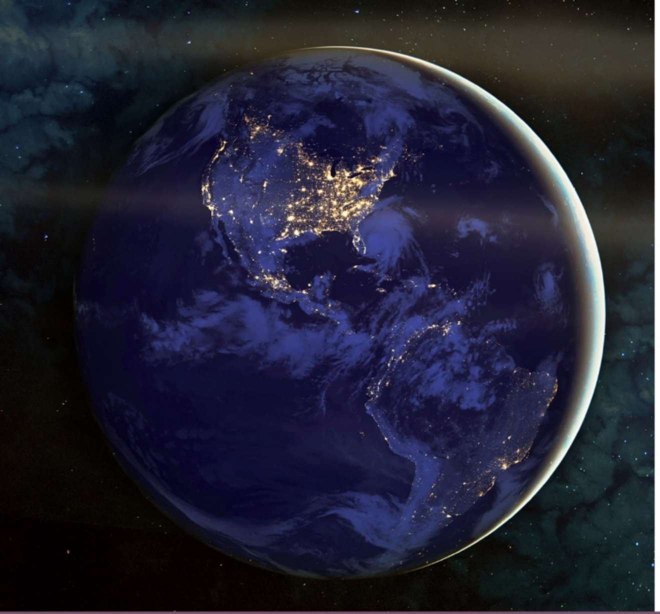

ANS Winter Meeting & Expo

2019 NUCLEAR TECHNOLOGY FOR THE U.S. AND THE WORLD

Thermal Neutron Scattering Cross Sections of U-10Mo

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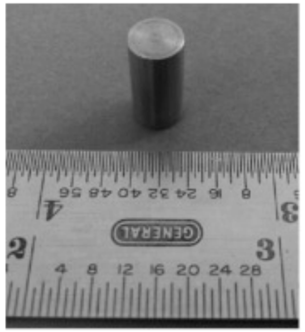
Introduction

- The U.S. National Security Administration Material Management and Minimization Reactor Conversion Program is actively working to convert research reactors from the use of high-enrichment uranium to low-enrichment uranium

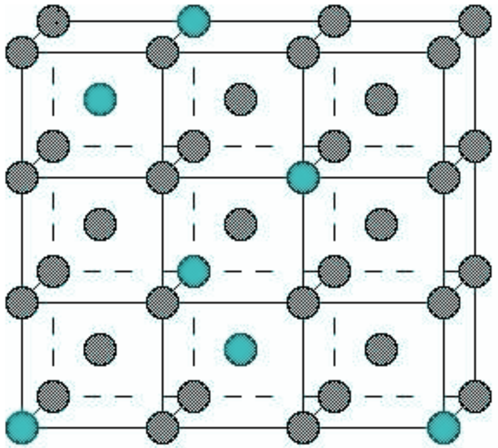
- LEU require a large increase in uranium density (> 15 gU/ cm^3)

- U-Mo alloys, such as U-10Mo (uranium with 10% molybdenum by weight), are under consideration as very high density fuels

- U is alloyed with Mo to preserve the high-temperature BCC phase at lower temperatures



U10Mo sample
Source: Vineet et al., J. Nucl. Mater., 465,pp. 805-813, 2015

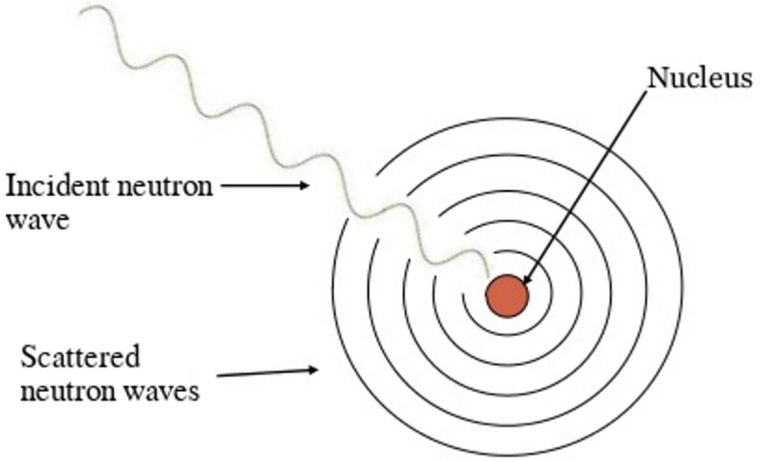


BCC substitutional alloy
Source: http://courses.chem.psu.edu

Introduction

Slowing down of fission neutrons in a reactor can be treated in two parts:

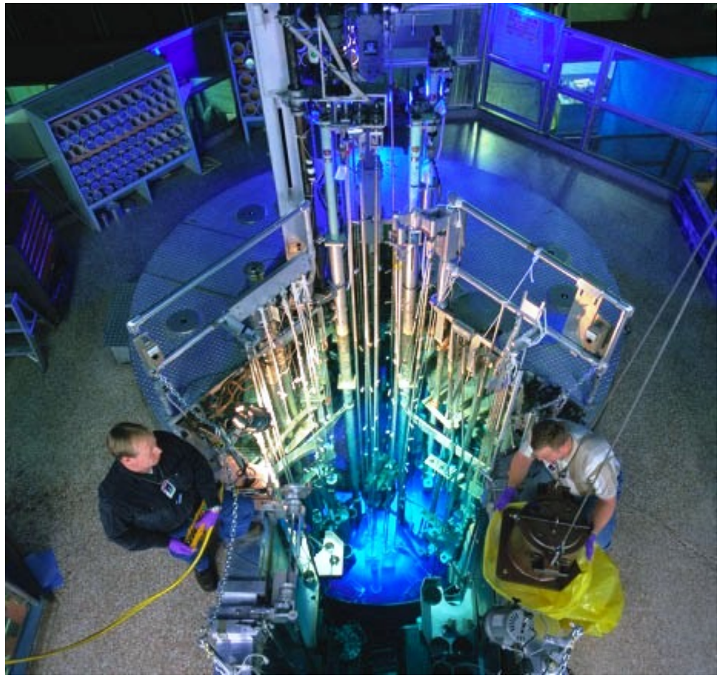
- Above 1 eV :
  - Atoms can be treated as unbound
  - Free-atom neutron scattering cross sections can be used
- Below 1 eV :
  - Energy of neutrons is of the same order as the quantized energy states associated with the vibrations of atoms
  - Interference effects can occur
  - These effects influence the energy and spatial distributions of the thermal neutron population
  - Bound thermal neutron scattering cross sections are needed



Neutron scattering from a single nucleus
Source:https://www.slideshare.net/upvita/neutronscattering

Introduction

- Current transport simulations of U-10Mo rely solely on free atom models which can render large uncertainties in neutron transport calculations
- Knowledge of thermal neutron scattering cross sections are needed for:
  - Accurate prediction of thermal neutron spectrum
  - Reactor physics parameters such as neutron lifetimes, and Doppler and reactivity coefficients



University of Missouri Research Reactor
Source: http://www.themaneater.com/photos

Thermal Neutron Scattering Theory

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi k_B T}\sqrt{\frac{E'}{E}}\left[\sigma_{coh} S(\alpha,\beta) + \sigma_{inc} S_s(\alpha,\beta)\right]$$

$$S(\alpha,\beta) = S_s(\alpha,\beta) + S_d(\alpha,\beta)$$

S_s → no interference (incoherent)

S_d → Interference (coherent)

elastic: S_d^0, S_s^0

inelastic: $S_d^1 + S_d^2 + S_d^3 + \cdots$, $S_s^1 + S_s^2 + S_s^3 + \cdots$

$$S_d = S_d^0 + S_d^1 + S_d^2 + S_d^3 + \cdots$$

$$S_s = S_s^0 + S_s^1 + S_s^2 + S_s^3 + \cdots$$

σ_{coh} → single atom effective coherent scattering cross section

σ_{inc} → single atom effective incoherent scattering cross section

$\alpha = \frac{E' + E - 2\mu\sqrt{E'E}}{Ak_BT}$ → momentum transfer

$\beta = \frac{E' - E}{k_BT}$ → energy transfer

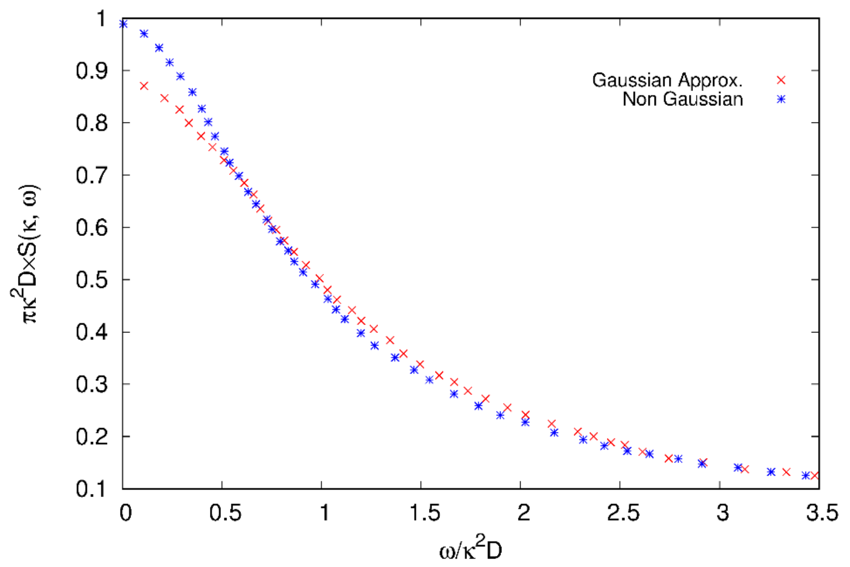
μ → cosine of the scattering angle

Inelastic Scattering Cross Section for an Alloy

- Calculated with:
  - Incoherent approximation
  - Gaussian approximation

- Phonon density of states needed to calculate the scattering law

- NJOY does not need to be modified



Incoherent scattering law
Adapted from: Nijboer et al., Physica, 32, pp. 415-432, 1966

$$\sigma = \frac{1}{2k_B T}\sqrt{\frac{E'}{E}}\sum_k x_k \sigma_b^k S_s^k(\alpha,\beta)$$

x: fraction of atoms of type k

σ_b^k: single atom effective total scattering cross section

S: self scattering law of atom of type k

Elastic Scattering Cross Section for an Alloy

$$\sigma = \frac{\pi \hbar^2}{2mNVE} \sum_{E_{i<E}} e^{-4WE_i} \sum_{\tau_i} \frac{1}{\tau_i} \left| \sum_{j=1}^{N} \sqrt{\frac{\sigma_{c,j}}{\sigma_{c,T}}} e^{2\pi i \vec{\tau_i} \cdot \vec{d_j}} \right|^2$$

→ High-symmetry material (NJOY)

$$\sigma = \frac{\pi \hbar^2}{2mNVE} \sum_{E_{i<E}} \left| \sum_{k} x_k \sqrt{\sigma_c^k} e^{-2W_k E_i} \right|^2 \sum_{\tau_i} \frac{1}{\tau_i} \left| \sum_{j=1}^{N} e^{2\pi i \vec{\tau_i} \cdot \vec{d_j}} \right|^2$$

→ Disordered Alloy

- Approximations:
  - Ignore diffuse scattering
  - Incoherent part negligible
  - Debye Waller factor depends only on the atomic species
- Implemented by modifying NJOY

$E_i = \frac{\hbar^2 \tau_i^2}{2m}$ Bragg edges

x: fraction of atoms of type *k*

W : Debye-Waller factor (calculated from the PDOS)

τ_i: reciprocal lattice vectors

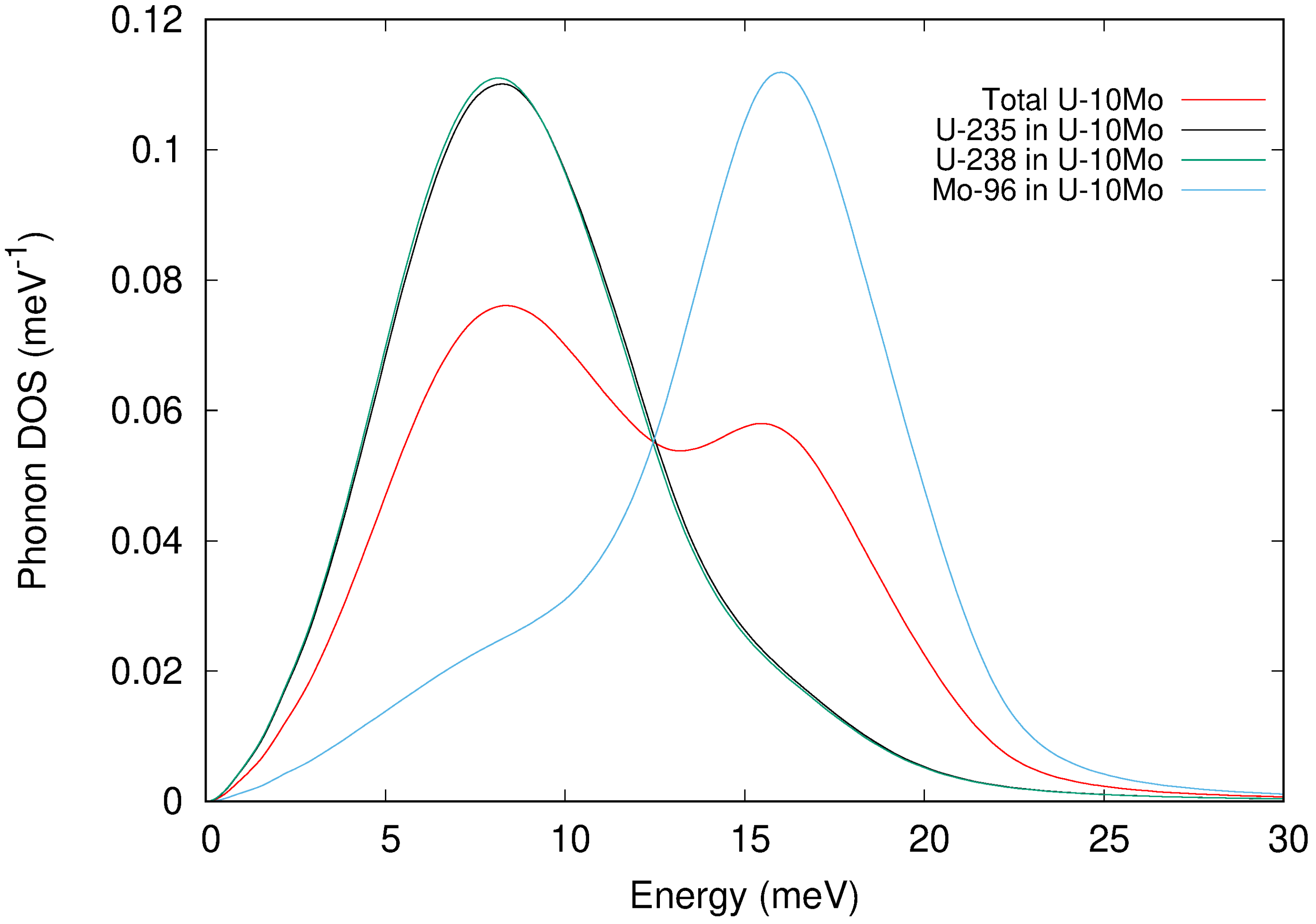
d_j: atomic position of the j atom in the unit cell

Methods

- Calculated the PDOS of U-10Mo using:
  - Molecular dynamics
  - Velocity Autocorrelation Function Method
  - U-10Mo modeled as a random distribution of ^{96}Mo, ^{235}U, and ^{238}U (20 at. % ^{235}U enrichment with 10 wt.% Mo)
  - 21x22x23 BCC primitive unit cells

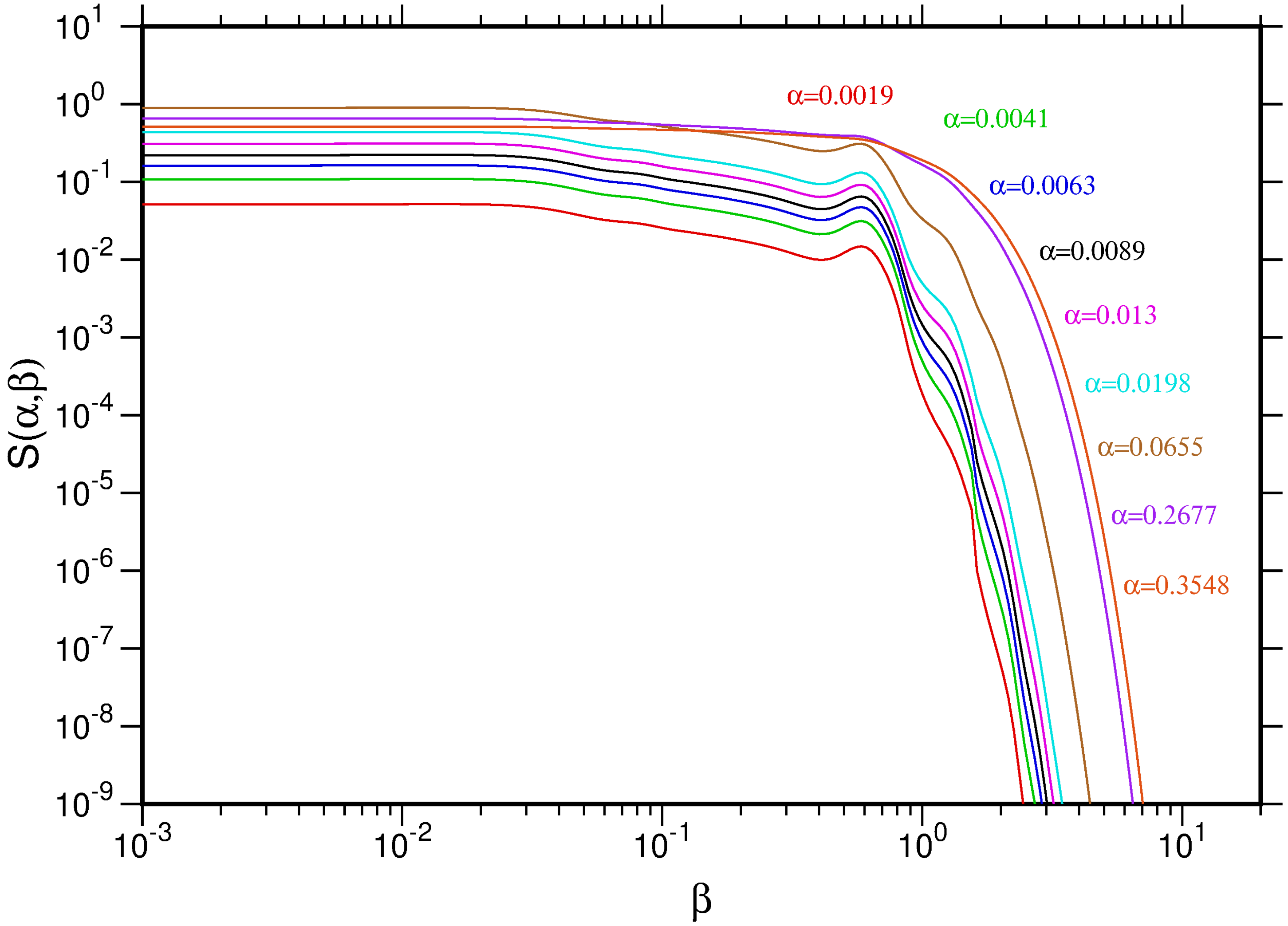
- Used NJOY to calculate the cross sections:
  - Incoherent inelastic cross section using the Gaussian Approximation
  - Coherent part calculation was implemented by modifying the LEAPR module of NJOY

Results: Phonon Density of States of U-10Mo at 300 K

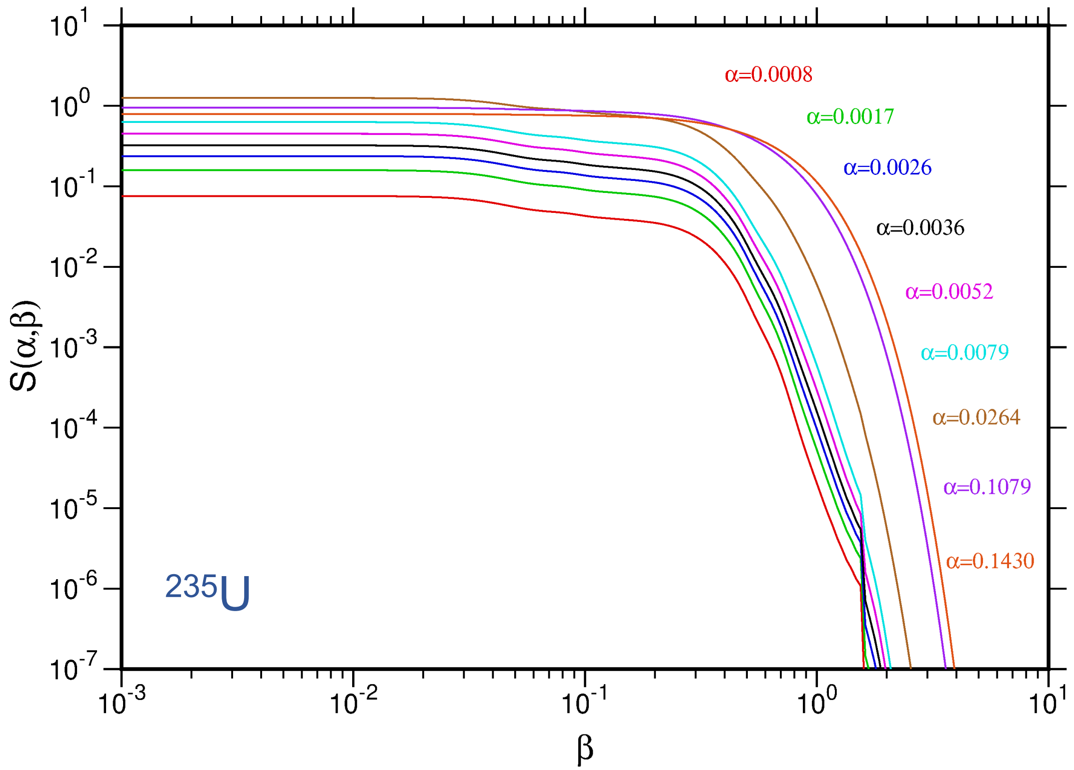


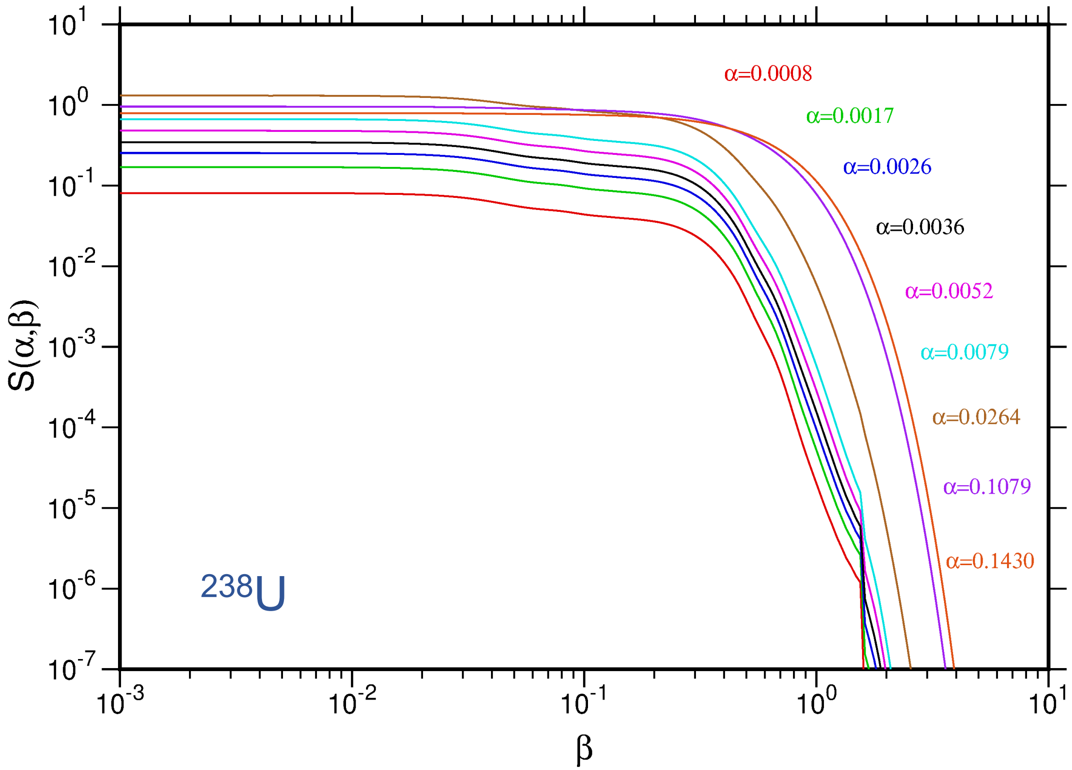
Partial phonon DOS are required to calculate the thermal neutron scattering cross sections

Results: Scattering Law of ^{96}Mo in U-10Mo at 300K



Results: Scattering Law of ^{235}U and ^{238}U in U-10Mo at 300K





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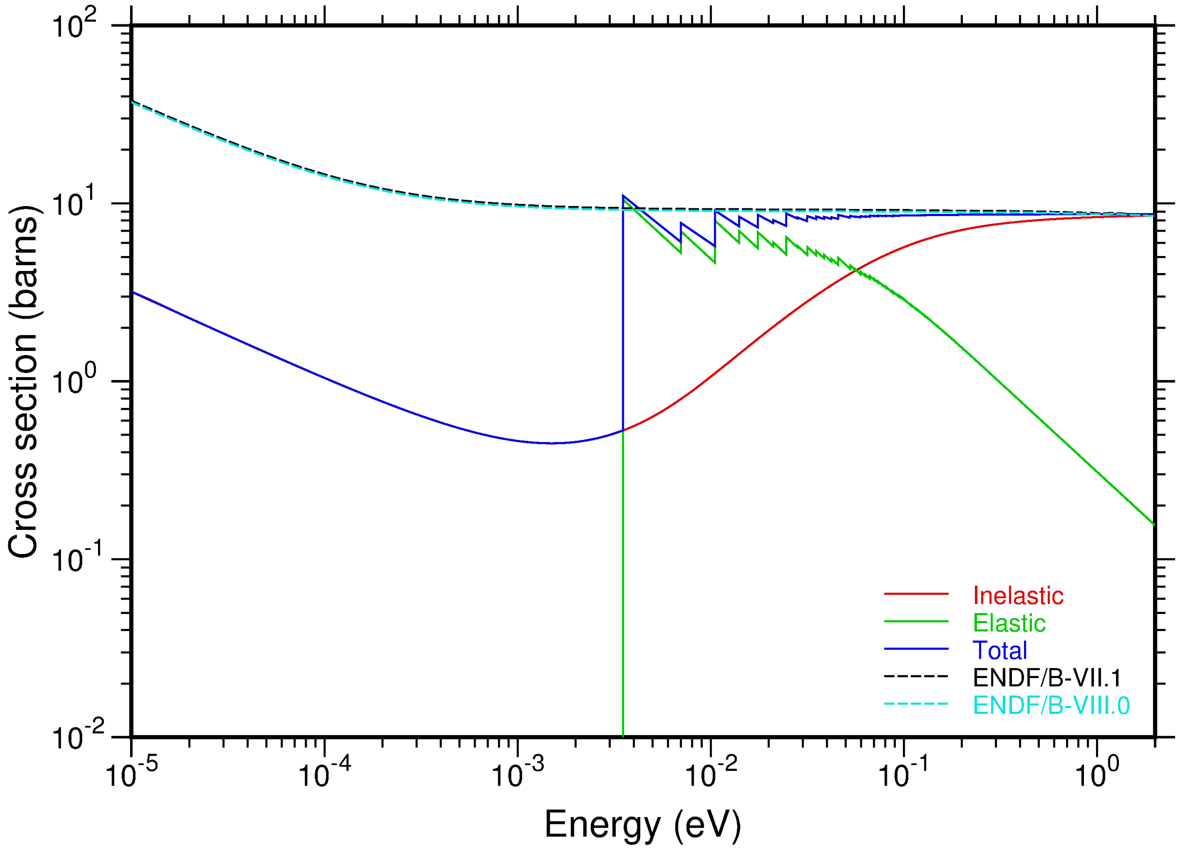
Results: Total thermal neutron scattering cross sections of U-10Mo at 300K



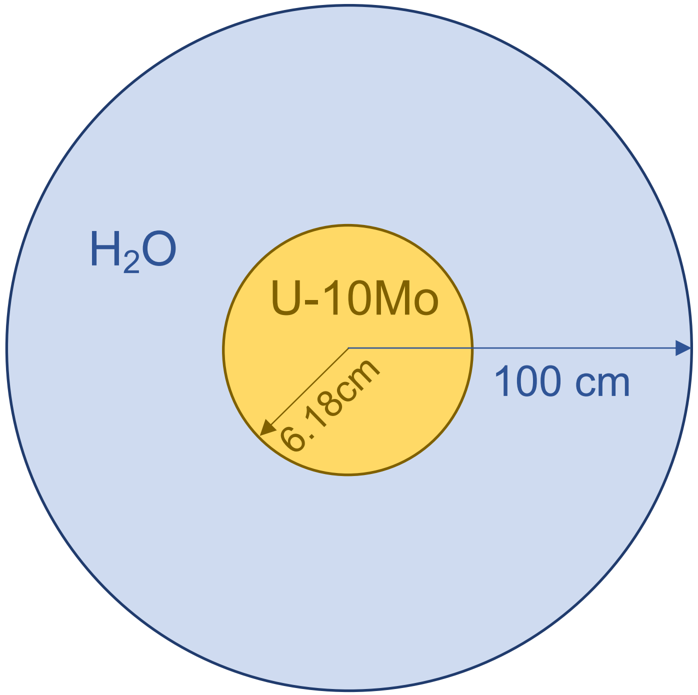
Free-nucleus cases (ENDF/B-VII.1 and ENDF/B-VIII.0)[1,2] are a linear combination of the three nuclei weighted by atom fractions

[1] Chadwick, M.B., et al. *ENDF/B-VII.1 nuclear data for science and technology*, Nucl. Data Sheets. 112, 12, 2887-2996 (2011).

[2] Brown, D.A., et al. *ENDF/B-VIII.0*, Nucl. Data Sheets. 148, 1-142, (2018).

Results: Effects on criticality

Criticality as predicted with the thermal cross section from a simple MCNP model of U-10Mo fuel with 20 at.% ^{235}U



Library	k_{eff}	Change
Free-atom (ENDF/B-VII.1)[1]	0.4241	-55.39%
Free-atom (ENDF/B-VIII.0)[2]	0.4238	-55.41%
U-10Mo thermal	0.9505	-0-

$$\text{Change} = \frac{k_{\text{eff}}^{f} - k_{\text{eff}}^{th}}{k_{\text{eff}}^{th}}$$

[1] Chadwick, M.B., et al. *ENDF/B-VII.1 nuclear data for science and technology*, Nucl. Data Sheets. 112, 12, 2887-2996 (2011).
[2] Brown, D.A., et al. *ENDF/B-VIII.0*, Nucl. Data Sheets. 148, 1-142, (2018).

Conclusions

- The thermal neutron scattering cross sections of the U-10Mo alloy enriched at 20 at.% ^{235}U were calculated using a modified version of NJOY
- The calculated scattering cross sections show that consideration of binding effects causes deviations from the free-atom model
- A non-negligible increase in the k_{eff} was found when employing the thermal neutron scattering cross sections

Results: Effects on criticality

Criticality as predicted with the thermal cross section from a simple MCNP model of U-10Mo fuel with 20 at.% ^{235}U

Library	k_{eff}	Change
Free-atom (ENDF/B-VII.1)[1]	0.4241	-0-
Free-atom (ENDF/B-VIII.0)[2]	0.4238	0.06%
U-10Mo thermal (including U235 and U238 data)	0.9505	124.2%
U-10Mo thermal (not including U235 thermal data)		

[1] Chadwick, M.B., et al. *ENDF/B-VII.1 nuclear data for science and technology*, Nucl. Data Sheets. 112, 12, 2887-2996 (2011).
[2] Brown, D.A., et al. *ENDF/B-VIII.0*, Nucl. Data Sheets. 148, 1-142, (2018).

Effects on Criticality

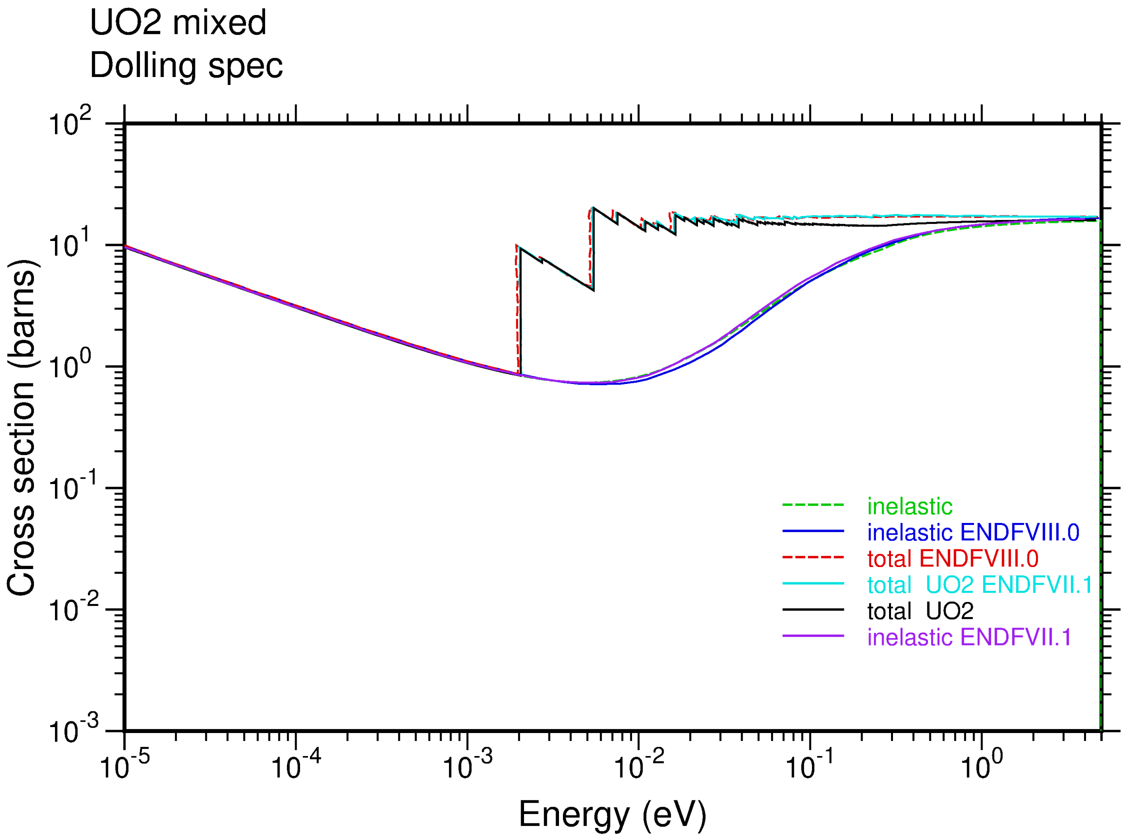
Criticality as predicted with the thermal cross section from a simple MCNP model of fuel with 2.55% enrichment

Cross Section	keff	Δk_{eff}
U10Mo 300K (U-238 / Mo-96)	0.51164	- 4.82 %
U10Mo 300K (U-235/Mo-96)	0.97542	81.46%
BCC U 300K (U238)	0.53753	-0-
U10Mo 1113K (U238-Mo96)	0.50758	-5.45%
BCC U 1113K (U-238)	0.53757	0.13%
free atom U238 1113k	0.53685	-0-

[1] Trkov, A., et al. *ENDF/B-VI and ENDF/B-VII*, National Nuclear Data Center, BNL, Upton, NY (2012)

Thermal Scattering Cross Sections of UO2

- Calculated using:
  - Available PDOS[1]
  - Averaged Debye Waller Factor W=WU + 2WO
- Compared to data from ENDFVII.1 [2] and ENDFVIII.0 [3] evaluations



[1] Dolling,G., et al. Can J. Phys, 43, 1397 (1965)
[2] Trkov, A., et al. *ENDF/B-VI and ENDF/B-VII*, National Nuclear Data Center, BNL, Upton, NY (2012)
[3] Brown, D. A., et al., Nucl. Data Sheets, 148, 1–142 (2018).

Effects on Criticality

Criticality as predicted with the thermal cross section from a simple MCNP model of UO2 fuel

Run (nat. enr.)	Fast-data	Inelastic thermal	Elastic thermal	keff	Change (%)
U-235 data	Free-atom	---	---		
U238-data	Free-atom	---	---	0.16509	0.000
O-data	Free-atom	---	----		
U-235 data	Free-atom	---	---		
U238-data	Free-atom	ENDF8	ENDF8	0.3734	126.180
O-data	Free-atom	ENDF8	ENDF8		
U-235 data	Free-atom	---	---		
U238-data	Free-atom	calculated	calculated	0.16482	-0.164
O-data	Free-atom	calculated	calculated		
U-235 data	Free-atom	calculated	calcualted		
U238-data	Free-atom	calculated	calculated	0.21764	31.831
O-data	Free-atom	calculated	calculated		

Run (5%. enr)	Fast-data	Inelastic thermal	Elastic thermal	keff	Change (%)
U-235 data	Free-atom	---	---		
U238-data	Free-atom	---	---	0.24935	0.000
O-data	Free-atom	---	----		
U-235 data	Free-atom	---	---		
U238-data	Free-atom	ENDF8	ENDF8	---	---
O-data	Free-atom	ENDF8	ENDF8		
U-235 data	Free-atom	---	---		
U238-data	Free-atom	calculated	calculated	0.24923	-0.048
O-data	Free-atom	calculated	calculated		
U-235 data	Free-atom	calculated	calculated		
U238-data	Free-atom	calculated	calculated	0.60006	140.650
O-data	Free-atom	calculated	calculated		

[1] Trkov, A., et al. *ENDF/B-VI and ENDF/B-VII*, National Nuclear Data Center, BNL, Upton, NY (2012)

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