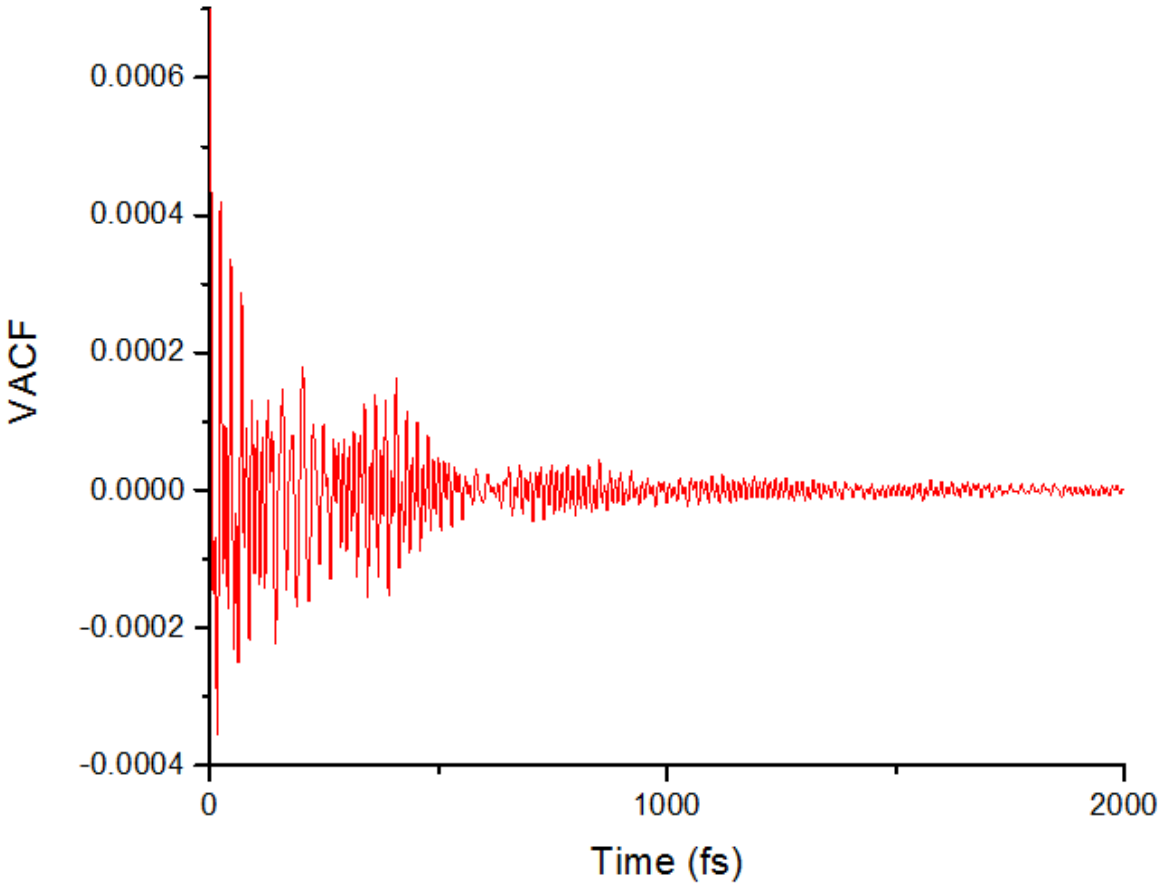
$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\beta t}e^{-\gamma(t,\rho(\omega))}dt$$

$$\left.\frac{d^2\sigma}{d\Omega dE}\right|_{inelastic} = \frac{\sigma}{2k_B T}\sqrt{\frac{E'}{E}}e^{-\frac{\beta}{2}}S(\alpha,\beta)$$

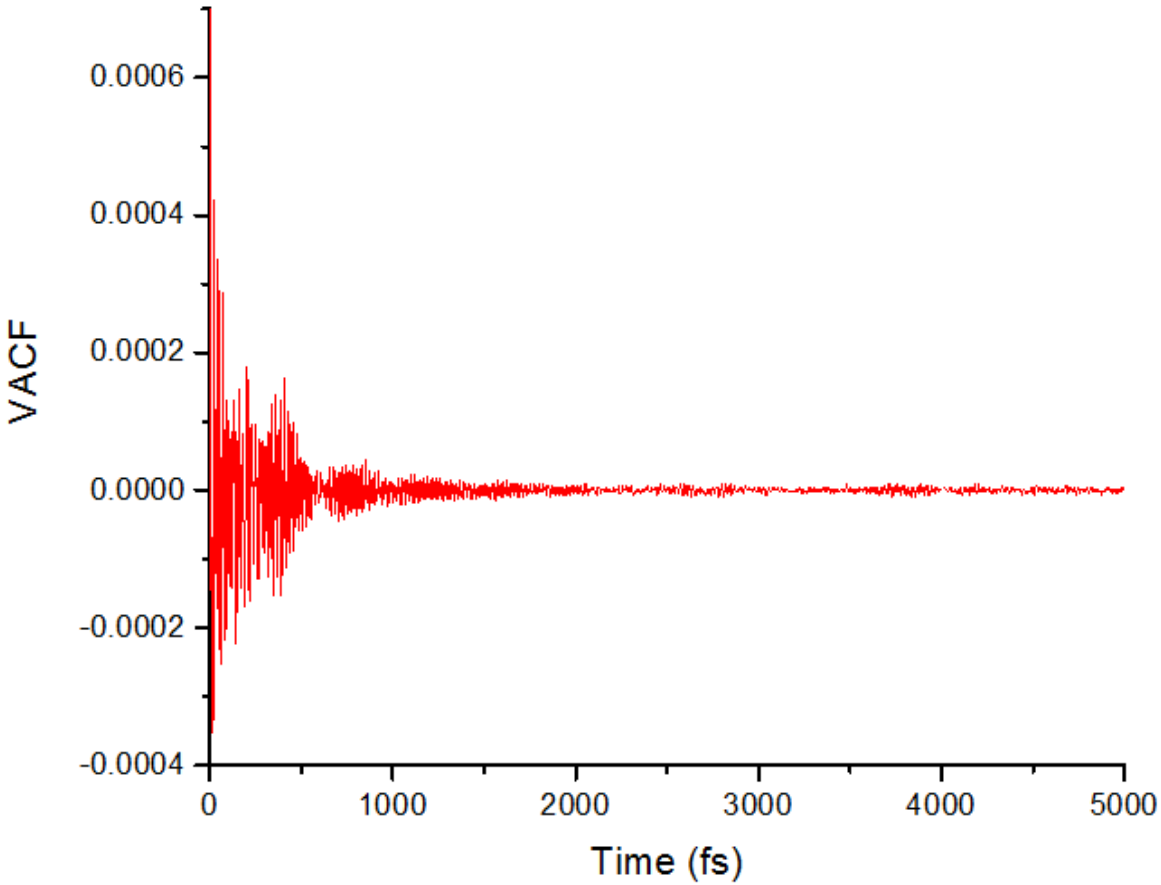
Polyethylene VACF



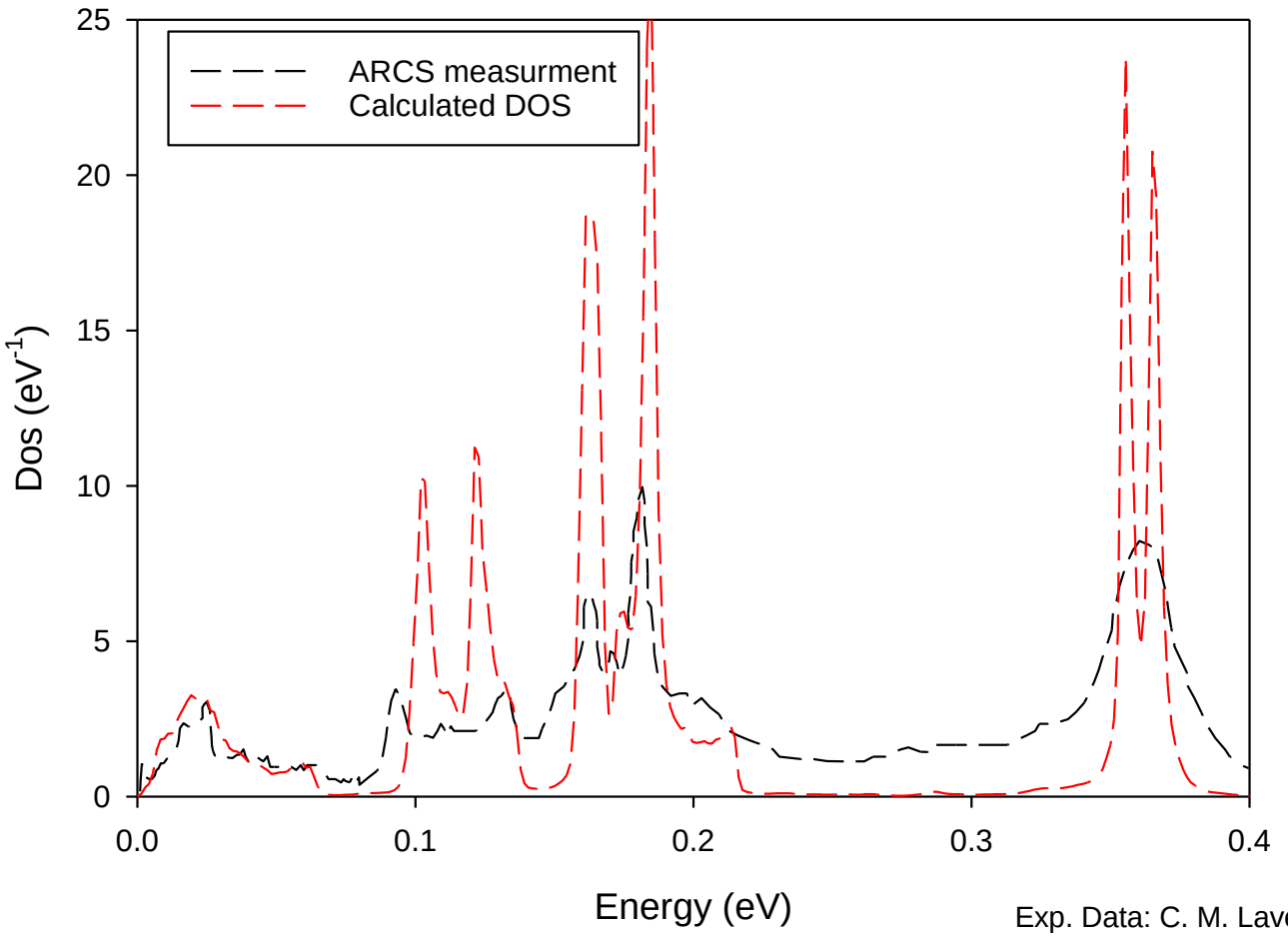
Polyethylene VACF



Polyethylene VACF

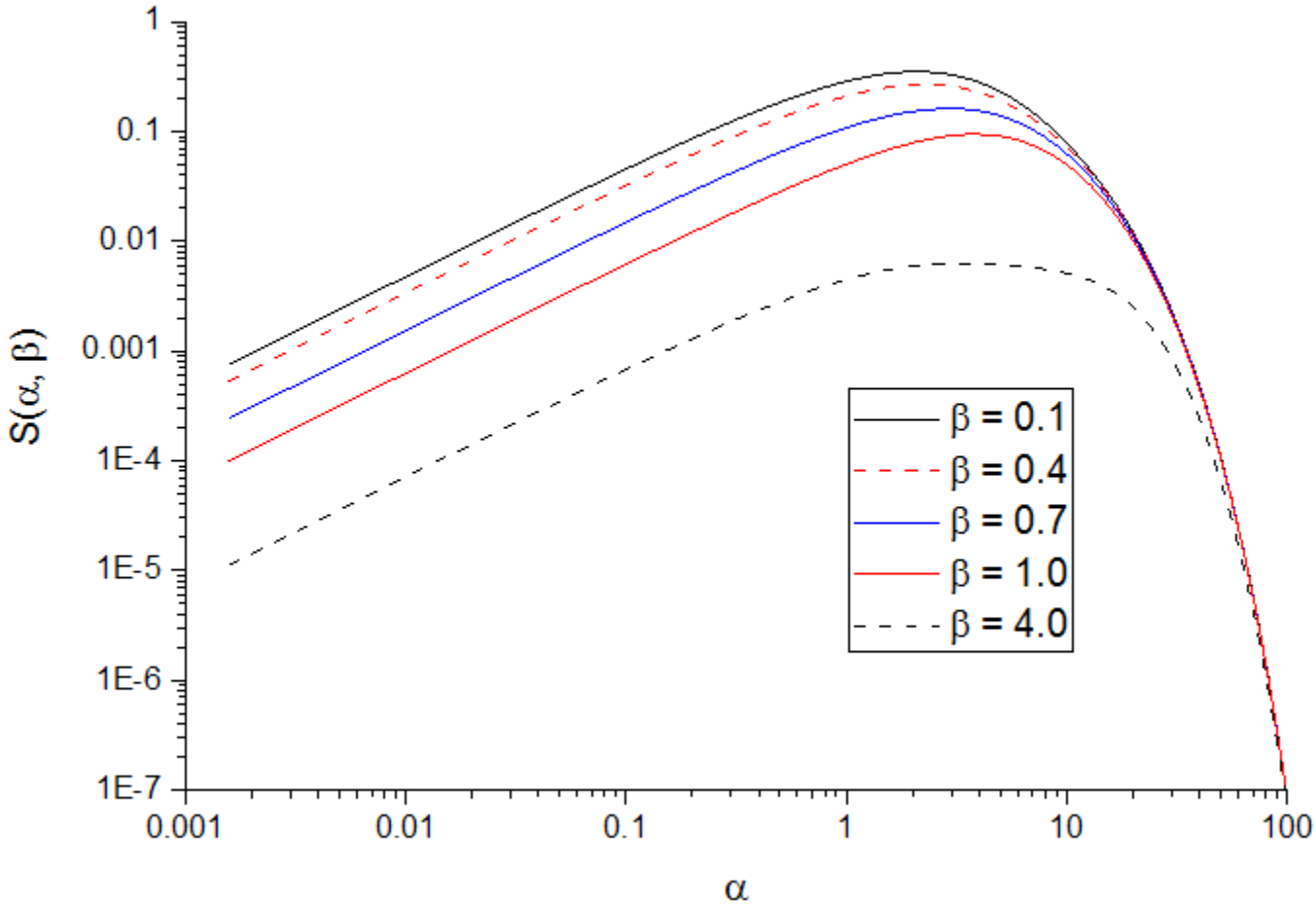


Density of States

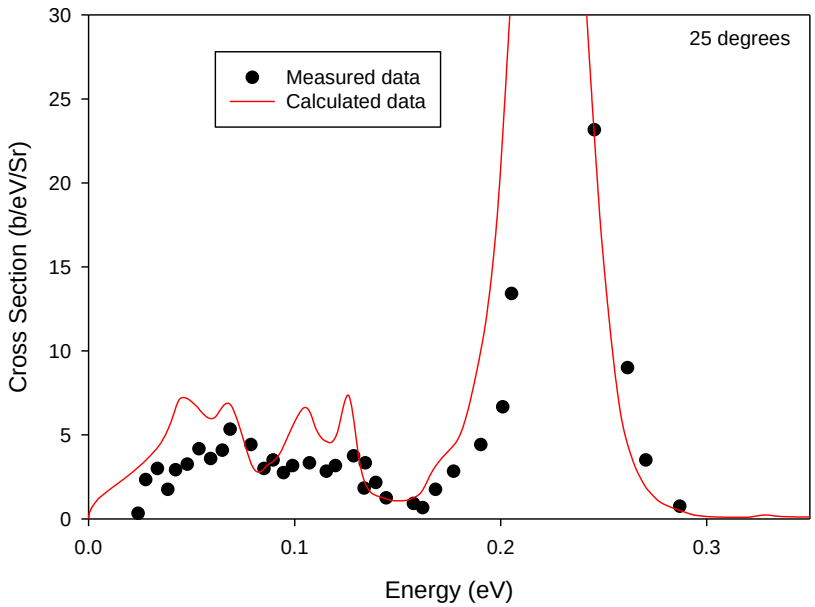


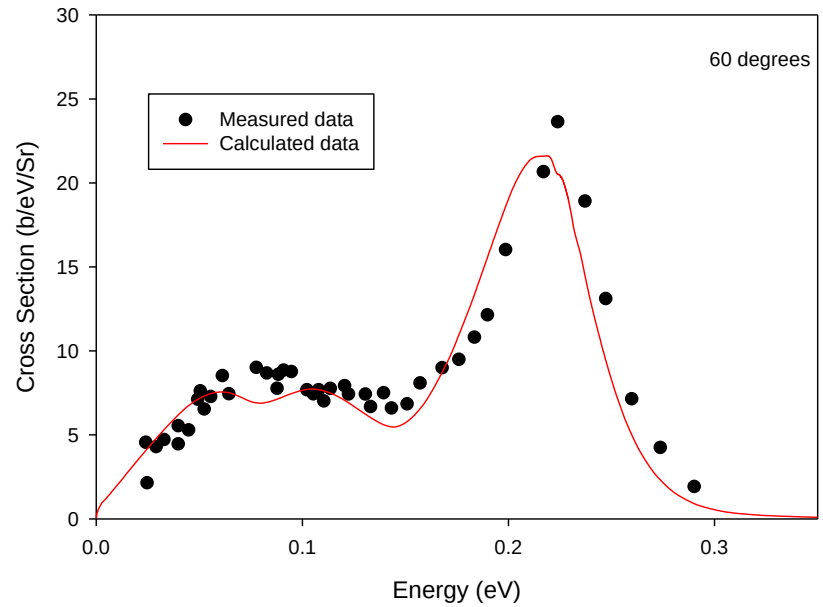
Exp. Data: C. M. Lavelle et al. , NIM A, 711, 166 (2013).

Thermal Scattering Law



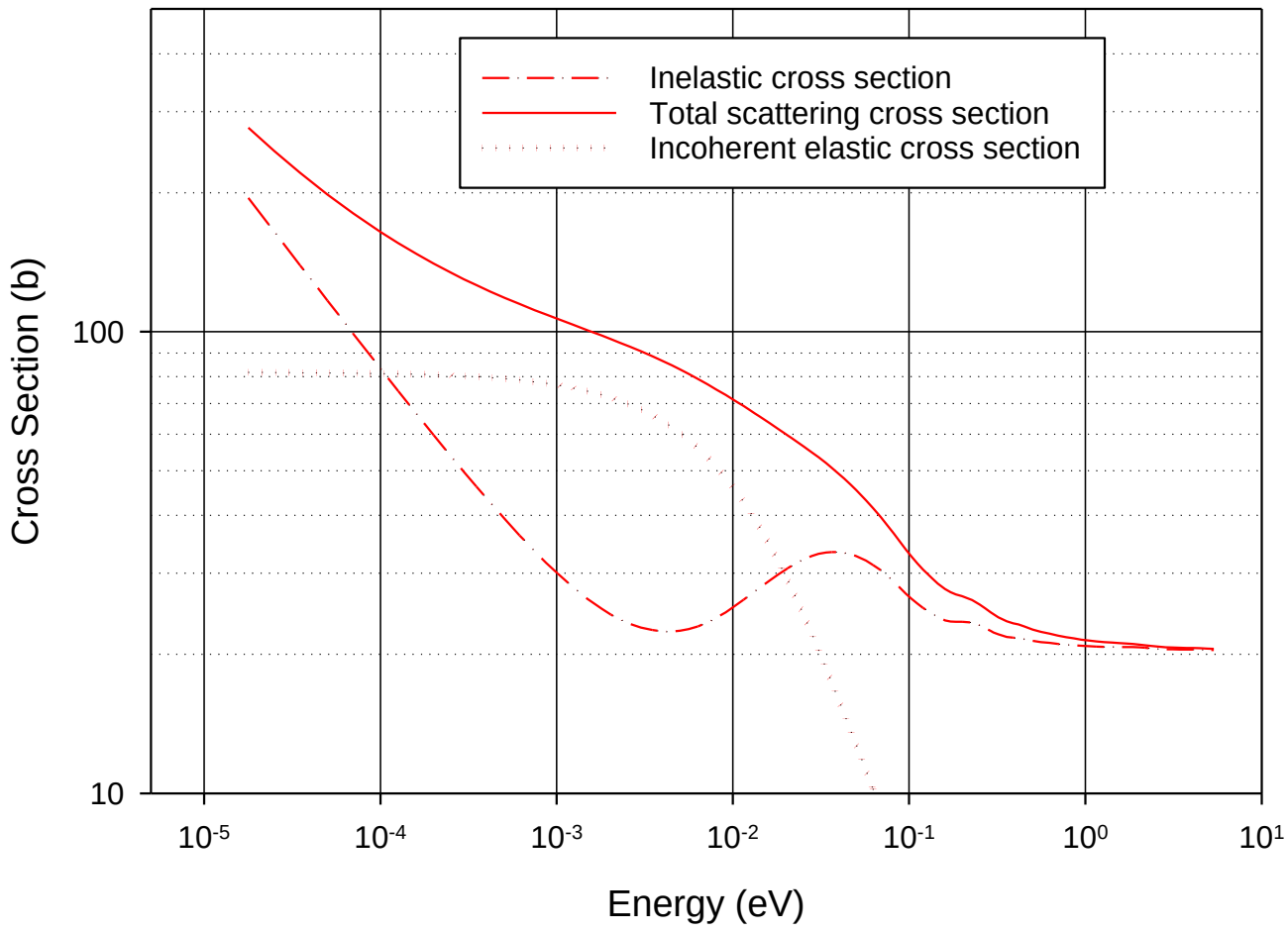
Differential Cross Section



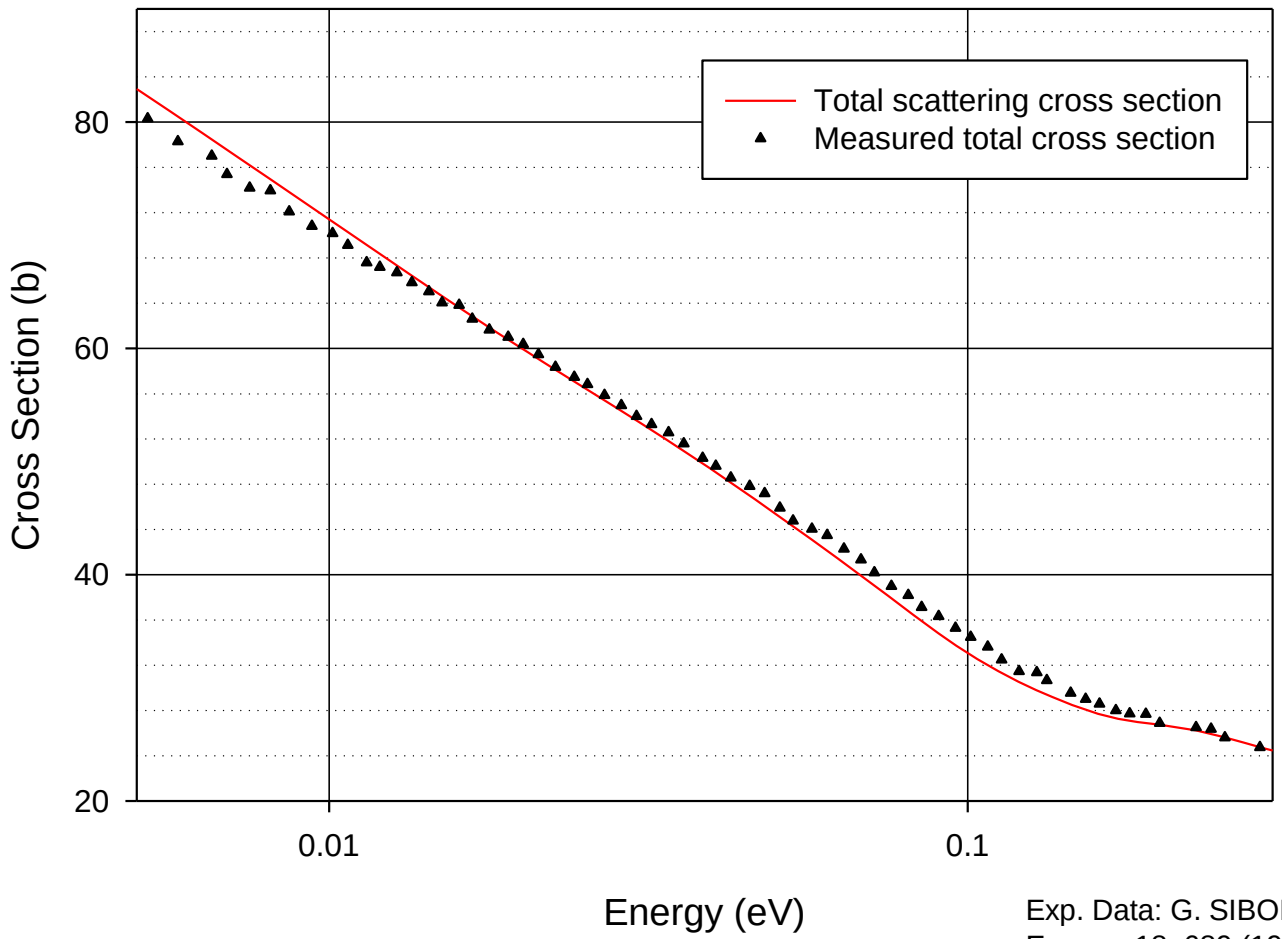


Exp. Data: R. E. Hill et al., NIM A, 538, 686 (2005).

Total Scattering Cross Section



Total Scattering Cross Section



Exp. Data: G. SIBONA et al., Anna. Nucl. Energy, 18, 689 (1991).

Polyethylene File 7

```
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1.636270+2 0.000000+0          0          0          1          2  40 7  2    2
         2          2                                               40 7  2    3
3.000000+2 2.716205+1 3.000000+2 2.716205+1                         40 7  2    4
                                                                    40 7  099999
1.400000+2 9.991673-1          0          1          0          0  40 7  4    1
0.000000+0 0.000000+0          0          0         12          1  40 7  4    2
4.087268+1 1.963720+2 9.991673-1 4.968212+0 0.000000+0 2.000000+0  40 7  4    3
1.000000+0 4.933334+0 1.189800+1 0.000000+0 0.000000+0 1.000000+0  40 7  4    4
0.000000+0 0.000000+0          0          0          1        200  40 7  4    5
       200          4                                               40 7  4    6
3.000000+2 0.000000+0          0          0          1        100  40 7  4    7
       100          4                                               40 7  4    8
1.572280-3 5.234086-4 1.795130-3 5.975359-4 2.049560-3 6.821499-4  40 7  4    9
2.340050-3 7.787328-4 2.671720-3 8.889769-4 3.050400-3 1.014807-3  40 7  4   10
3.482740-3 1.158416-3 3.976370-3 1.322317-3 4.539960-3 1.509358-3  40 7  4   11
5.183430-3 1.722796-3 5.918110-3 1.966338-3 6.756910-3 2.244203-3  40 7  4   12
7.714600-3 2.561198-3 8.808030-3 2.922795-3 1.005640-2 3.335201-3  40 7  4   13
1.148180-2 3.805532-3 1.310920-2 4.341788-3 1.496720-2 4.953085-3  40 7  4   14
1.708860-2 5.649809-3 1.951060-2 6.443655-3 2.227600-2 7.347967-3  40 7  4   15
2.543320-2 8.377686-3 2.903800-2 9.549856-3 3.315370-2 1.088356-2  40 7  4   16
3.785280-2 1.240035-2 4.321790-2 1.412435-2 4.934330-2 1.608259-2  40 7  4   17
5.633700-2 1.830534-2 6.432200-2 2.082618-2 7.343860-2 2.368227-2  40 7  4   18
8.384750-2 2.691473-2 9.573160-2 3.056845-2 1.093000-1 3.469236-2  40 7  4   19
1.247920-1 3.933937-2 1.424790-1 4.456546-2 1.626730-1 5.043017-2  40 7  4   20
1.857300-1 5.699506-2 2.120540-1 6.432177-2 2.421100-1 7.247176-2  40 7  4   21
2.764260-1 8.150194-2 3.156050-1 9.146205-2 3.603370-1 1.023904-1  40 7  4   22
4.114090-1 1.143079-1 4.697210-1 1.272112-1 5.362960-1 1.410634-1  40 7  4   23
6.123080-1 1.557866-1 6.990940-1 1.712490-1 7.981800-1 1.872544-1  40 7  4   24
9.113100-1 2.035309-1 1.040470+0 2.197207-1 1.187950+0 2.353766-1  40 7  4   25
1.356320+0 2.499540-1 1.548560+0 2.628284-1 1.768040+0 2.733076-1  40 7  4   26
2.018640+0 2.806712-1 2.304750+0 2.842184-1 2.631410+0 2.833377-1  40 7  4   27
3.004380+0 2.775855-1 3.430200+0 2.667702-1 3.916380+0 2.510240-1  40 7  4   28
4.471470+0 2.308484-1 5.105240+0 2.071131-1 5.828830+0 1.809961-1  40 7  4   29
6.654970+0 1.538625-1 7.598220+0 1.271018-1 8.675160+0 1.019553-1  40 7  4   30
```
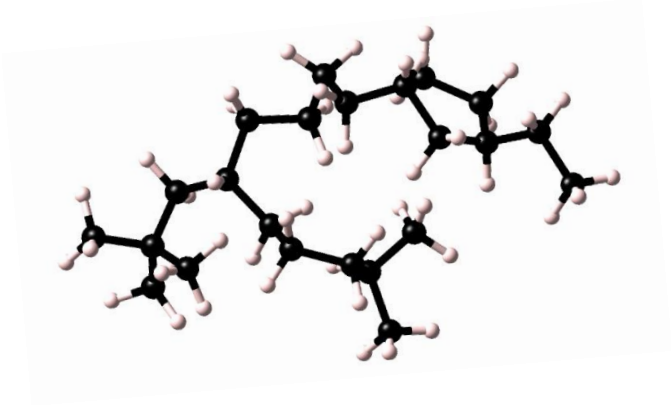
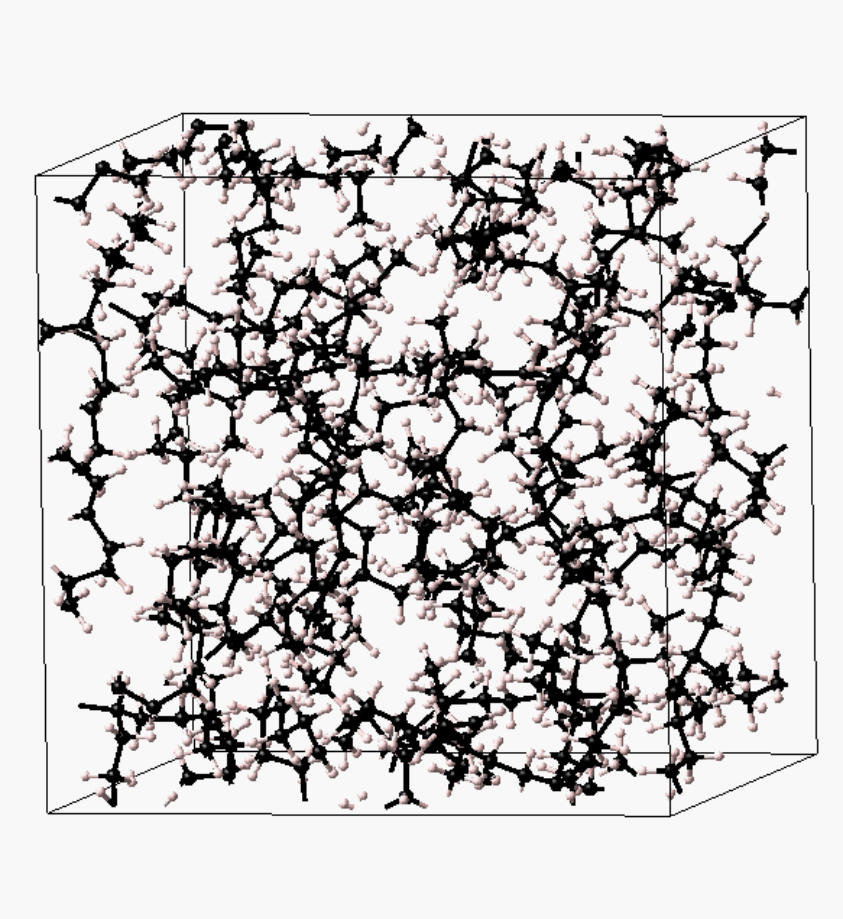

Lubricant Oil MD Model

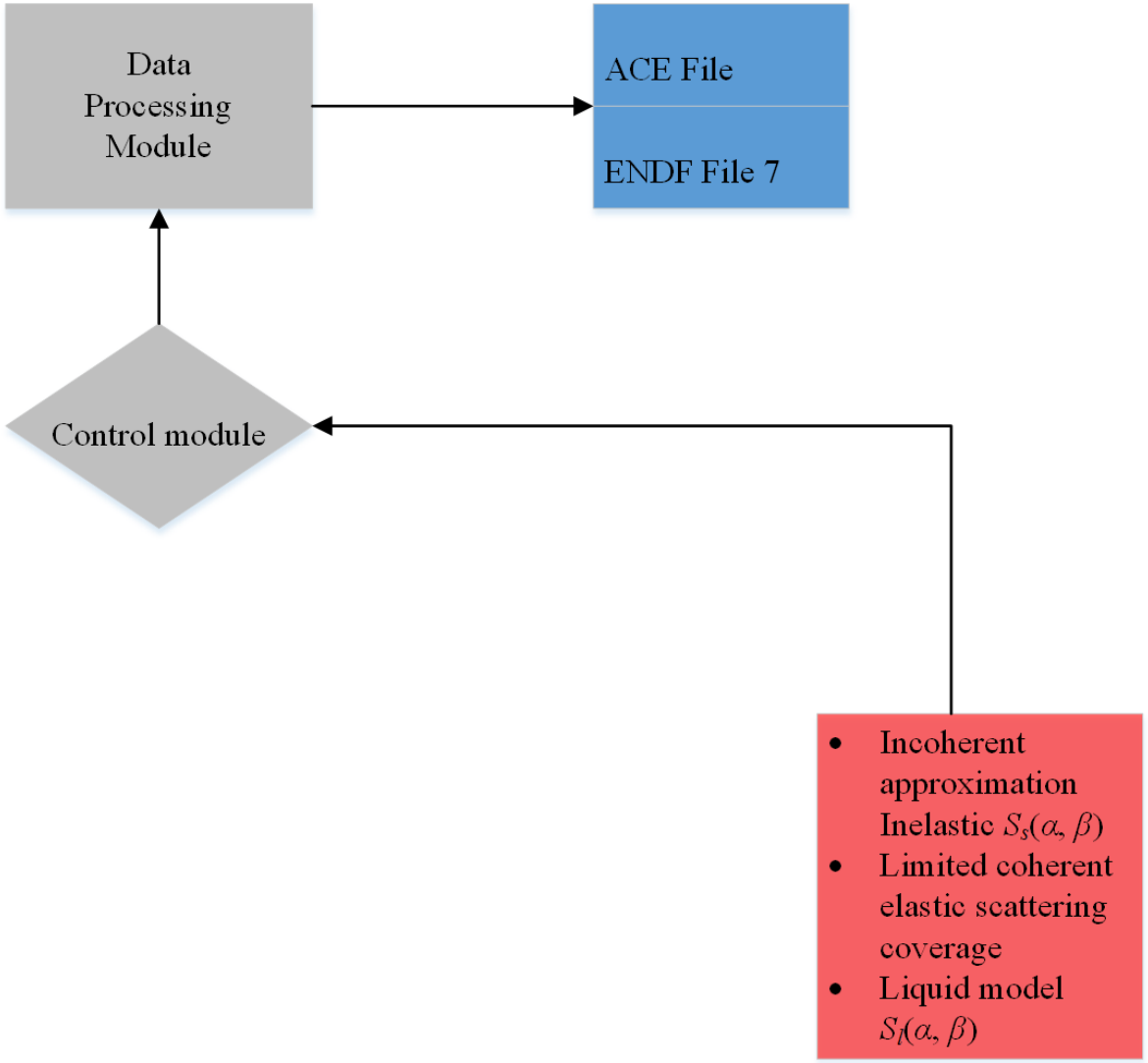
- Distilled and dewaxed heavy paraffinic mineral oil
- Example molecule

  C23H48
- Test model 20 molecules
- Verification of physical properties is underway

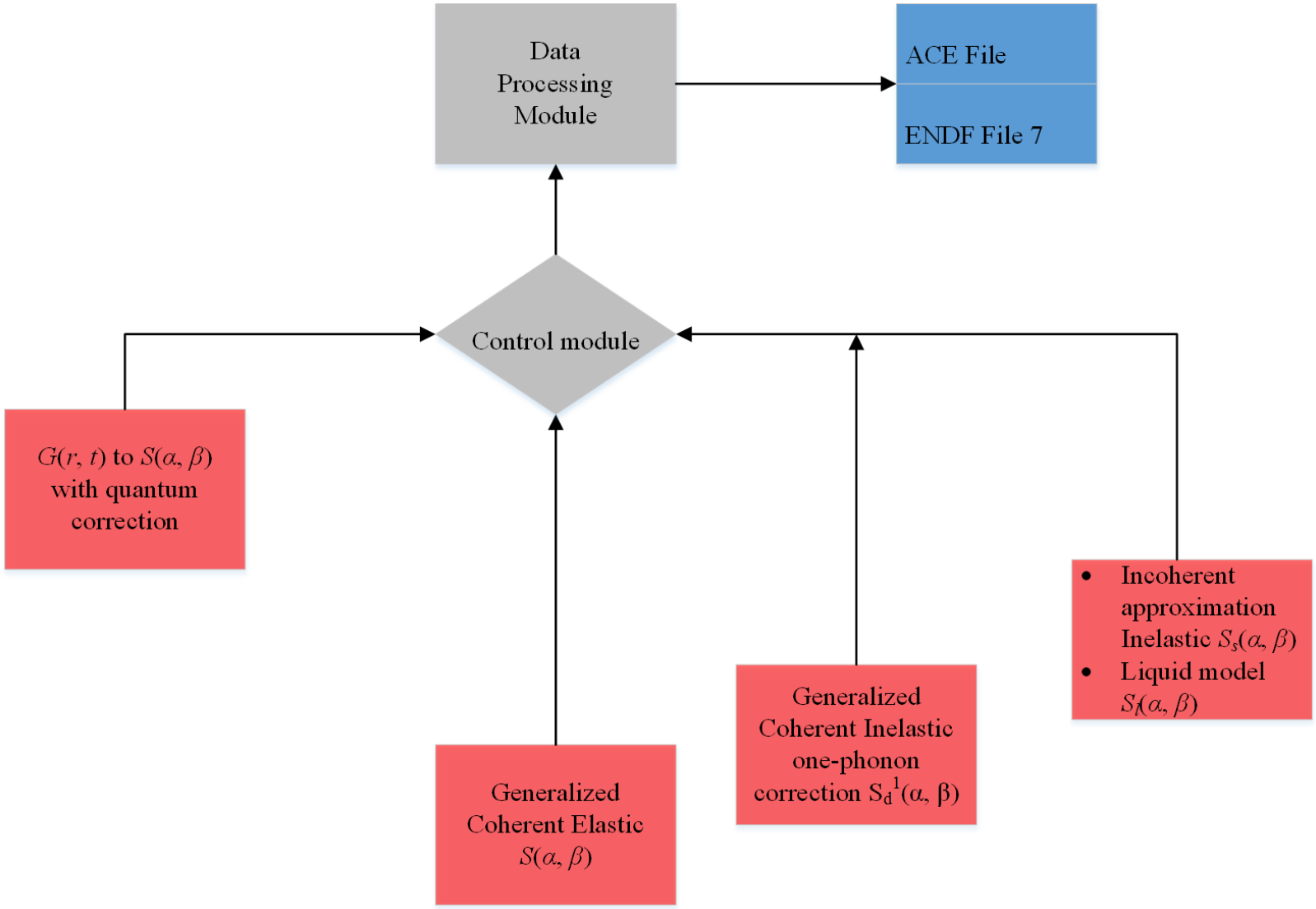




Next Generation Code



Next Generation Code



Coherent Elastic Scattering

	Current	Generalized (NCSU)
Supported structure	Hexagonal, FCC, BCC	Any crystal structure
Supported material	Graphite, beryllium, beryllium oxide, aluminum, lead, iron	Any material
Compound material	2 elements with ratio 1:1	Any number of elements with any ratio
Cubic Approximation	Yes	No
Atom sites approximation	Yes	No
Coherent Elastic Scattering Cross Section	Over Ewald Sphere	On every reciprocal space point
Need to modify source code if calculating other materials	Yes	No

Summary

- Generation of TSL File 7 libraries is proceeding
  - Polyethylene completed in FY'15
  - Polymethyl Methacrylate (Lucite) contributed to NNDC in FY'15
  - New materials are initiated
- Work on "next generation" TSL generation code is ongoing. FY'16 tasks include
  - Defining code flow and structure
  - Integration of a generalized coherent elastic scattering module
  - Completing a generalized coherent inelastic scattering module