CALCULATION OF THERMAL SCATTERING CROSS SECTIONS FOR SI AND BI

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OUTLINE

Thermal scattering cross sections needed for some thermal neutron filters

New code

Develop the code to calculate thermal scattering law from the scratch

LEAPR of NJOY

- LEAPR can calculate thermal scattering cross sections for materials including graphite, beryllium, hydrogen and solid methane.
- Modification was needed to calculate the thermal elastic cross sections for silicon and bismuth, because the module did not take into account the lattice structures of these crystals on which the thermal elastic scattering sensitively depends.

THERMAL ELASTIC SCATTERING

Thermal elastic scattering can be divided into two parts: coherent scattering and incoherent scattering.

For crystalline solids, scattered waves interfere with each other, resulting in so-called Bragg scattering, which is coherent elastic scattering.

The incoherent effect is important for hydrogenous materials including solid methane and zirconium hydride.

THERMAL ELASTIC SCATTERING – CROSS SECTIONS FOR POLYCRYSTAL

The coherent elastic cross section for a polycrystal is given by

$$\sigma_{coh} = \frac{n\pi^2\sigma_c}{Vk^2}\sum_{\boldsymbol{\tau}}^{\tau\leq 2k}\frac{1}{\tau}e^{-2W(\boldsymbol{\tau})}\left|F(\boldsymbol{\tau})\right|^2$$

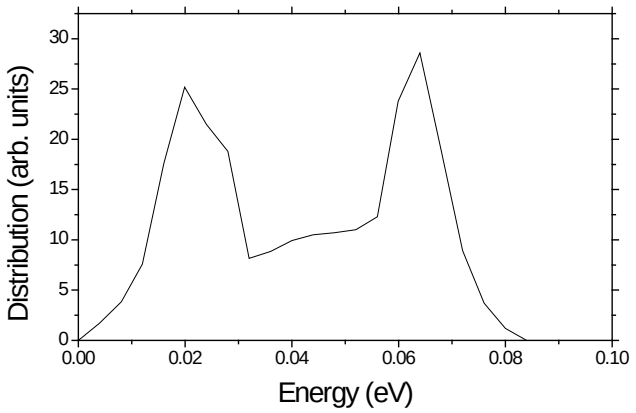
where n is the number of atoms in the primitive unit cell, V is the volume of the primitive unit cell, σ_c is the effective bound coherent scattering cross section for the material, $\boldsymbol{\tau}$ is the reciprocal lattice vector, $e^{-2W(\boldsymbol{\tau})}$ is the Debye-Waller factor, and $F(\tau)$ is the unit cell structure factor. The summation extends over all reciprocal lattice vectors whose magnitudes are not greater than $2k$.

THERMAL INELASTIC SCATTERING

Thermal inelastic scattering is important for all materials. The cross sections for thermal neutrons are calculated from the exact shape of the phonon frequency spectrum.

$$\sigma(E \to E', \mu) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}S(\alpha, \beta)$$

function of frequency spectrum

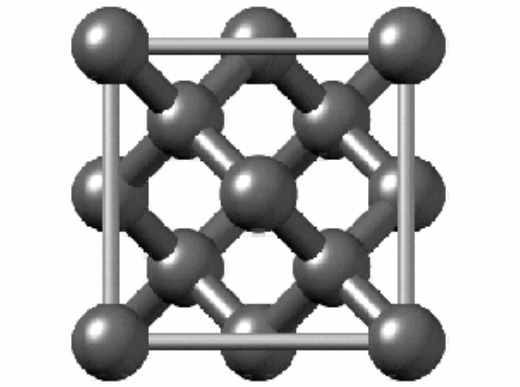


STRUCTURE OF SILICON LATTICE

Silicon has a diamond-like cube structure which consists of two interpenetrating fcc (face-centered cubic) lattices with one being replaced from the other by ¼ of the principal diagonal of the cube.

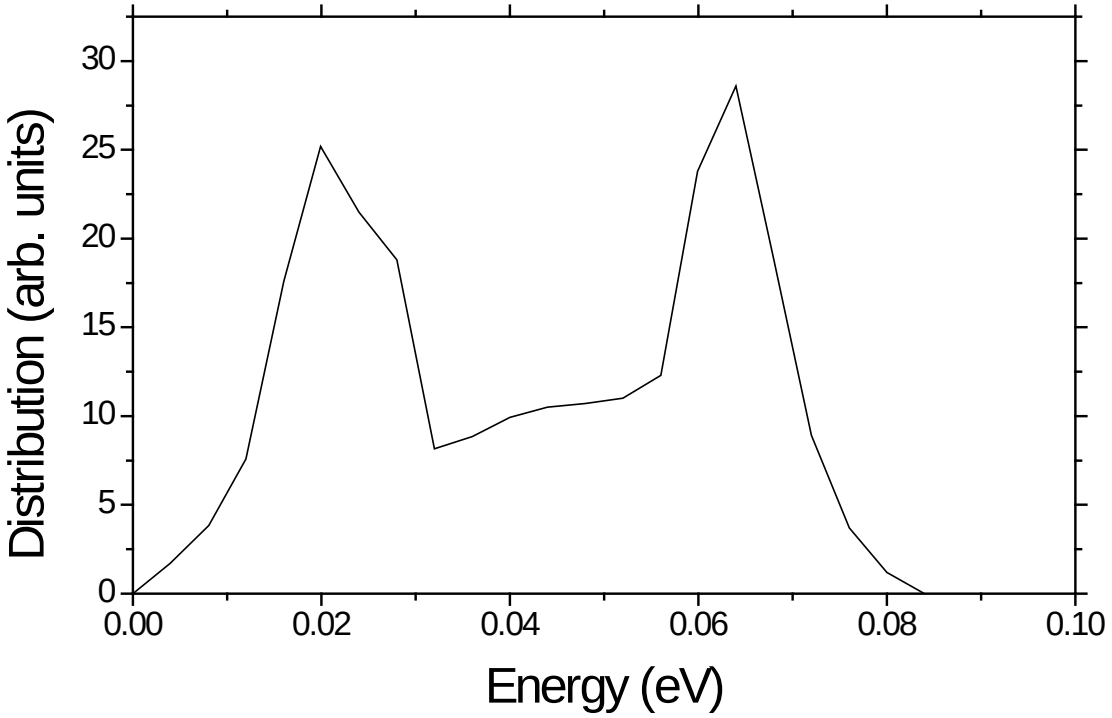
It can be simplified as a single fcc lattice with each lattice point having two identical atoms, one at (0,0,0), and the other at (1/4,1/4,1/4).

The lattice constant a is 5.42 Å.



Silicon – Phonon spectrum

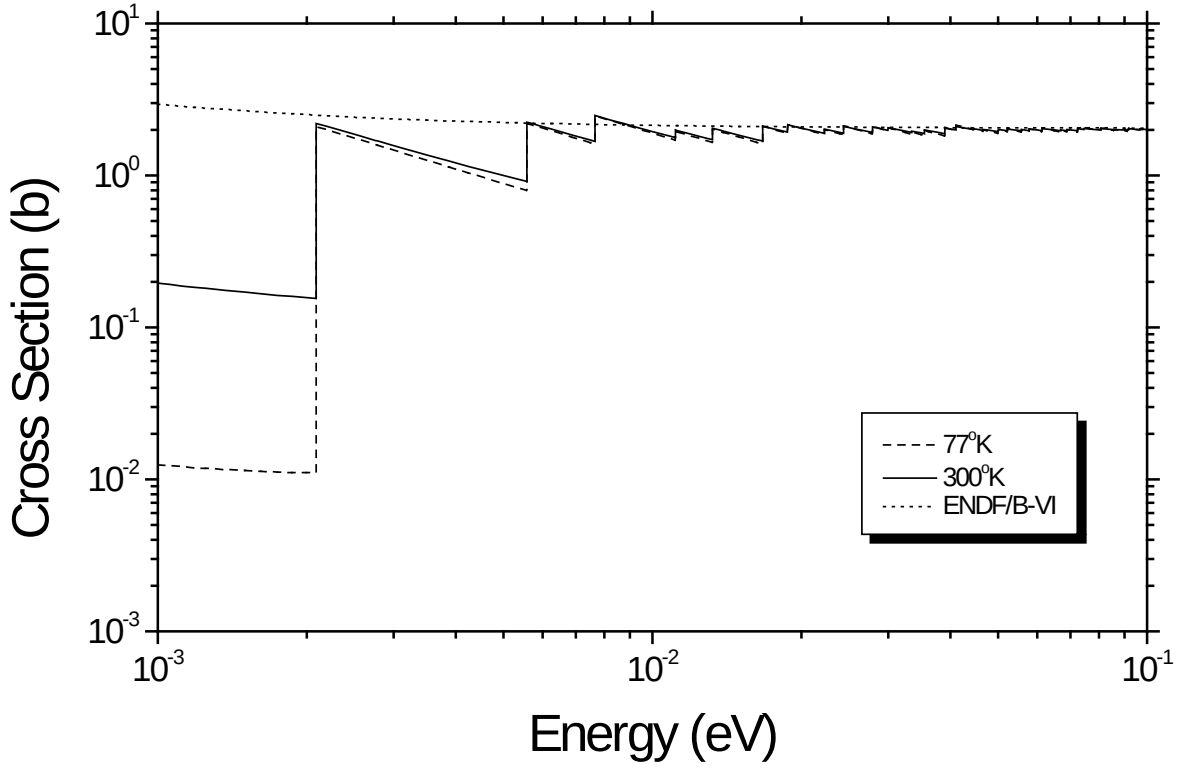
THE PHONON FREQUENCY SPECTRUM OF SILICON



The phonon frequency spectrum of silicon. It is that of coarse-grained silicon powders measured by Nesterenko et al.

Silicon - Results

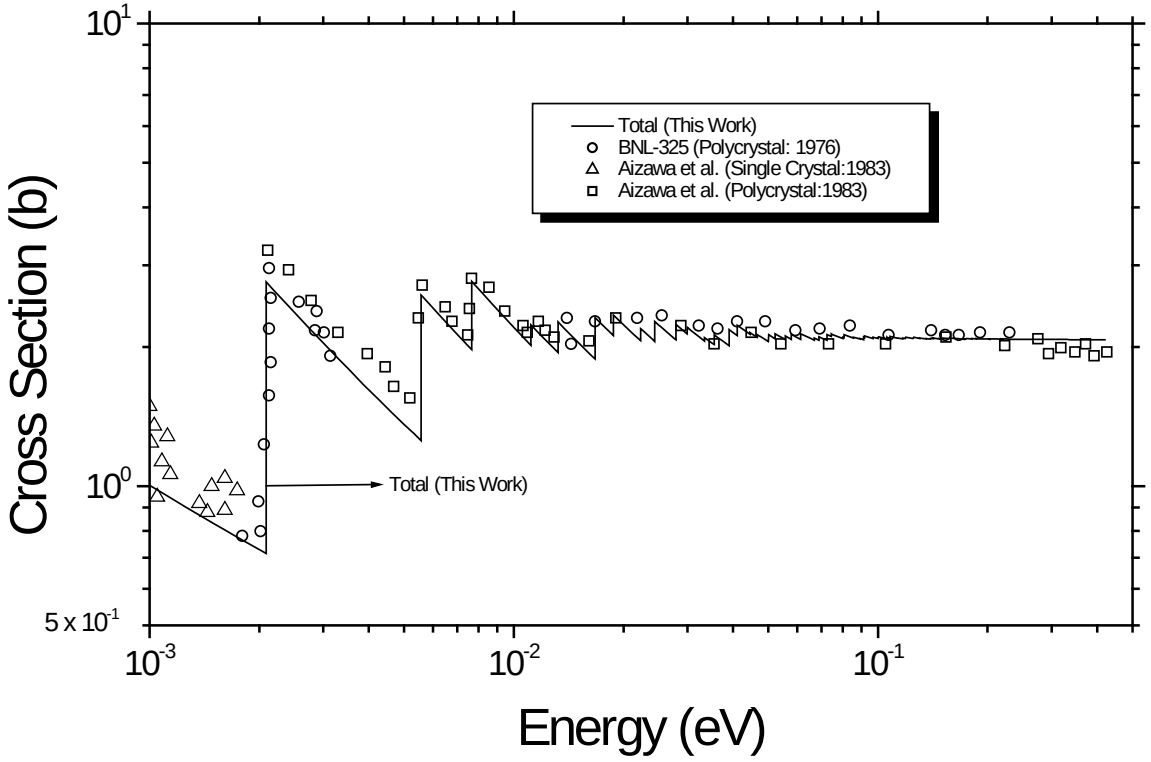
THE SCATTERING CROSS SECTIONS FOR POLYCRYSTALLINE SILICON



The calculated scattering cross sections for polycrystalline Si are compared with the elastic scattering cross sections from ENDF/B-VI. [*Young-Sik Cho et al. J. Korean Nucl. Soc. 31, p.631, 1999*]

Silicon - Results

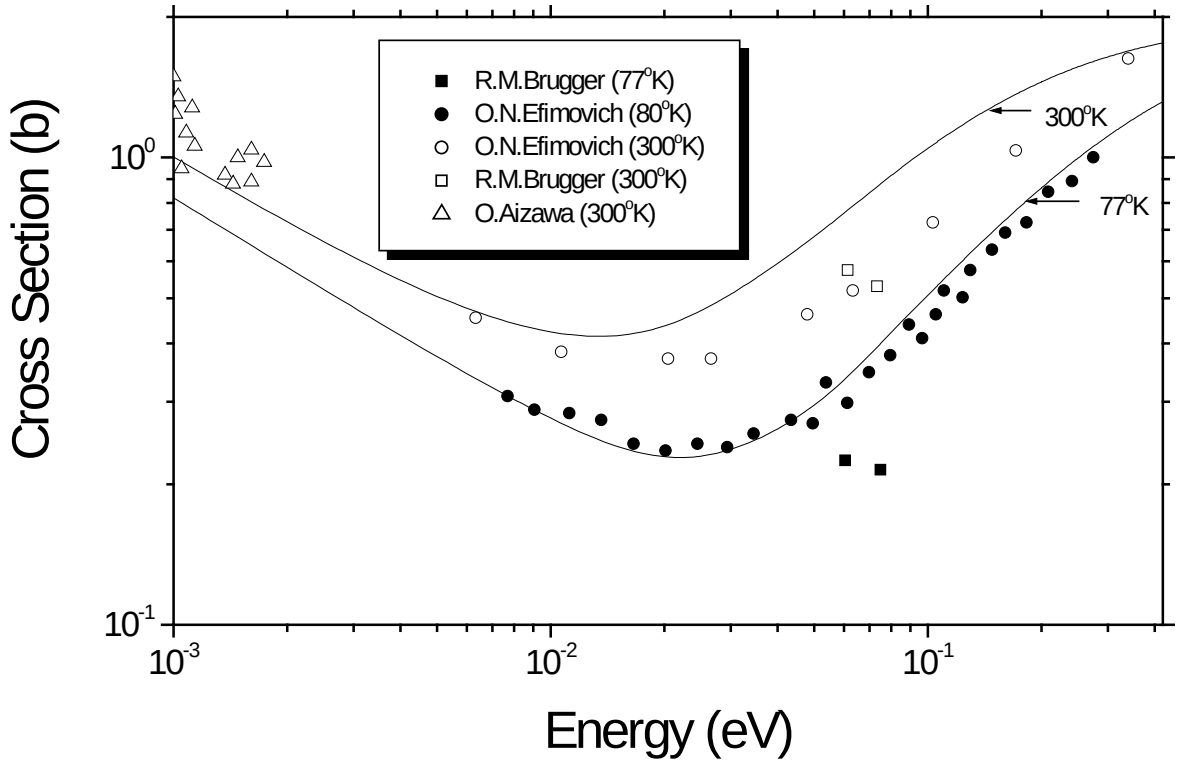
TOTAL CROSS SECTIONS AT 300^{0}K FOR POLYCRYSTALLINE SILICON



Total cross sections at 300°K for polycrystalline Si. The experimental data were given as the total cross sections, so for comparison, the theoretical total cross sections were obtained by adding the capture cross sections from ENDF/B-VI to the total scattering cross sections calculated in this work. [*Young-Sik Cho et al. J. Korean Nucl. Soc. 31, p.631, 1999*]

Silicon - Results

TOTAL CROSS SECTIONS AT 300°K FOR SINGLE CRYSTAL SILICON



Total cross sections at 300°K for single crystal Si. In the case of a single crystal, it was expected that the contribution of Bragg scattering would be very small, so the elastic scattering cross sections were not included for the comparison. [*Young-Sik Cho et al. J. Korean Nucl. Soc. 31, p.631, 1999*]

STRUCTURE OF BISMUTH LATTICE

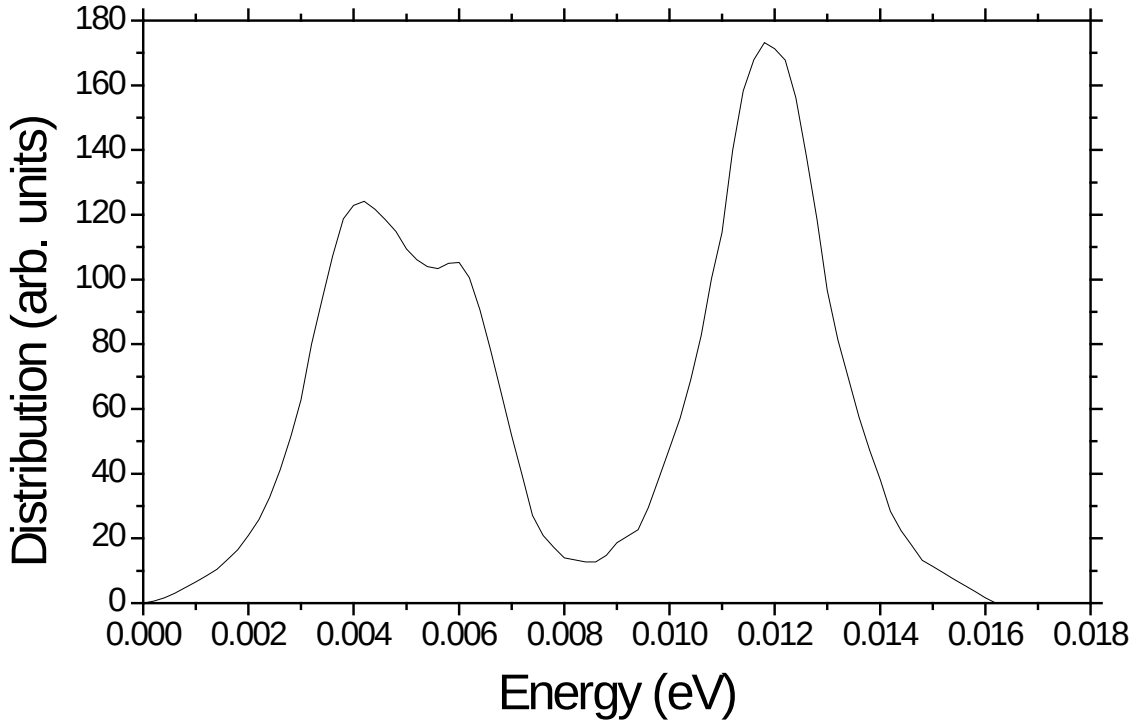
Bismuth has a rhombohedral structure with two atoms per unit cell.

The rhombohedral angle is 57.23° and the atomic positional parameter *z* is 0.23389 at 298°K.

The lattice constant a_H is 4.546 Å and c_H is 11.863 Å.

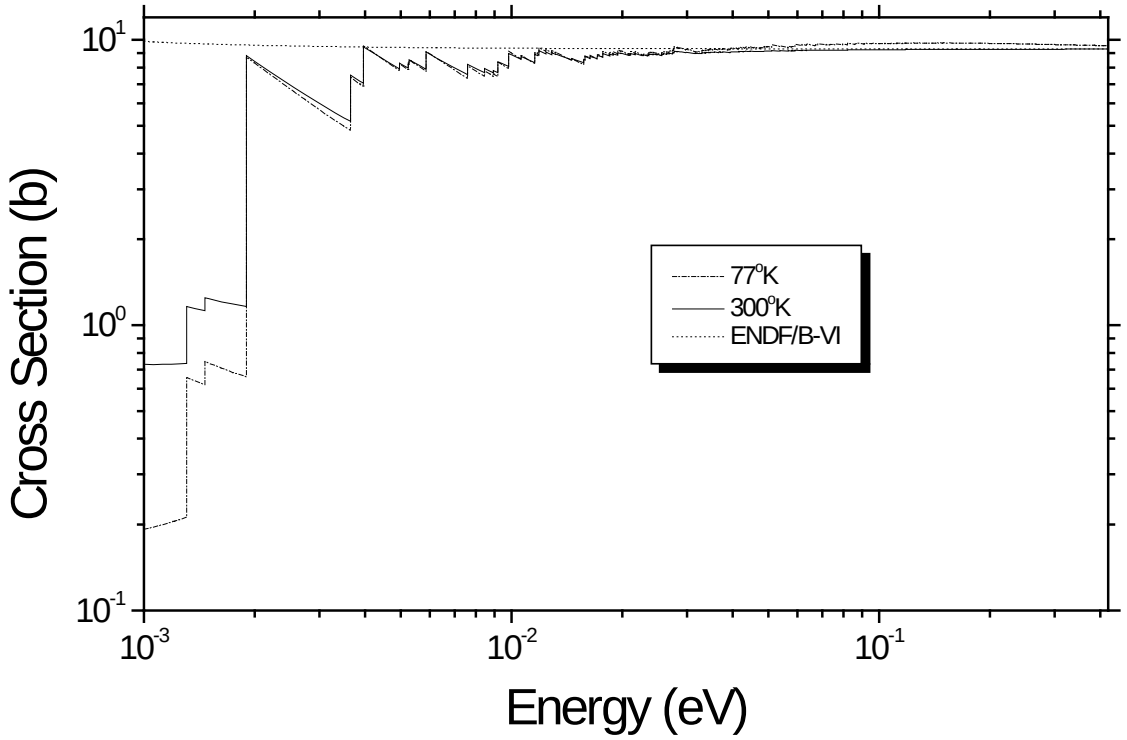
Bismuth – Phonon spectrum

THE PHONON FREQUENCY SPECTRUM OF BISMUTH



The phonon frequency spectrum of bismuth. It is taken from the results experimentally determined by Kress.

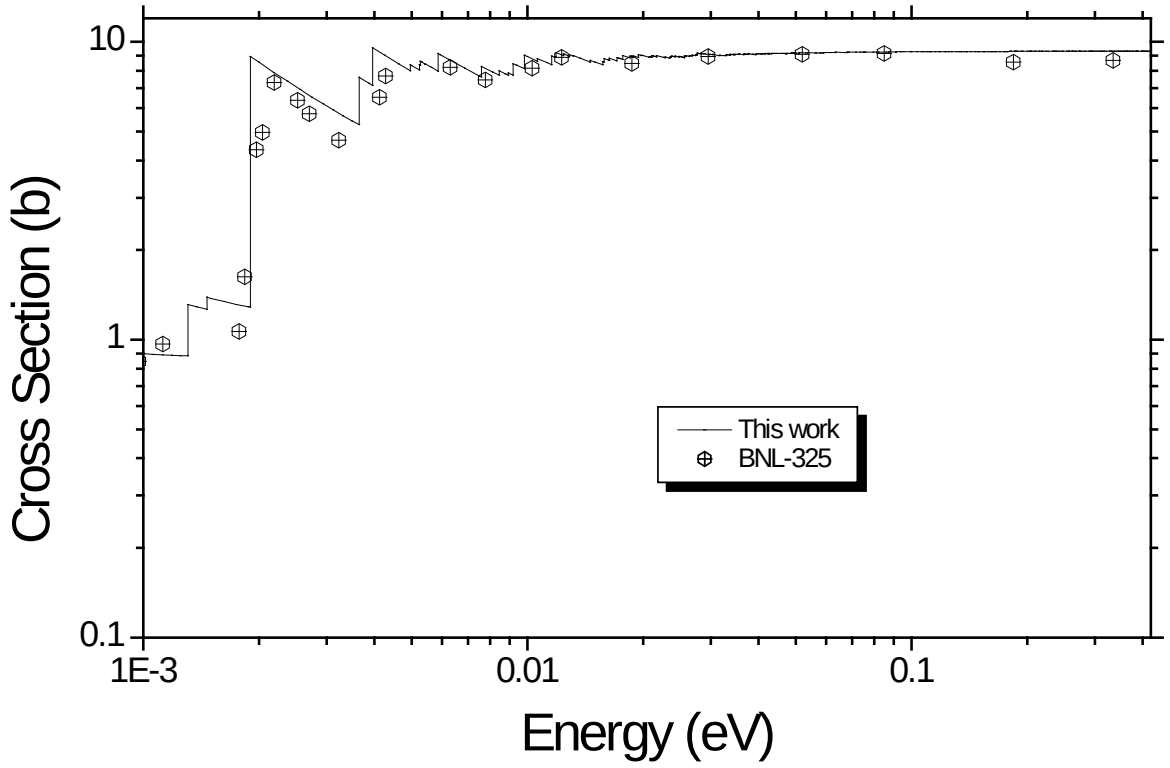
THE SCATTERING CROSS SECTIONS FOR POLYCRYSTALLINE BISMUTH



The calculated scattering cross sections for polycrystalline Bi are compared with the elastic scattering cross sections from ENDF/B-VI. [*Young-Sik Cho et al., p.176, ND2001*]

Bismuth - Results

TOTAL CROSS SECTIONS AT 300^{0}K FOR POLYCRYSTALLINE BISMUTH



Total cross sections at 300°K for polycrystalline Bi. The experimental data were given as the total cross sections, so for comparison, the theoretical total cross sections were obtained by adding the capture cross sections from ENDF/B-VI to the total scattering cross sections calculated in this work. [*Young-Sik Cho et al., p.176, ND 2001*]