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Thermal Neutron Scattering Data for LiF and BeF₂

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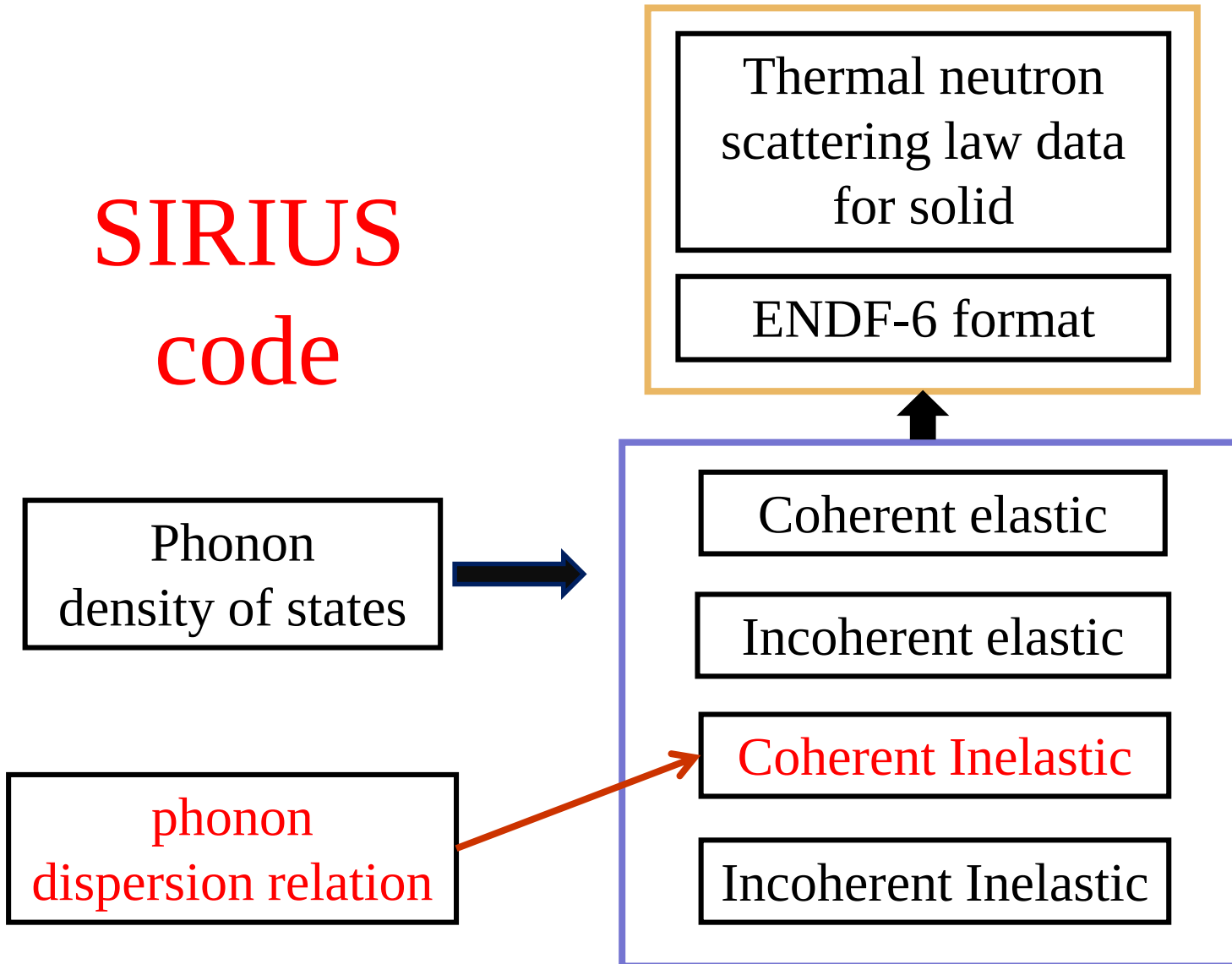
Introduction

Thermal neutron scattering data are widely used in nuclear engineering applications.

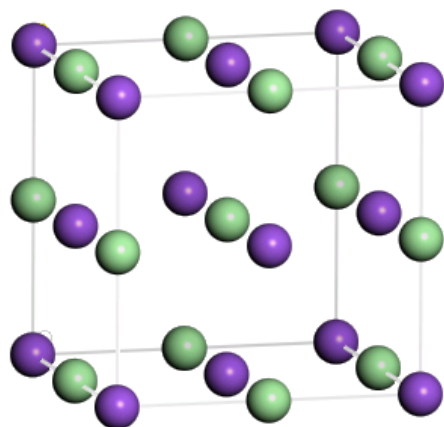
- 1950s- Now
 - Code: GASKET, LEAPR module in NJOY code system.
 - TSL Sublibraries: about 23 moderators.
- New requirements for the Generation-*IV* reactor design **need more TSL data.**
 - In molten salt reactor: LiF, BeF₂ and so on
 - No these TSL data in libraries. So this work is trying to give these TSL data for future use.

Theory and code

SIRIUS code



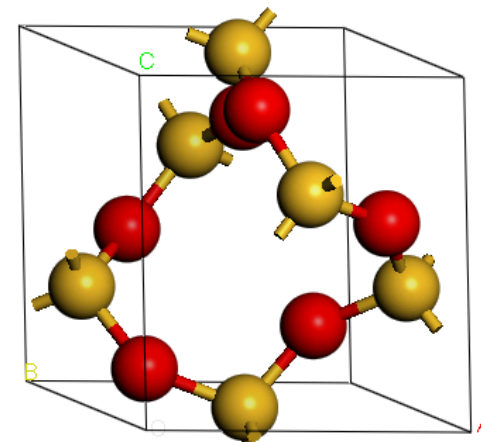
The phonon densities of states



LiF

Supercell
3x3x3

FCC, $a=4.026$

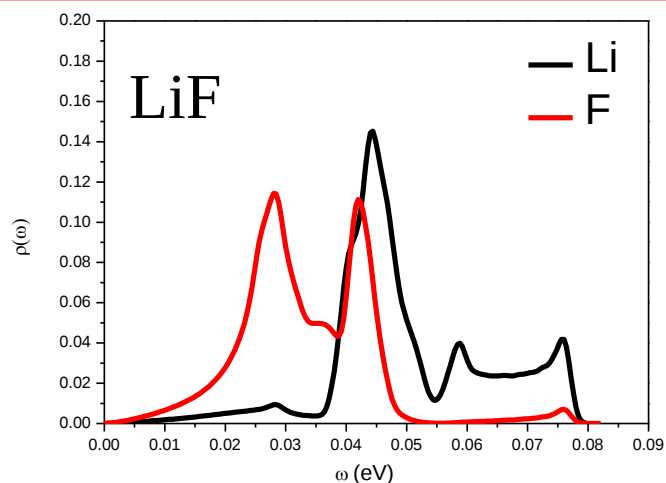


BeF₂

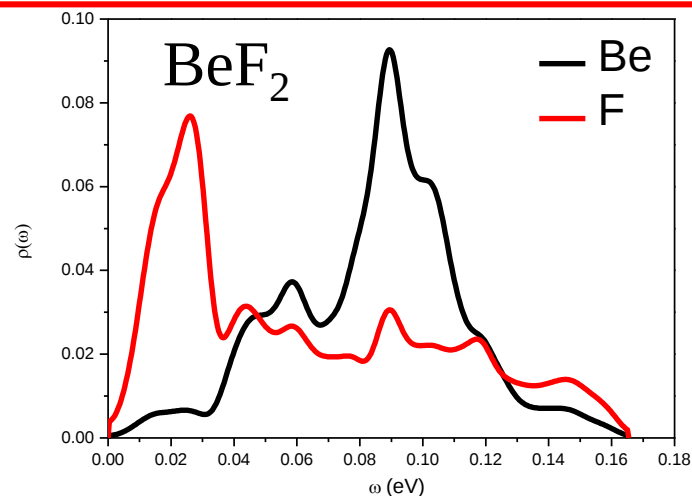
Supercell
2x2x2

α -quartz, $a=4.85$, $c=5.335$

Hellman-Feynman Theorem combined with a lattice dynamics direct method



PDOS



TSL data for ^7LiF

Bound atom
scattering cross section



^7Li
 ^{19}F

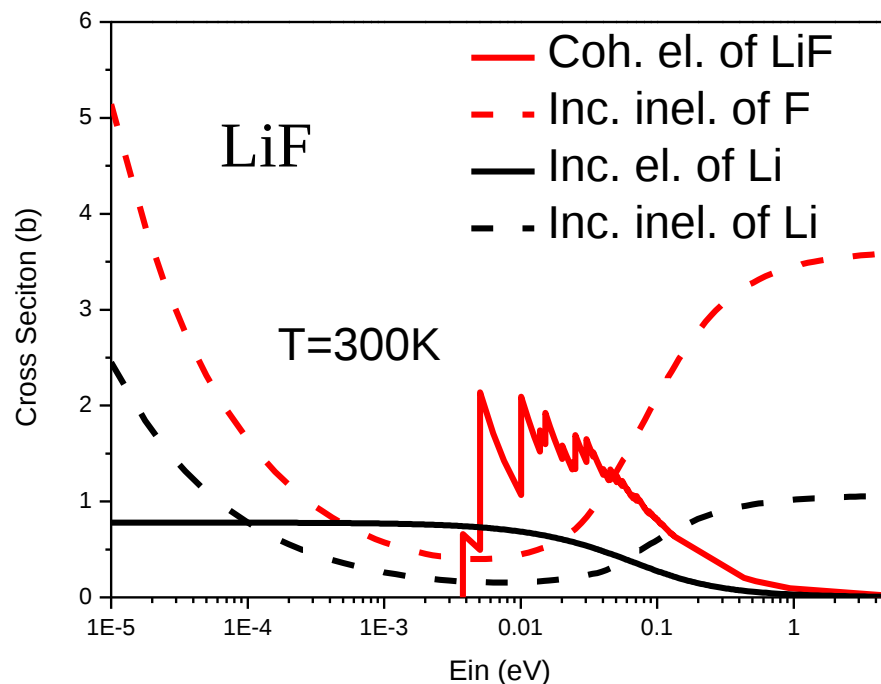
Coherent **Incoherent**

0.619b

0.78b

4.017b

0.0008b



Li: Both coherent + Incoherent
elastic

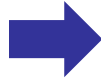


Cohherent elastic of LiF
Incoherent elastic of Li
Incoherent inelastic of Li
Incoherent inelastic of F

The thermal neutron scattering
cross sections at 300K

TSL data for BeF₂

Bound atom
scattering cross section



⁹Be
¹⁹F

Coherent

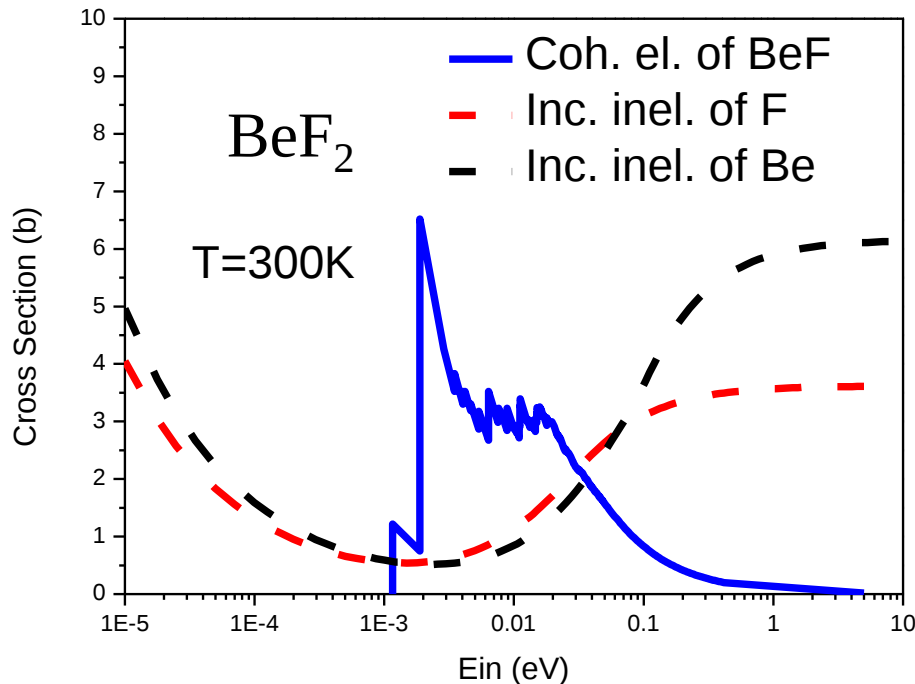
Incoherent

7.63b

0.0018b

4.017b

0.0008b



BeF₂: only Coherent elastic



Coherent elastic of BeF₂
Incoherent inelastic of F
Incoherent inelastic of Be

The thermal neutron scattering
cross sections at 300K



Conclusion

- SIRIUS code is used to generate TSL data for solid.
- TSL data for LiF and BeF₂ crystals are given,
However experimental data are need to validate these data.

Thank you
for your attention!