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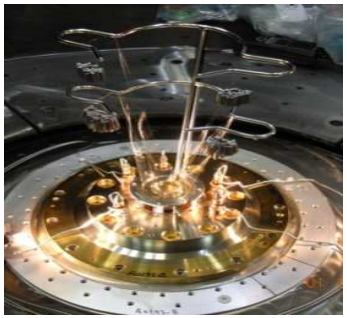

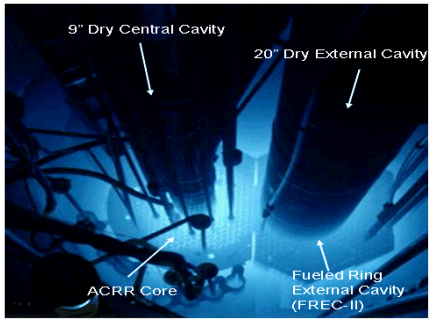

A Rigorous Treatment of Uncertainty Quantification for Silicon Damage Metrics

Presented at: IAEA Technical Meeting (F4-TM-52919): Nuclear Reaction Data and Uncertainties for Radiation Damage

June 13-16, 2016

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Org. 1300, Radiation and Electrical Sciences

U.S. DEPARTMENT OF ENERGY

NNSA

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FOCUS OF WORK:

RIGOROUS QUANTIFICATION OF THE UNCERTAINTY IN SILICON DISPLACEMENT DAMAGE METRICS USED IN ASSESSING SEMICONDUCTOR RESPONSE

Develop a covariance matrix to describe the silicon damage function as reflected in the ASTM E722 standard.

Outline of Presentation

- Definitions
  - Displacement kerma
  - Damage energy
- Uncertainty
  - Types
  - Treatment
    - Sensitivities to parameters
    - Method of Characterization

Sources of Uncertainty Considered

- **Nuclear Data**
  - Natural isotopic abundance
  - Cross sections
  - Recoil atom spectra
- **Damage Partition Function**
  - Electronic potential
  - Nuclear (lattice atom) scattering potential
- **Displacement Threshold**
  - Displacement threshold energy, E_d
  - Formulation of damage energy
- **Model Defect**

TOPIC:
TERMINOLOGY AND DEFINITIONS

Kerma

Displacement kerma

Damage energy

NIEL

1-MeV(Si) equivalence fluence

Displacement model

Radiation Damage Metrics Considered

- **Material**
  - ^{28}Si
  - ^{nat}Si
- **Response**
  - Displacement kerma
  - NRT damage energy
  - 1-MeV(Si)-equivalent damage

Kerma

$$K = {dE_{tr}}/{dm}$$

$$K = \int \Phi_E \cdot E \cdot \frac{\mu_{tr}}{\rho} \cdot dE$$

- **Kerma, *K*, (for ionizing uncharged particles) is the quotient of dE_{tr} by *dm*, where dE_{tr} is the mean sum of the initial kinetic energies of all charged particles liberated in a mass *dm* of a material by the uncharged particle incident on a mass *dm* of a material.**
- **μ_{tr}/ρ is he mass energy transfer coefficient**

Microscopic Displacement Kerma Factor

$$\kappa^{dpa}(E) = \sum_{i,j_i} \sigma_{i,j_i}(E) \int_0^{\infty} dT_{R,j_i} \int_{-1}^{1} d\mu \cdot f_{i,j_i}\left(E, \mu, T_{R,j_i}\right) \cdot {}^{ion}T_{dam}\left(T_{R,j_i}\right)$$

- **Summation over all open reaction channels, *i*, and all emitted particles, *j*.**
- **$T_{R,j,i}$ is the recoil particle energy**
- **$f_{i,j}$ is the energy distribution for outgoing ions $T_{R,j,i}$**
- **$^{ion}T_{dam}(T_{ri,j})$ is the damage energy from recoil ion $T_{R,j,i}$**
- **Energy integral for $T_{R,j,i}$ goes from 0 to ∞**

NIEL – Non-ionizing Energy Loss

$$NIEL^{T_{\min}}(E) = \frac{N_A}{A'_L} \cdot \sum_i \sigma_i(E) \cdot \int_{T_{min}}^{\infty} dT_R \int_{-1}^{1} d\mu \cdot f_i(E, \mu, T_R) \cdot {}^{ion}T_{dam}(T_R)$$

- **Energy integral over T_R goes from T_{min} to ∞.**
- **T_{min} is defined differently by different authors, but it is most commonly set to E_d, the displacement threshold energy.**
- **Issue – there is non-ionizing energy from neutron interactions less than E_d. The energy goes into lattice phonons.**
- **Note, most of the "damage energy" also goes into phonons and lattice heating. The rest goes into changes in lattice binding energy.**

Energy Partition for 50 keV ^{28}Si Ion in Si Lattice

- SRIM calculation of Silicon ion energy deposition
- Ionization and Frenkel pair formation come from primary ion and from displaced secondary recoil atoms
- 91.76% of non-ionizing damage energy goes into phonons

Energy Loss Mechanism: (50 keV Si ion in Si lattice, range = 736 A, straggle = 290 A)	Percent of Energy Deposition	
	Primary Ion	Recoil Atoms
Ionization	30.50	25.67
Vacancies	0.23	3.38
Phonons	0.77	39.44

Displacement Kerma

- **Displacement kerma, K^{dpa}, is equal to the microscopic kerma factor multiplied by number of atoms per unit mass in the target material and the incident particle fluence.**

Ionization Kerma

- **Ionization kerma, K^{ion}, is obtained by subtracting the displacement kerma. K^{dpa}, from the total kerma, K.**
- **Note, if one formulates this in terms of the NIEL, then the non-ionizing energy less than E_d needs to be addressed as a separate subtracted term.**

Neutron Damage Energy

$$ {}^{n}\sigma_{dam}(E) = {}^{n}T_{dam}(E) = \sum_{i,j_i} \int \sigma_{i,j_i}(E) \cdot K_{i,j_i}^{recoil}\left(E \rightarrow T_{j_i}\right) \cdot {}^{ion}T_{dam}(T_{j_i}) \cdot dT_{j_i} $$

$$ {}^{n}E_{dam}(E) = \frac{{}^{n}\sigma_{dam}(E)}{\sigma(E)} $$

- **Damage energy, or neutron damage energy cross section, typically has units of eV-b or MeV-mb. This is the term computed in NJOY-2012**
- **$^{n}E_{dam}$ is an effective damage energy**
- **$\sigma(E)$ is the total neutron cross section**
- **The lower integration bound is model-dependent**

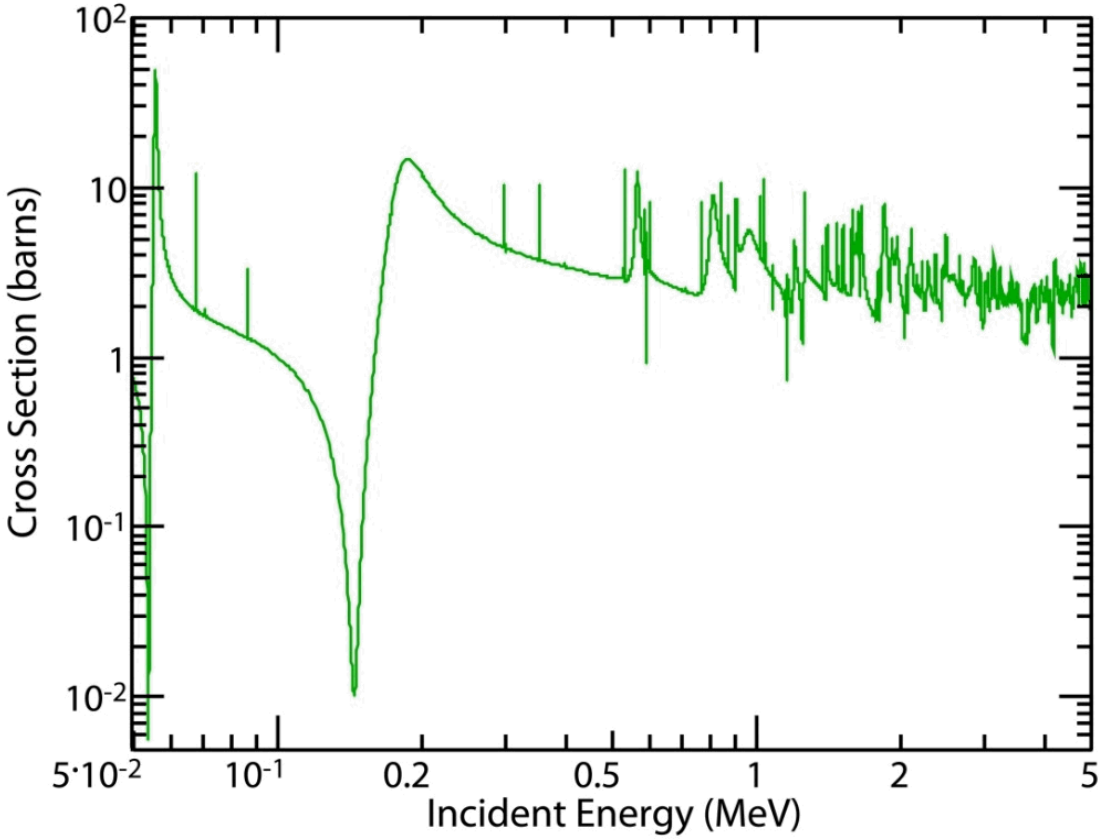
1-MeV(Si) Equivalent Neutron Fluence

$$\kappa_{Si}^{dpa}(E) = A \cdot E\left(1 - e^{-B/E}\right)$$

$$\kappa_{Si-\mathrm{Re}f}^{dpa} = \kappa_{Si}^{dpa}(1\,MeV)$$

- **Reference kerma is taken from a fit to avoid sensitivity to resonances in the region**
- **1-MeV(Si)-n/cm^2 is the macroscopic {damage energy | displacement kerma} divided by the reference 1-MeV value, $\kappa^{dpa}_{Si\text{-}Ref}$**
- **The community-intended metric is "damage energy" since it should correlate with observed damage, but this term has been described using "displacement kerma" in the past.**

Silicon Total Cross Section



- **Resonance structure exists in the 1-MeV region**

Historical Fitting Data for Reference Value

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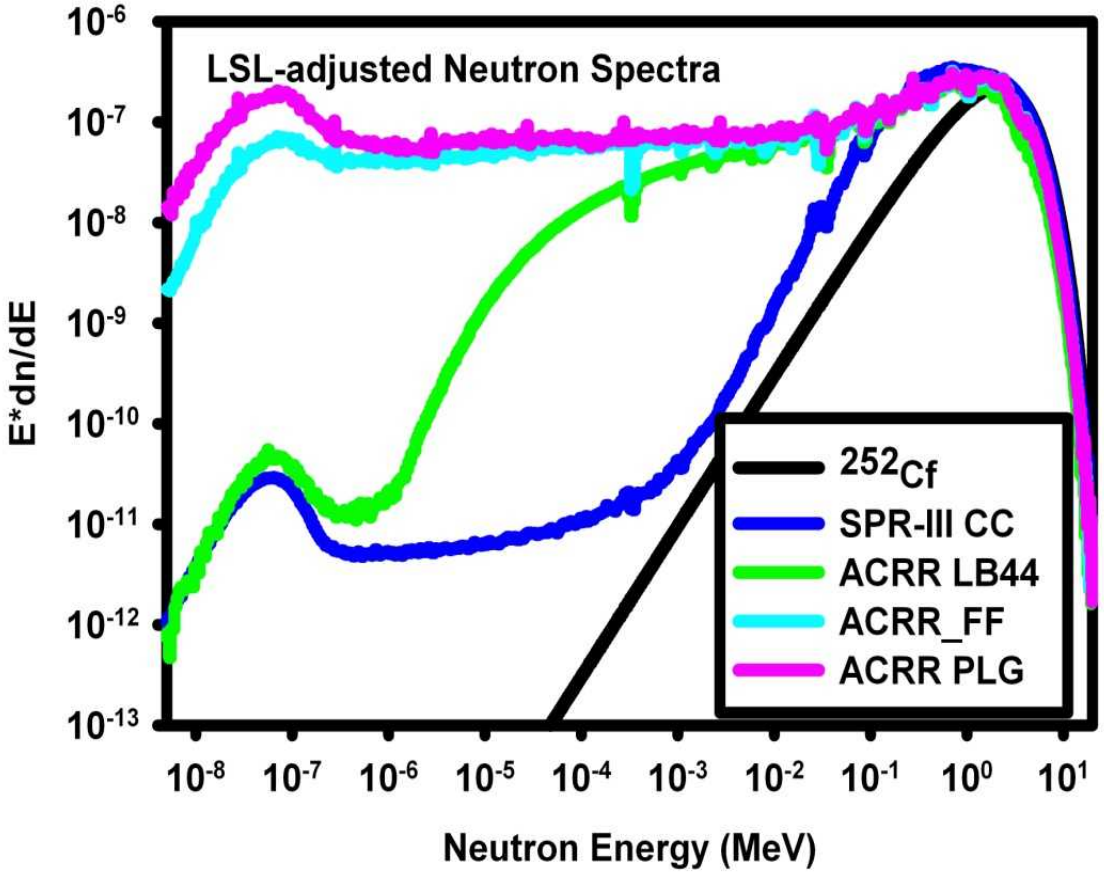
1-MeV(Si) Ref.	A Coeff.	B Coeff	Weighting Function
95.9	124.0	1.49	SPR-III Cavity, EXX4 Disp. Kerma
94.0	163.0	0.86	TRIGA with boral weighting, EX44 Disp. Kerma
100.1	129.3	1.49	SPR-III Cavity, Verbinski Disp. Kerma
96.9	192.6	0.70	TRIGA with boral weighting, Verbinski Disp. Kerma
93.6	146.7	0.99	SPR-III Cavity, Bendel Disp. Kerma
90.8	177.0	0.70	TRIGA with boral weighting, Bendel Disp. Kerma

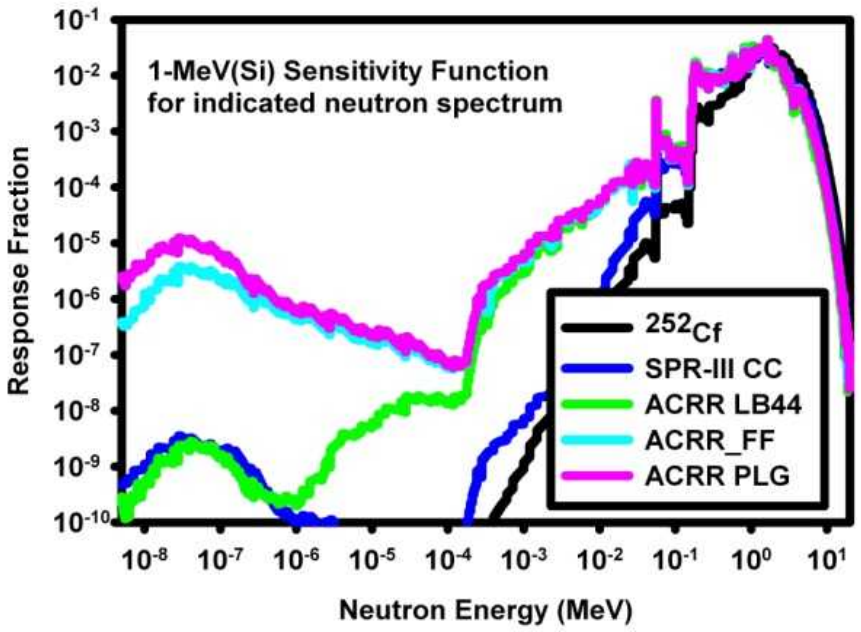
Reactor Energy-dependent Spectra Investigated for Weighting Fitting Response



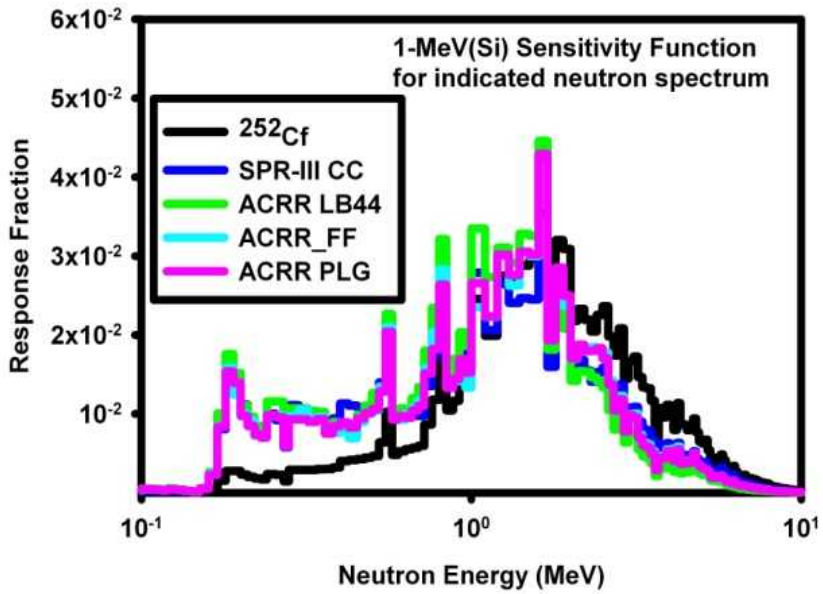
- **Used suite of SNL-based reactor environments and reference benchmark fields**

Energy-dependent Sensitivity Functions for 1-MeV(Si) fir Various Reactor Spectra

Total Energy Sensitivity



High Energy Region



Characteristics of Reactor Spectra

Identifier	Avg. Eng. [MeV]	1-MeV(Si) disp. kerma/(n/cm^2) [MeV-mb]/(n/cm^2)]	[10% | 90%] 1-MeV(Si) Sensitivity Range	[5% | 95%] 1-MeV(Si) Sensitivity Range
^{252}Cf Spontaneous Fission	2.1227	100.4940	[0.6740 | 4.969]	[0.444 | 6.06]
SPR-III Central Cavity	1.2580	78.00787	[0.2607 | 4.078]	[0.199 | 5.179]
ACRR PbB_4C Bucket	0.7496	53.25974	[0.2321 | 3.016]	[0.285 | 4.239]
ACRR Free-field Cavity	0.5947	38.19648	[0.2467 | 3.663]	[0.189 | 4.737]
ACRR PLG Bucket	0.4709	30.39959	[0.2448 | 3.626]	[0.188 | 4.746]

Sensitivity of Fit for Reference Value to Energy Groups and Fit Region

1-MeV(Si) Ref.	A/B Coeff.	Fit Region	Response
94.59	181.8 ± 0.22% 0.7345 ± 0.25%	[0.05, 4.66]	89-grp., ENDF/B-VII.1 with Robinson
95.17	186.5 ± 0.10% 0.7138 ± 0.15%	[0.05, 4.66]	640-grp., ENDF/B-VII.1 with Robinson
92.19	150.2 ± 0.27% 0.95 ± 0.25%	[0.5, 5.00]	89-grp., ENDF/B-VII.1 with Robinson
90.69	138.6 ± 0.14% 1.06 ± 0.12%	[0.5, 5.00]	640-grp., ENDF/B-VII.1 with Robinson

- Uniform weighting used in this analysis

Observations on Sensitivity of Fitting on the Ref. Displacement Kerma

- From this fitting one observes:
  - Insensitive to the number of energy groups used
  - Some sensitivity to the fitting region
- From historical data:
  - Some sensitivity to the weighting spectrum
  - Strong sensitivity to the response function

Generic Formulation of the Displacement Model

$$ {}^{type}\nu_d\left(E_d, {}^{ion}T_{dam}\right) = {}^{type-A}\Lambda(E_d, {}^{ion}T_{dam}) \square {}^{type-B}\varsigma_d(E_d, {}^{ion}T_{dam}) \square {}^{type-C}\xi({}^{ion}T_{dam}) $$

- ${}^{type}\upsilon_d$ is the number of Frenkel pairs (FP)
- ${}^{type\text{-}A}\Lambda(E_d, {}^{ion}T_{dam})$ is a threshold function
- ${}^{type\text{-}B}\zeta_d(E_d, {}^{ion}T_{dam}$ is a FP generation efficiency
- ${}^{type\text{-}C}\xi({}^{ion}T_{dam})$ is a residual defect survival

- Formulation designed to capture all current types displacement models
- Threshold function permits the formulation to use a lower integration bound of 0

Existing Displacement Models

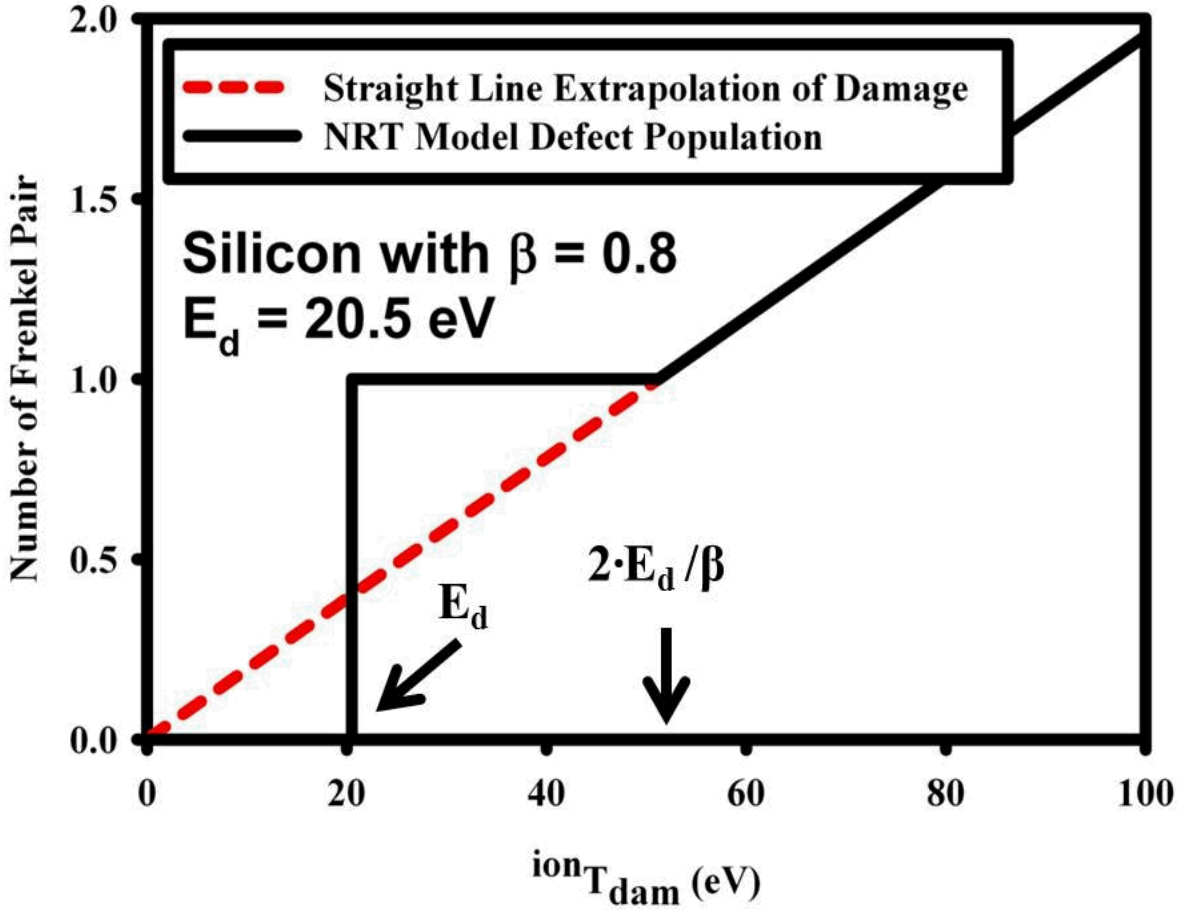
- Original Kinchin-Pease
- Sharp-transition Kinchin-Pease
- Robinson-Sigmund Modification
- Norgett-Robinson-Torrens (NRT)
- Snyder-Neufeld
- Neufeld-Snyder
- Bacon
- Athermal Recombination-corrected Displacement (arc-dpa)
- Replacement per atom (rpa)

NRT Displacement Model

$$ {}^{NRT}\nu_d\left(E_d, {}^{ion}T_{dam}\right) = \begin{cases} 0 & 0 \le {}^{ion}T_{dam} < E_d \\ 1 & E_d \le {}^{ion}T_{dam} < 2 \cdot E_d / \beta \\ \beta \cdot {}^{ion}T_{dam} / \left(2 \cdot E_d\right) & 2 \cdot E_d / \beta \le {}^{ion}T_{dam} < \infty \end{cases} $$

- **β is an atomic scattering correction and is taken to 0.8, a value close to the *ζ (m=1)* value in the Robinson-Sigmund analysis**

Energy-dependence of NRT FP Creation in Si



- Note treatment near E_d threshold energy

NRT Expression in our Formulation

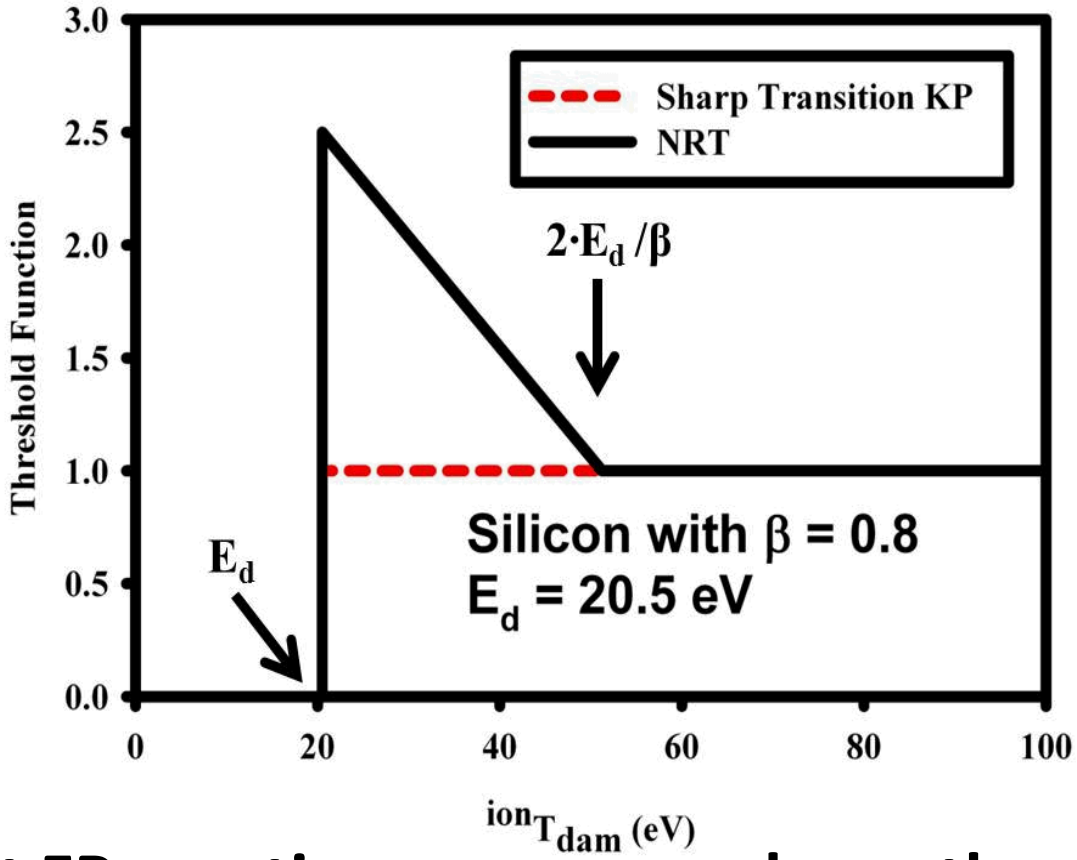
$$ {}^{NRT}\nu_d\left(E_d, {}^{ion}T_{dam}\right) = {}^{NRT}\Lambda(E_d, {}^{ion}T_{dam}) \square {}^{defect}\varsigma[(\beta \square {}^{ion}T_{dam})/(2 \square E_d)] \square {}^{null}\xi({}^{ion}T_{dam}) $$

$$ {}^{defect}\varsigma\left(X\right) = X \qquad {}^{null}\xi_d\left({}^{ion}T_{dam}\right) = 1 $$

- **Note arguments in the various terms in the above expression.**
- **We use a constant FP generation efficiency, hence a constant reference energy to create a defect.**
- **A more compact model-specific notation uses:**

$$ {}^{NRT}\varsigma_d\left(E_d, {}^{ion}T_{dam}\right) = {}^{defect}\varsigma[(\beta \square {}^{ion}T_{dam})/(2 \square E_d)] $$

NRT Threshold Function in this Formulation



- **Constant FP creation energy produces the enhanced threshold-dependent efficiency:** $^{NRT}\Lambda_d\left(E_d, {}^{ion}T_{dam}\right)$

NRT-based Damage Energy

$$\overset{n}{\underset{NRT=E_d}{}} T_{dam}(E) = \sum_{i,j_i} \int_0^{\infty} \sigma_{i,j_i}(E) \square K_{i,j_i}^{recoil}\left(E \to T_{j_i}\right) \square^{NRT} \Lambda_d[E_d, {}^{ion} T_{dam}(T_{j_i})] \square^{ion} T_{dam}(T_{j_i}) \cdot dT_{j_i}$$

- **Formulation:**
  - **uses a lower integration bound of 0**
  - **while capturing the treatment of the threshold near E_d**

Issue: NJOY-2012 Treatment of Damage Energy

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- Damage is partitioned into ionization and displacement components
  - Displacement component includes:
    - Binding energy
    - Energy that goes into phonons
- Actual displacements cannot occur for very small damage energies. This is captured in the displacement threshold energy model, i.e. the Kinchin-Pease or NRT defect production model.
- Robinson's damage partition is defined down to a zero energy
- Issue: damage energy in NJOY-2012 is artificially truncated at E_d
  - It uses a sharp-threshold Kinchin-Pease model
  - It does not support easy computation of displacement kerma

TOPIC:
UNCERTAINTY

Type ⇨ Nuclear Data ⇨ Natural Abundance

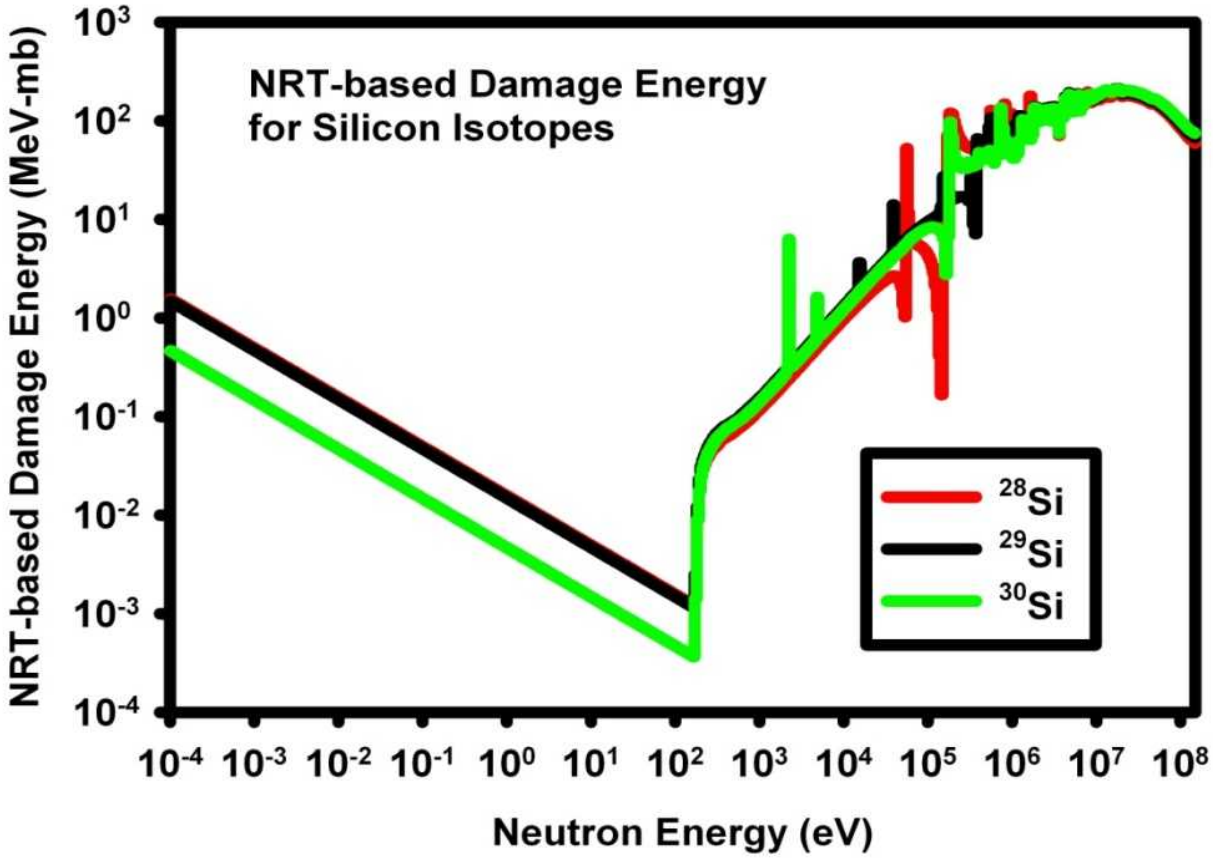
Nuclear Data Used

Isotope	ENDF/B MAT Designator	Natural Abundance (%)[2,3]	Weight Fraction	Number Fraction	Mass Excess (MeV) [1,2]
^{28}Si	1425	92.223 (19)	0.918665	0.92223	-21.4927
^{29}Si	1428	4.685 (8)	0.048336	0.04685	-21.8950
^{30}Si	1431	3.092 (11)	0.032999	0.03092	-24.4329

[1]Mass excess correction applied using 1 amu = 931.494013 MeV
[2]Data from Reference [Tu11]
[3]Uncertainties in last significant figures are given in parenthesis.

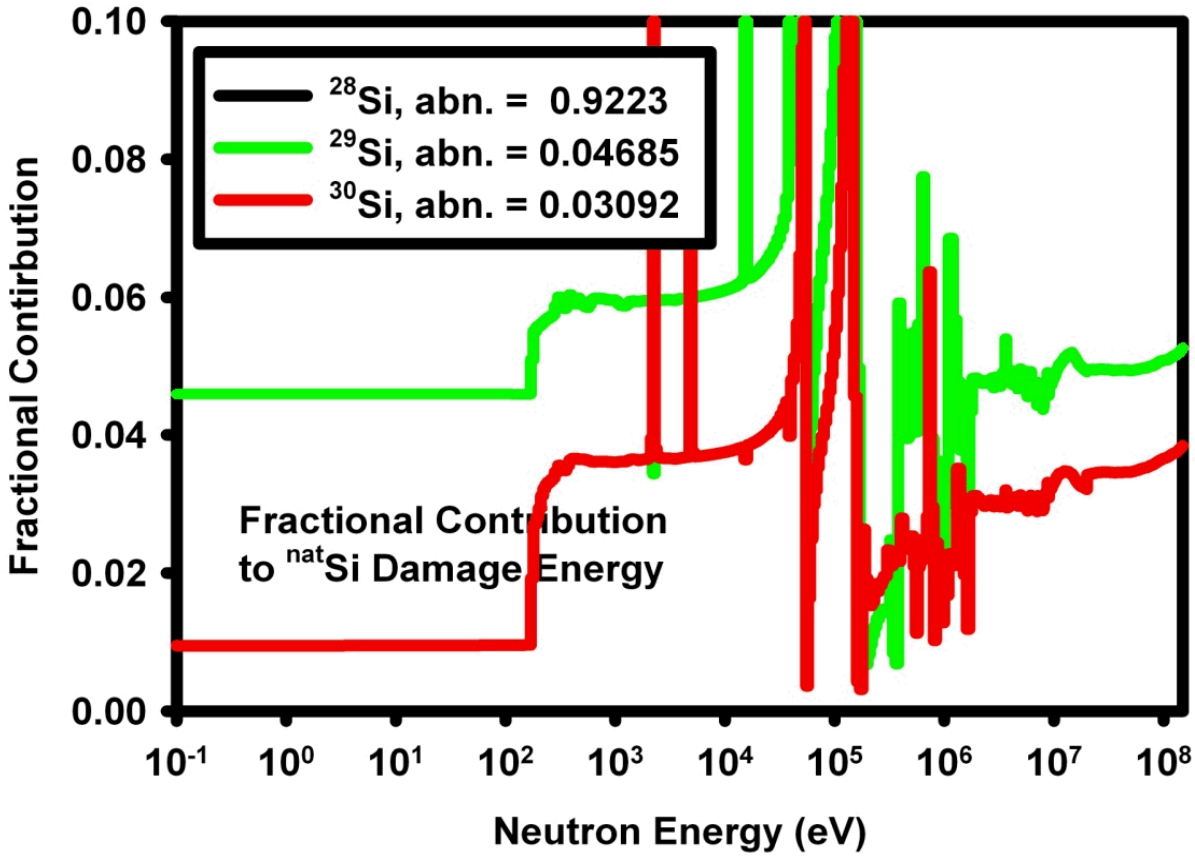
- Uncertainty in natural abundance is small enough that it has no effect in the overall analysis
- The combination of radiation metrics for the Silicon isotopes is an important consideration

NRT-based Damage Energy for Silicon Isotopes



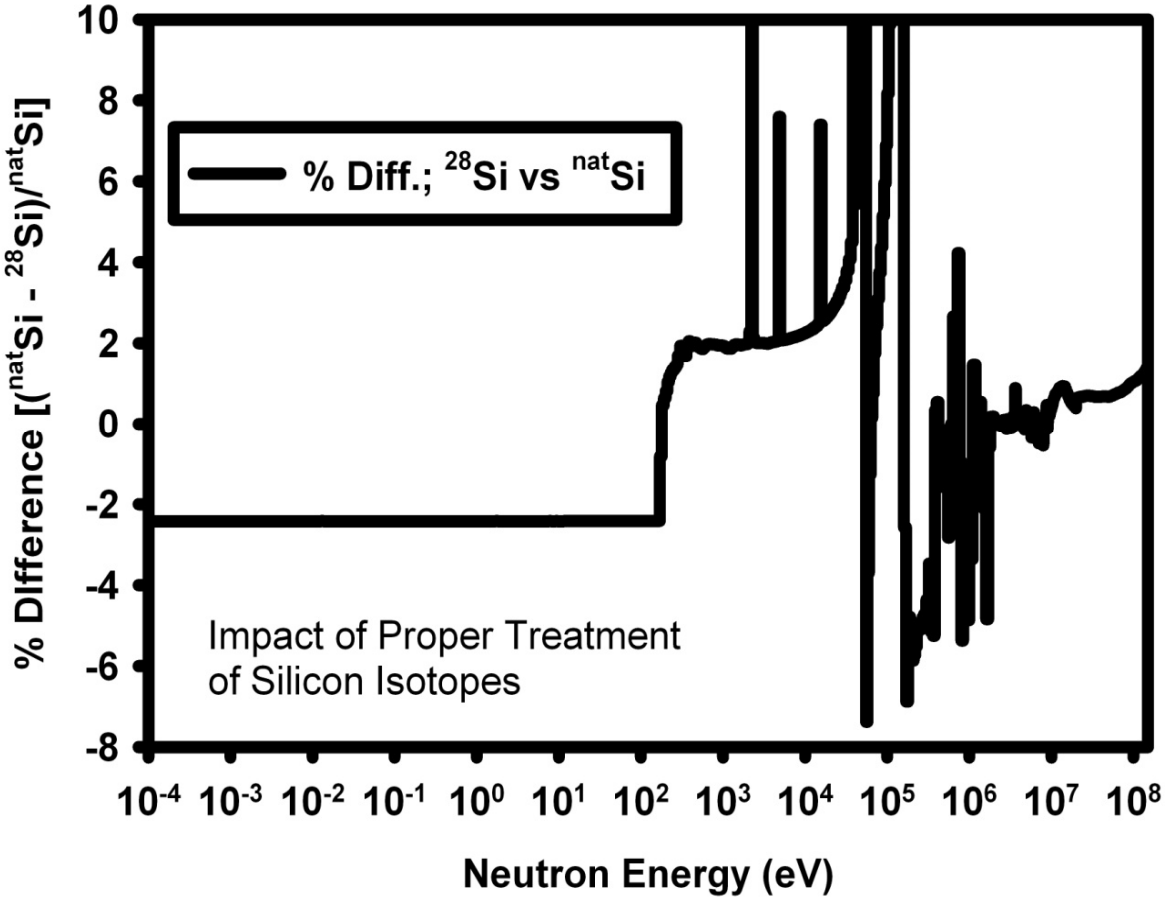
- **Damage energy from silicon isotopes are similar but have a different resonance structure**

Fractional Contributions from Silicon Isotopes to NRT-based Damage Energy



- **Weighting is dominated by the natural abundance**

Difference Between ^{28}Si and ^{nat}Si NRT-based Damage Energy



- **Except for some resonance structure, the ^{28}SI damage energy is within the uncertainty of the ^{nat}Si damage energy**

TOPIC:
UNCERTAINTY

Type ⇨ Nuclear Data ⇨ Cross Sections

Treatment ⇨ Sensitivity

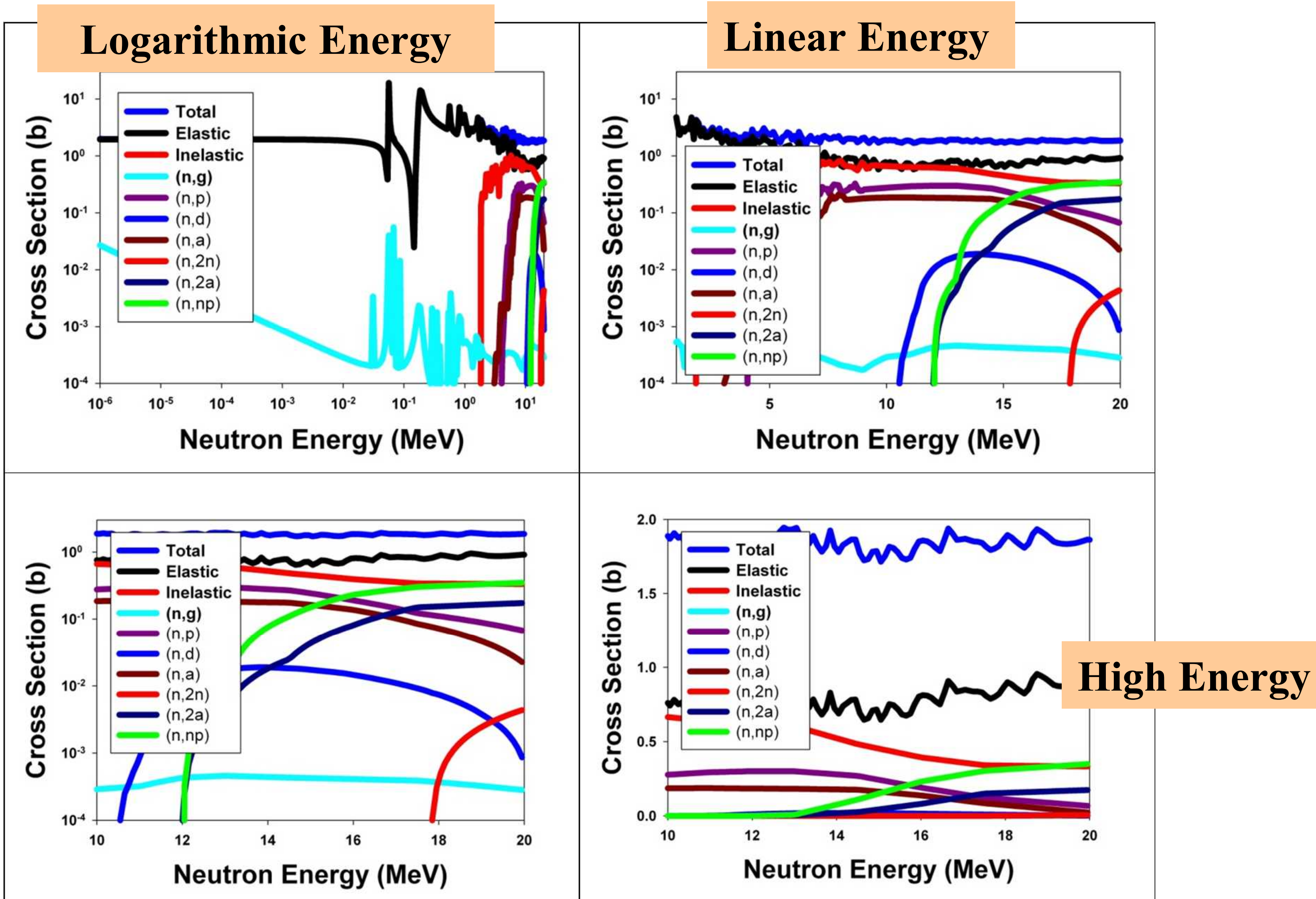
^{28}Si Reaction Channels (1/2)

Number	Reaction	Q-value (MeV)	Threshold Energy (MeV)	ENDF/B-VII.1	TENDL-2015
1	Elastic (MF=2)	0.0	1.e-5	Yes	Yes
2	Discrete Inelastic (MF=51-90)	-1.77903	1.84317	Yes	Yes
3	Continuum Inelastic (MF=91)	Evaluation dependent (~-9.0)	Evaluation dependent (~9.3245)	Yes	Yes
4	(n,γ) (MF=102)	8.4736	0.0	Yes	Yes
5	(n,p) (MF=103)	-3.85996	3.99912	Yes	Yes
6	(n,α) (MF=107)	-2.65362	2.74929	Yes	Yes
7	(n,2n) (MF=16)	-17.17977	17.79916	Yes	Yes
8	(n,nα) (MF=22)	-9.98414	10.34410	Yes	Yes
9	(n,np) (MF=28)	-11.58506	12.00274	Yes	Yes
10	(n,d) (MF=104)	-9.36049	9.69797	Yes	Yes
11	(n,2nα) (MF=24)	-9.36049	9.69797	No	Yes
12	(n,n2α) (MF=29)	-19.30070	19.99655	No	Yes
13	(n,nd) (MF=32)	-22.41840	23.22666	No	Yes
14	(n,nt) (MF=33)	-27.52643	28.51885	No	Yes

^{28}Si Reaction Channels (2/2)

Number	Reaction	Q-value (MeV)	Threshold Energy (MeV)	ENDF/B-VII.1	TENDL-2015
15	(n,n^{3}He) (MF=34)	-23.23124	24.06880	No	Yes
16	(n,2np) (MF=41)	-24.6297	25.53143	No	Yes
17	(n,n2p) (MF=44)	-19.85619	20.57207	No	Yes
18	(n,npα) (MF=45)	-21.67683	22.45835	No	Yes
19	(n,t) (MF=105)	-16.16177	16.74383	No	Yes
20	(n,^{3}He) (MF=106)	-12.13815	12.57577	No	Yes
21	(n,2α) (MF=108)	-19.30070	19.99655	No	Yes
22	(n,3α) (MF=109)	-19.88746	20.60447	No	Yes
23	(n,2p) (MF=111)	-13.41280	13.89638	No	Yes
24	(n,pα) (MF=112)	-14.71741	15.24802	No	Yes
25	(n,pd) (MF=115)	-17.63162	18.26730	No	Yes
26	(n,pt) (MF=116)	-22.46748	23.27751	No	Yes
27	(n,dα) (MF=117)	-19.88746	20.15358	No	Yes

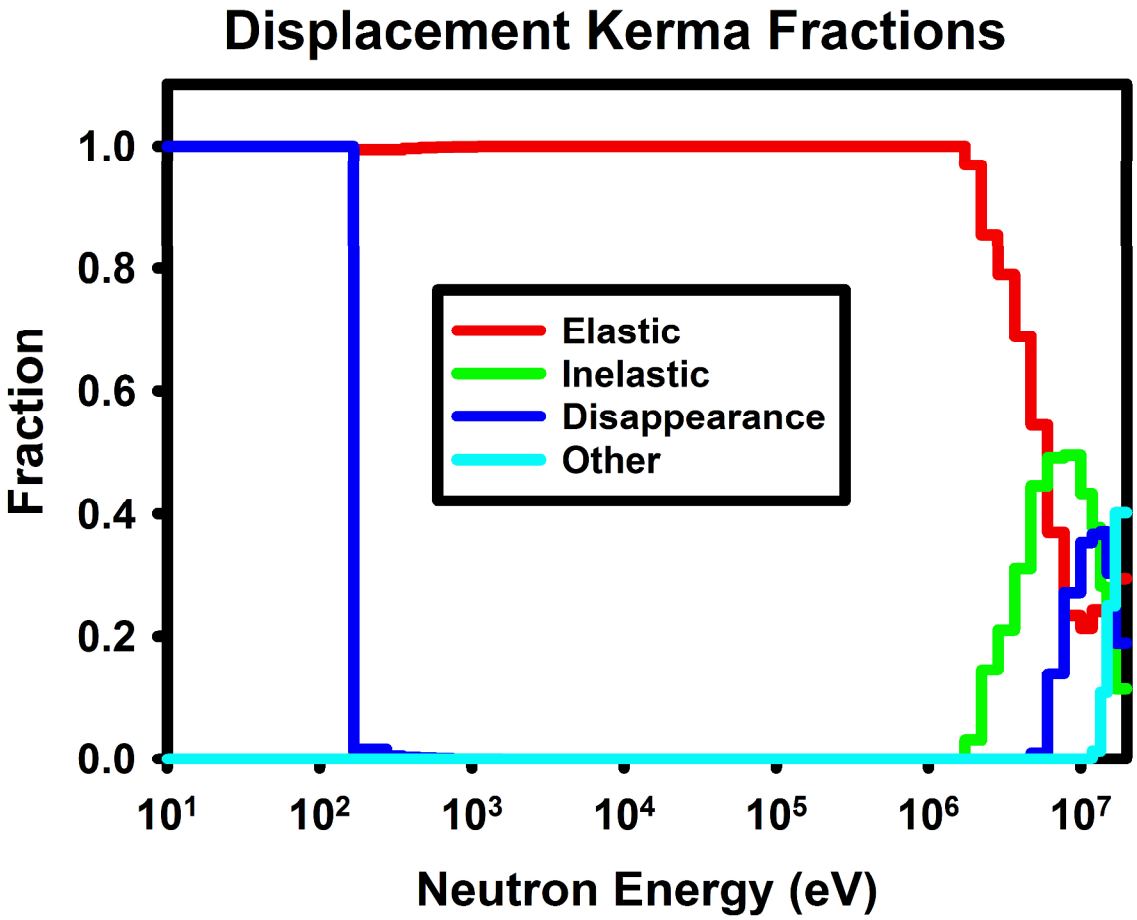
Silicon Cross Section Partition



NJOY reports several displacement kerma components

- Total (MT=444)
- Elastic (MT = 445): « MT = 2
- Inelastic (MT=446): « MT = 51 - 91
- Disappearance (MT=447): « MT = 102-120
- There is an "other" component:
  - Obtained by subtracting components from total
  - Includes transmutation channels with a neutron in the exit channel, e.g., (n,nα), (n,np), (n,2n), (n,2nα), (n,n2α)
    - MTs for TENDL ^{28}Si include 16, 22, 24, 28, 29

Fractional Composition of ^{28}Si Displacement Kerma



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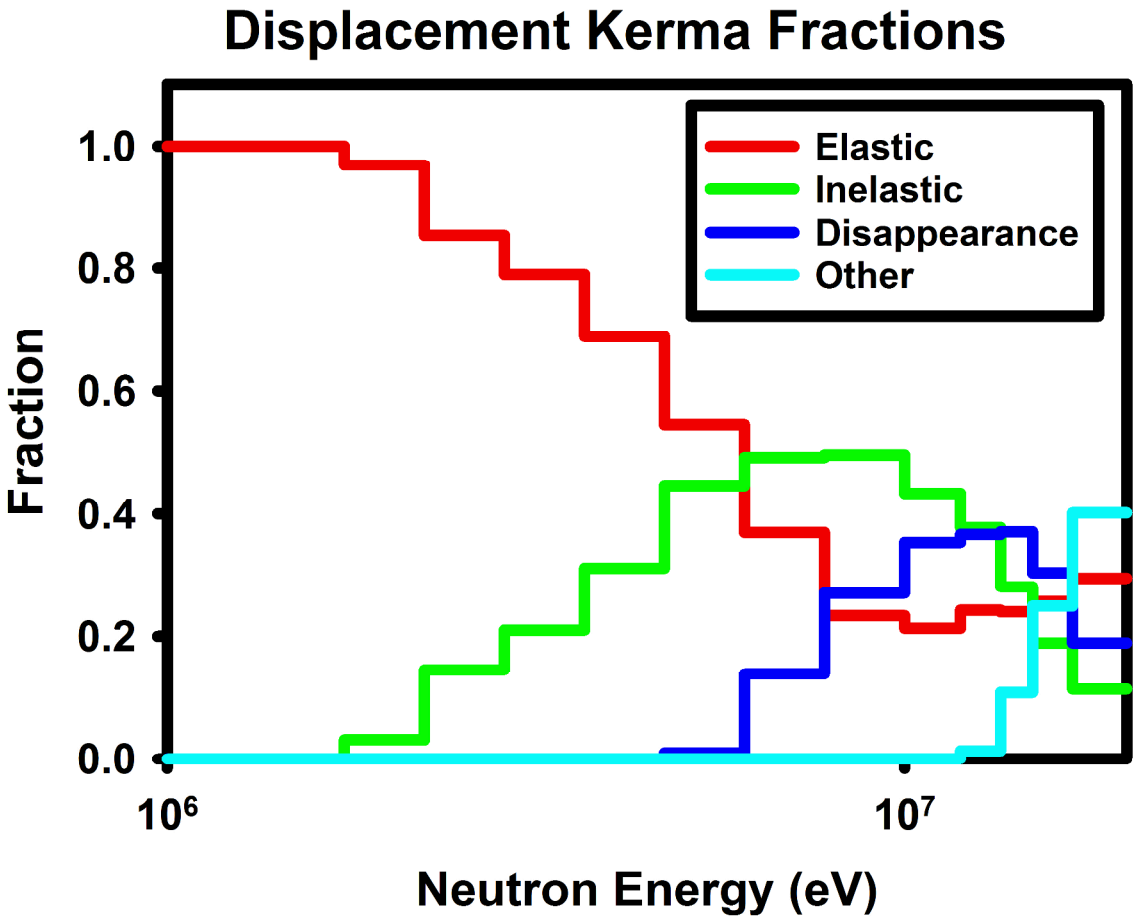
Fractional Composition of ^{28}Si Displacement Kerma



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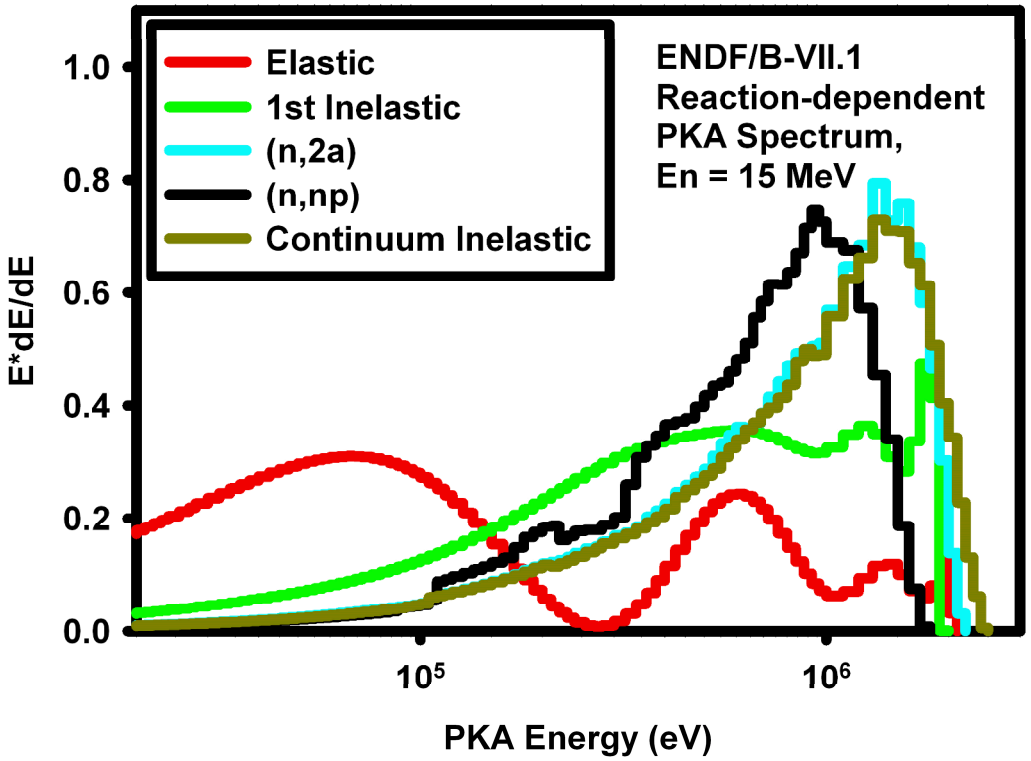
TOPIC:
UNCERTAINTY

Type ⇨ Nuclear Data ⇨ PKA Recoil Spectra

Treatment ⇨ Sensitivity

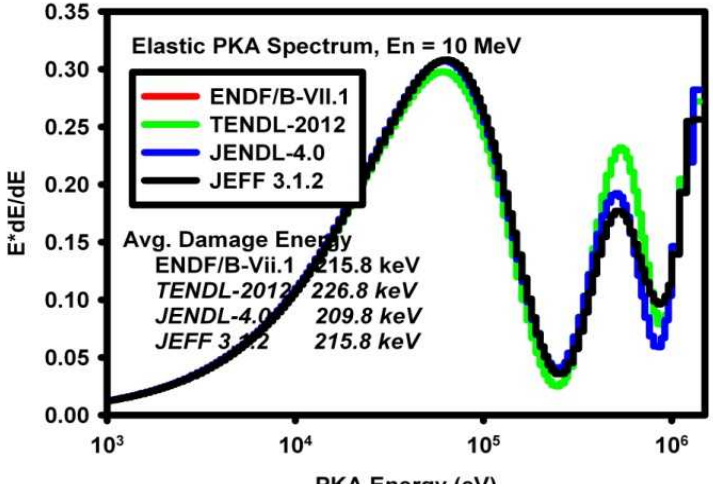
15 MeV Neutron-induced ^{28}Si PKA Recoil Spectra



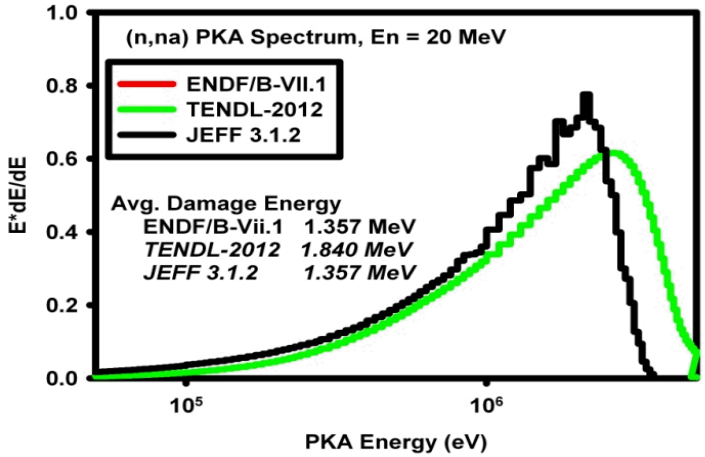
- PKA spectra are strongly dependent upon the neutron energy and reaction channel
- One sensitivity metric is the variation seen between evaluated nuclear data files

Uncertainty in Silicon Recoil Spectra: Reaction and Energy Dependent

Some Good

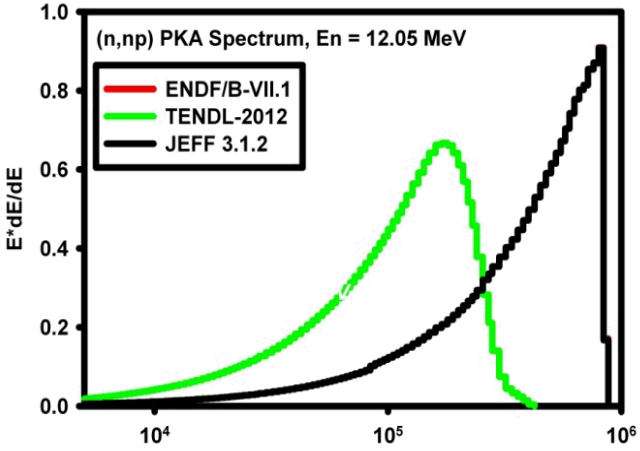


Elastic
10 MeV

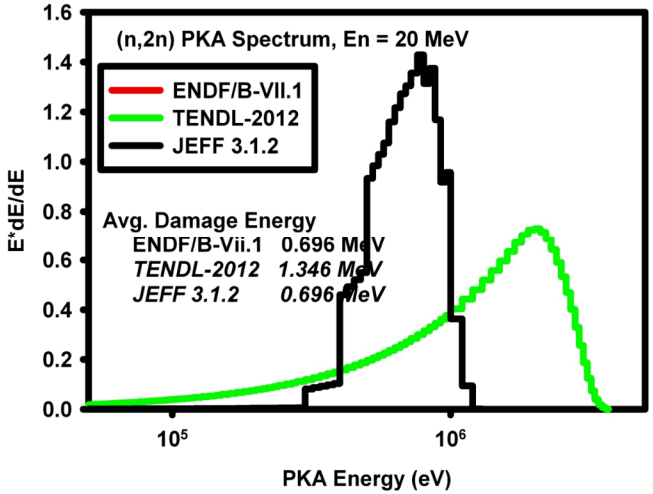


(n,nα)
20 MeV
(E_t = 10.3 MeV)

Some Poor

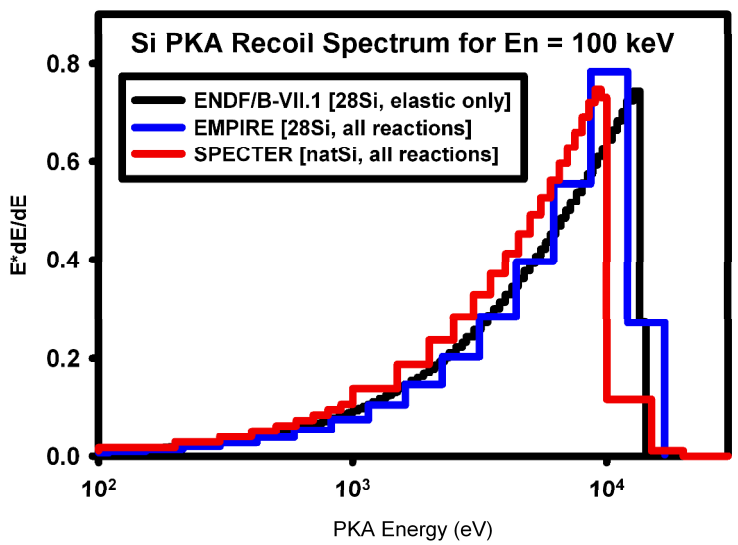


(n,np)
12.4 MeV
(E_t = 12 MeV)

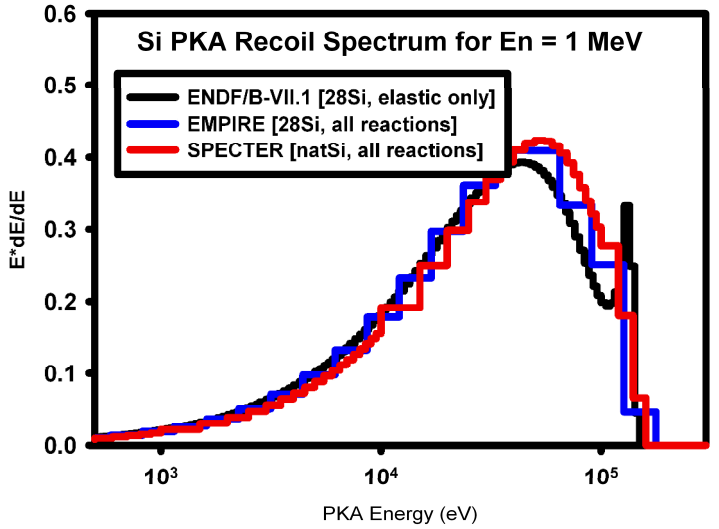


(n,2n)
20 MeV
(E_t = 17.8 MeV)

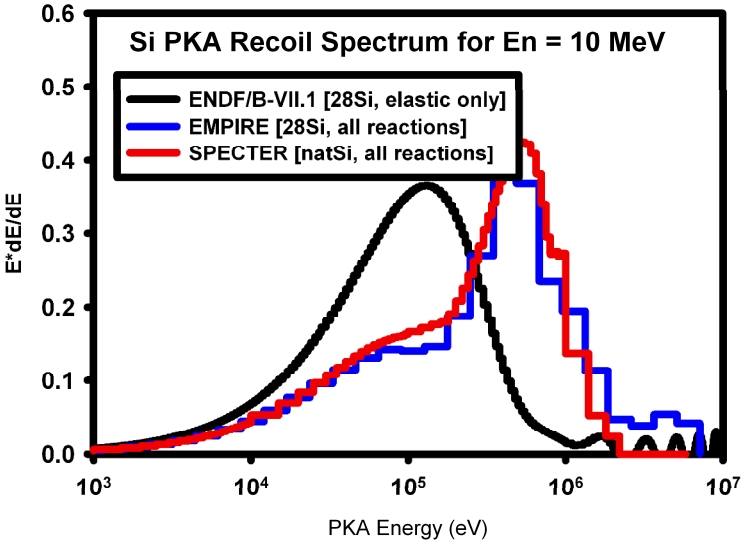
Variation in PKA Recoil Spectrum: SPECTER vs EMPIRE



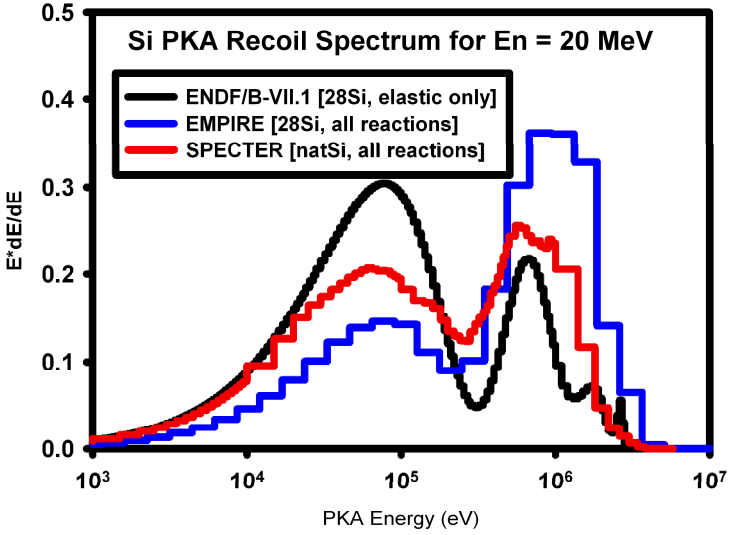
100 keV



1 MeV



10 MeV



20 MeV

TOPIC:
UNCERTAINTY

Type ⇨ Nuclear Data ⇨ Cross Sections & PKA Recoil Spectrum

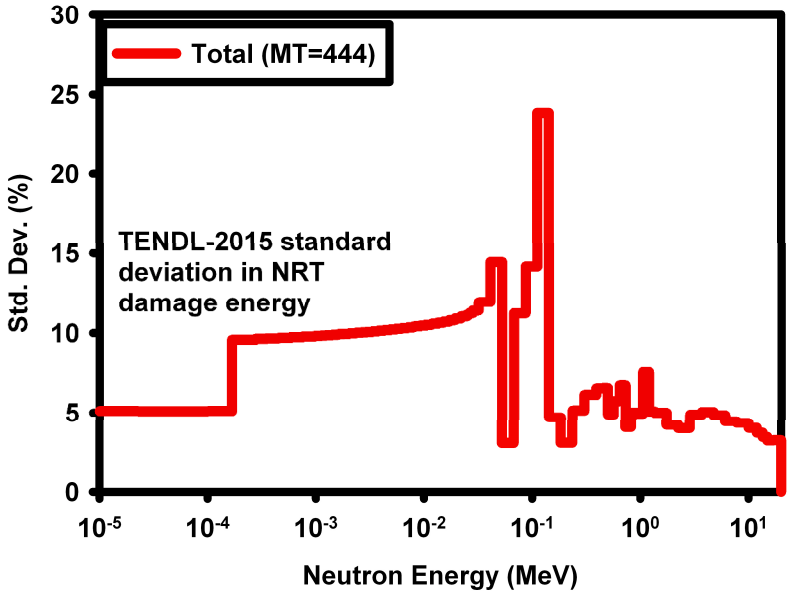
Treatment ⇨ Method of Characterization

Analysis Methodology

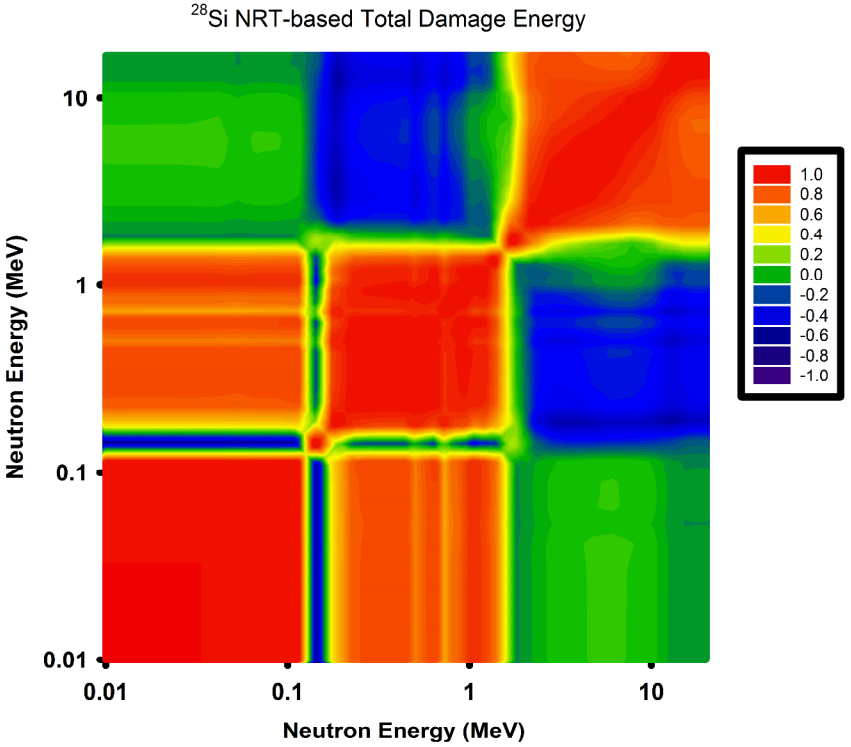
- Use a Total Monte Carlo (TMC) approach to characterize uncertainty and capture nonlinear uncertainty propagation
- Based on use of TENDL-2015 library
  - Many thanks to A. Koning (IAEA/NRG) and D. Rochman (PSI/NRG) for providing the 297 element random libraries for ^{28}Si.
- Cross Section Processing
  - NJOY-2012 used in processing
    - Analysis up to 150 MeV using SAND-IV 770 group structure
    - 89-group representation for uncertainty representation
  - Baseline ^{28}Si prototype, later will extend to ^{29}SI, ^{30}Si
- Selection of 9 random TENDL-2015 draws used in plots:
  - Random draws: 31, 49, 83, 134, 175, 207, 212, 255, 284
  - Complete 297 sample used for covariance in 89-groups

Covariance Matrix for ^{28}Si Total (MT=444) NRT-based Damage Energy (Total Range)

Standard Deviation

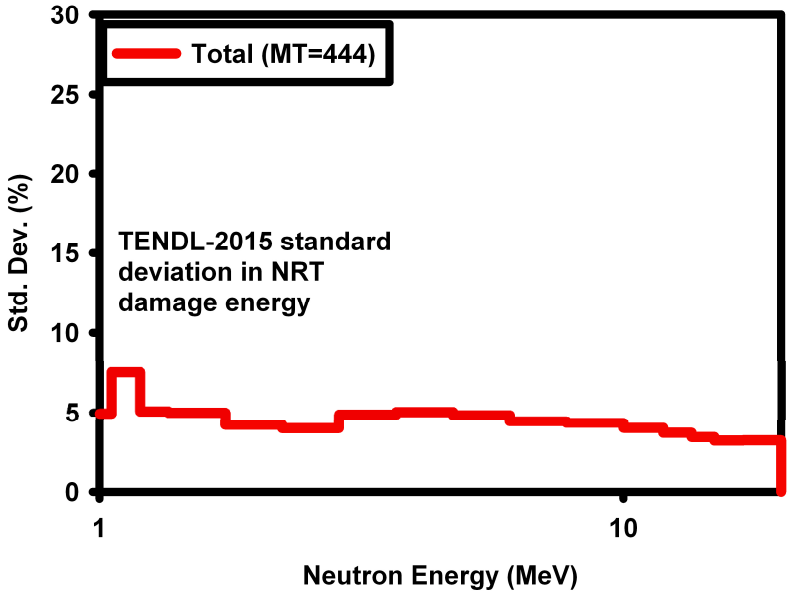


Correlation Matrix

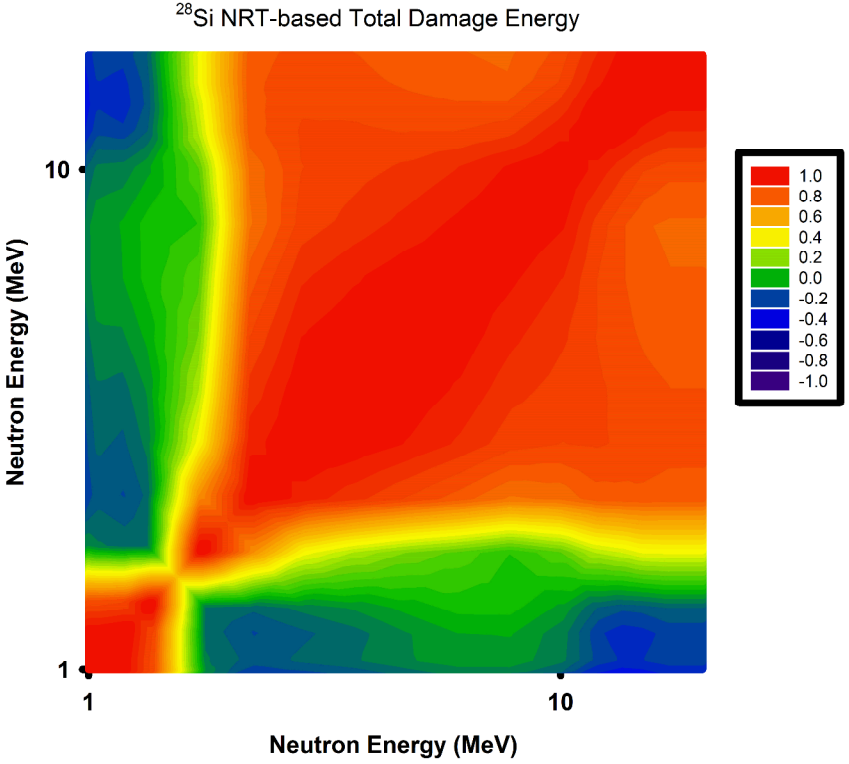


Covariance Matrix for ^{28}Si Total (MT=444) NRT-based Damage Energy (High Energy)

Standard Deviation

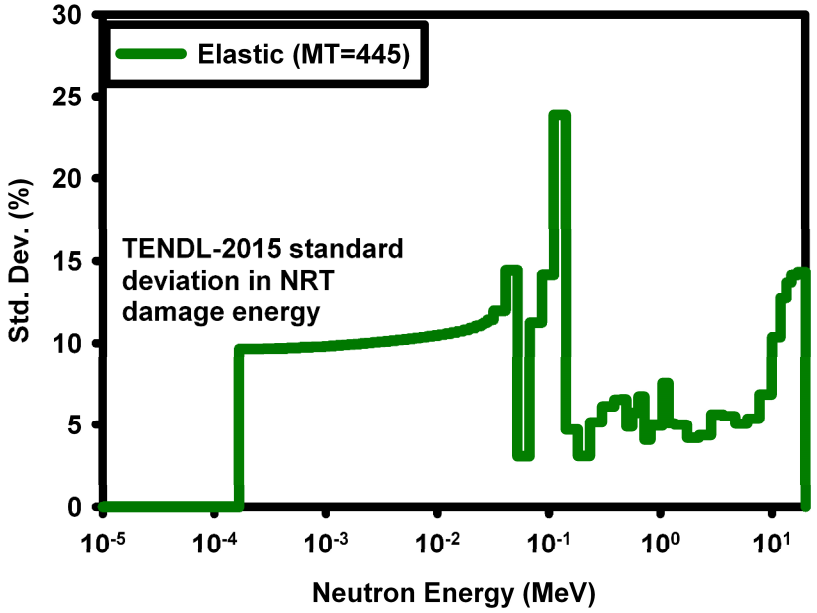


Correlation Matrix

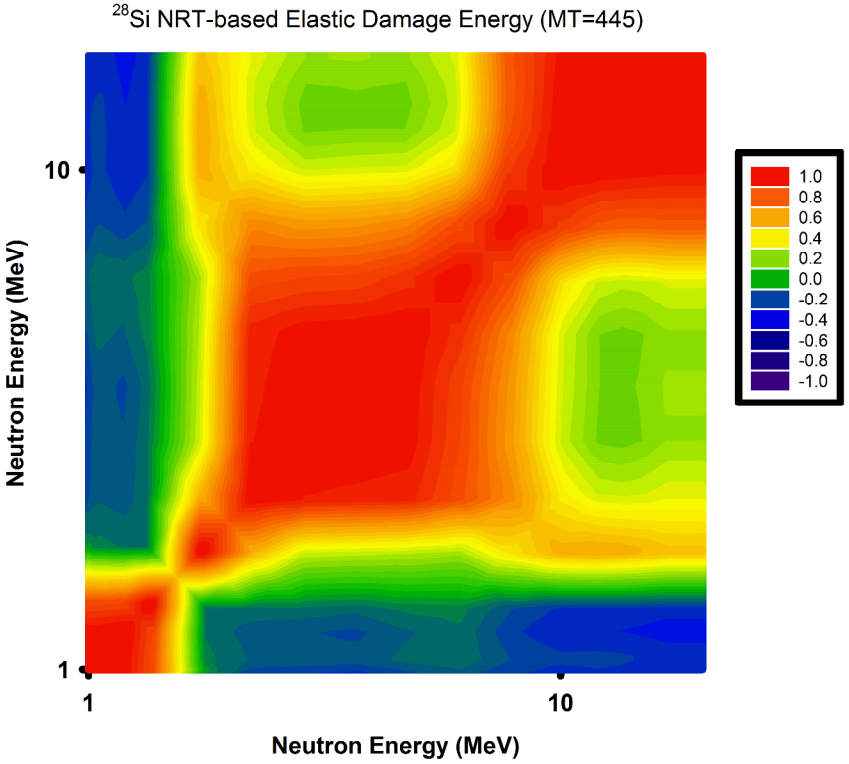


Covariance Matrix for ^{28}Si Elastic (MT=445) NRT-based Damage Energy

Standard Deviation

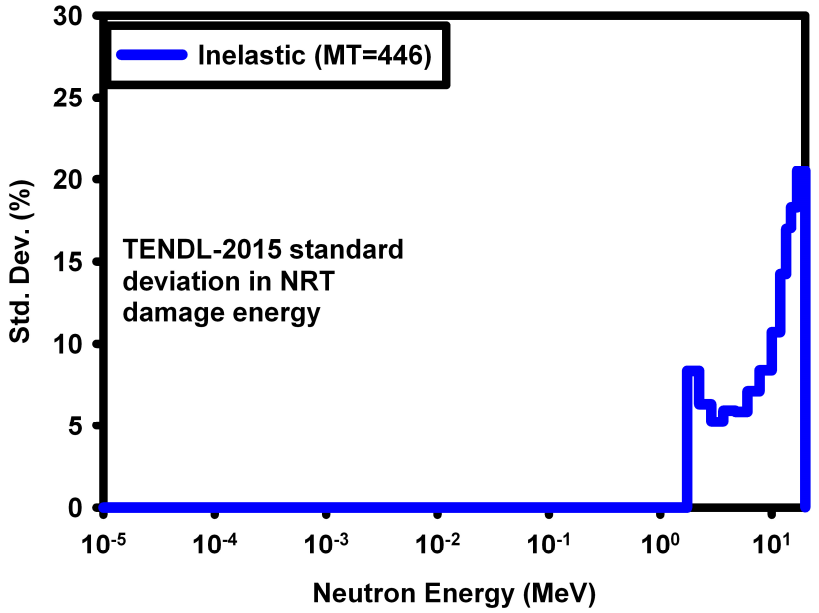


Correlation Matrix

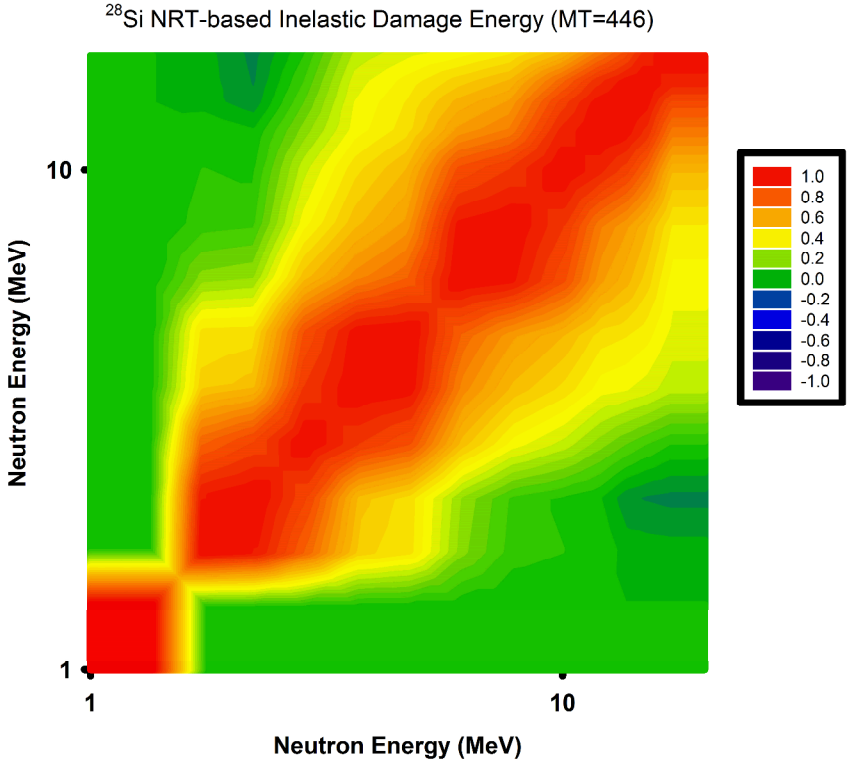


Covariance Matrix for ^{28}Si Inelastic (MT=446) NRT-based Damage Energy

Standard Deviation

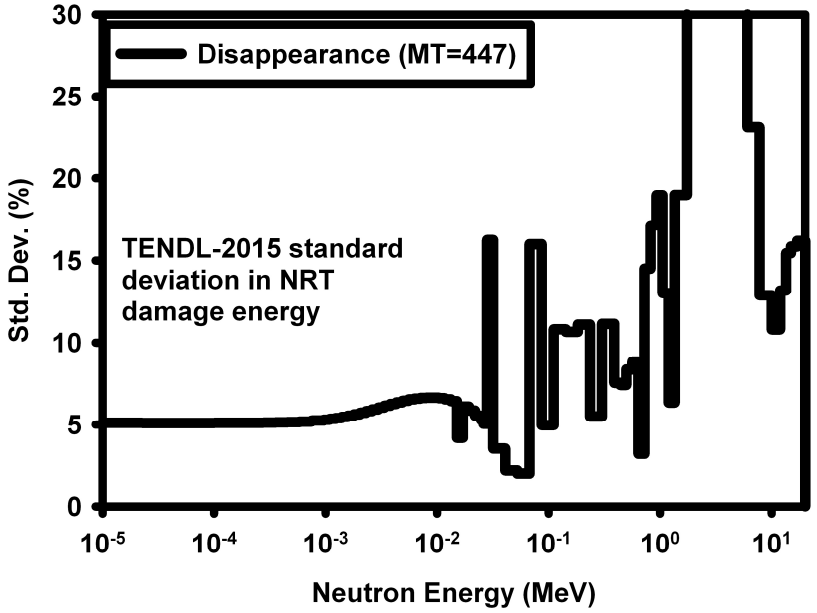


Correlation Matrix

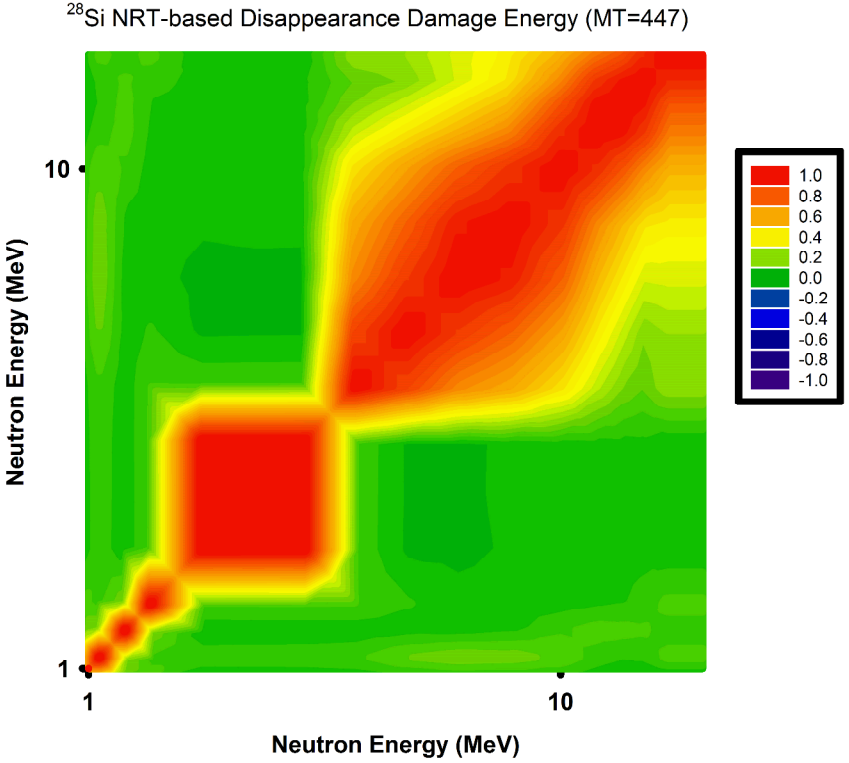


Covariance Matrix for ^{28}Si Disappearance (MT=447) NRT-based Damage Energy

Standard Deviation

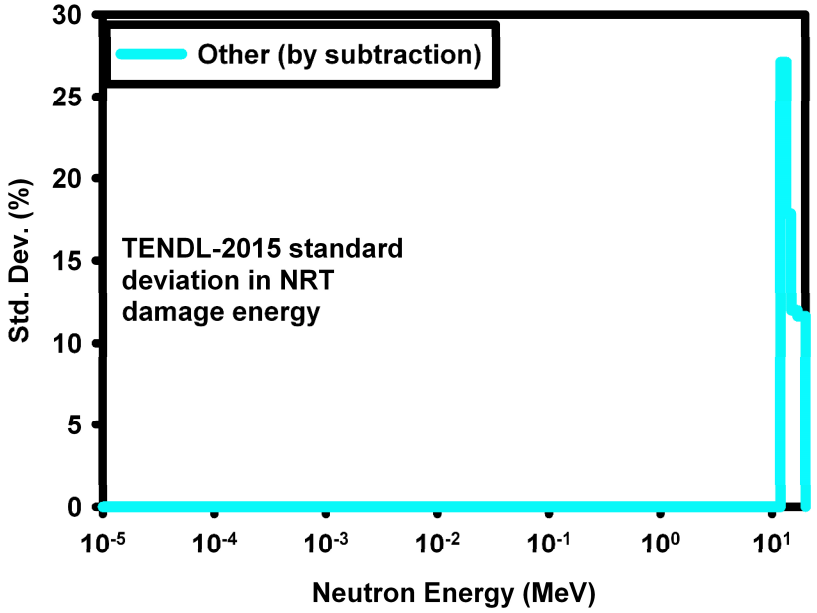


Correlation Matrix

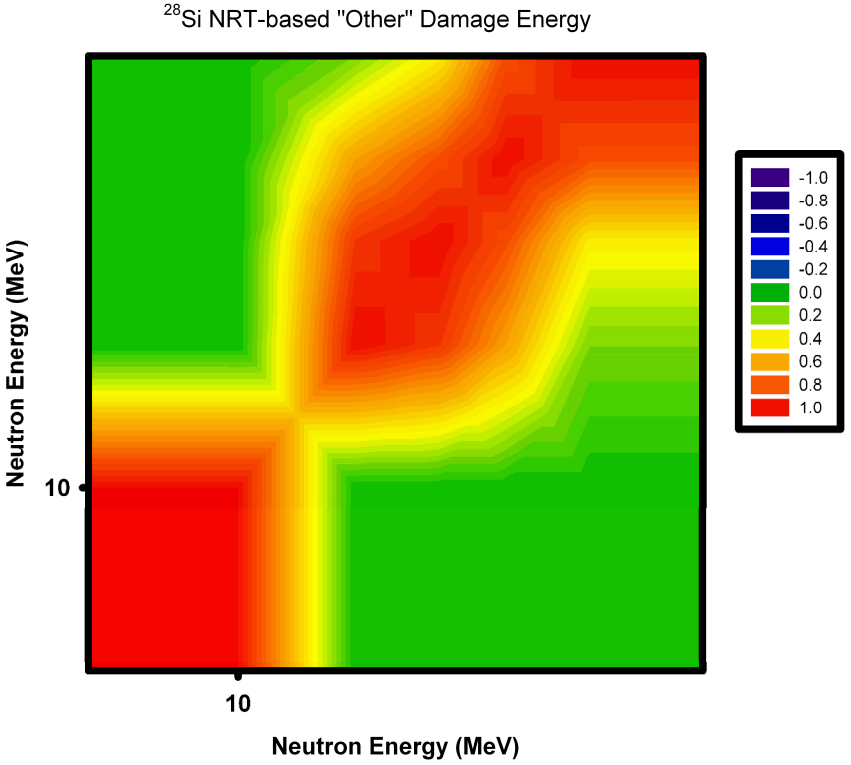


Covariance Matrix for ^{28}Si "other" NRT-based Damage Energy

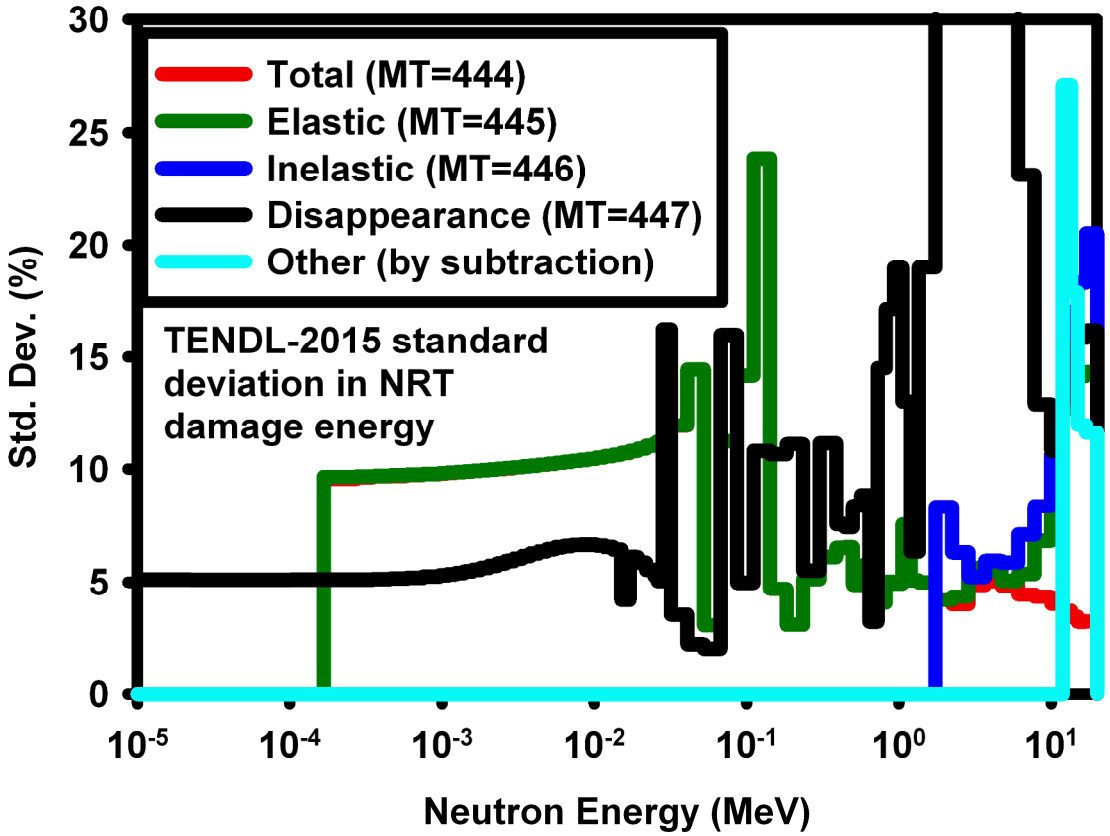
Standard Deviation



Correlation Matrix



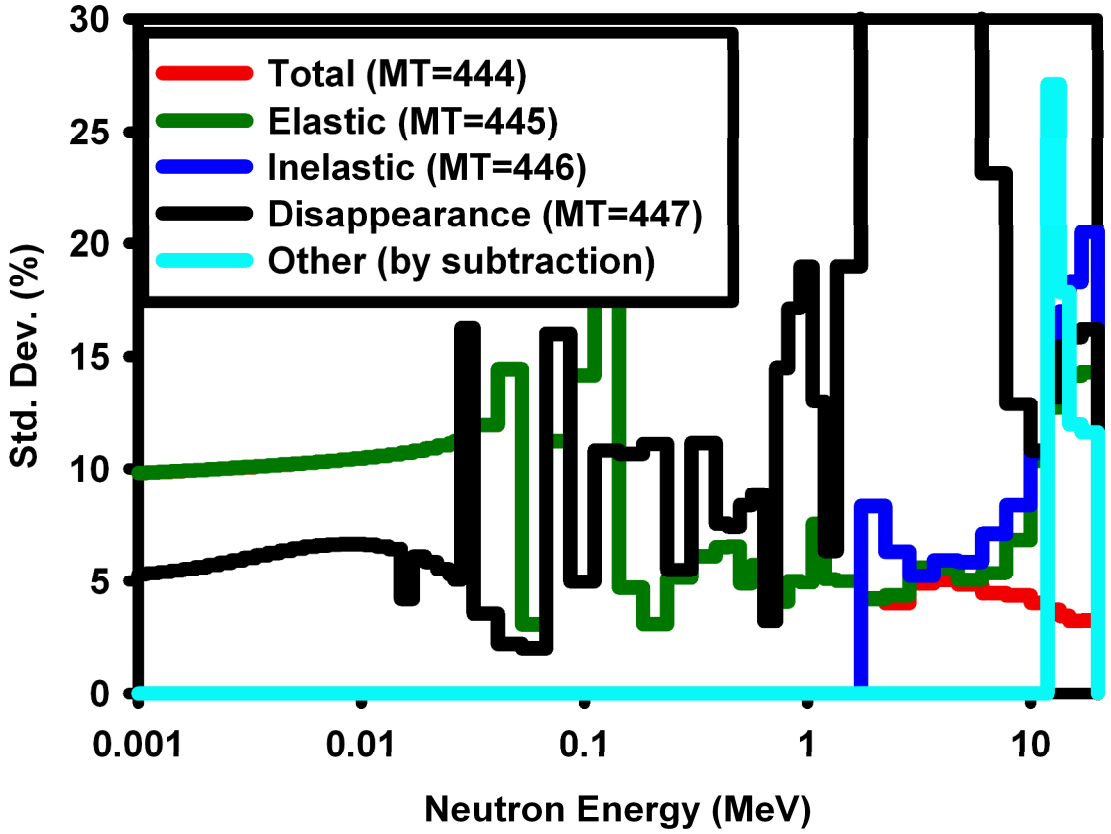
Uncertainty of TENDL-2015 ^{28}Si Displacement Kerma Components



Note: total (red) curve merges with elastic (green) and then disappearance (black) curve

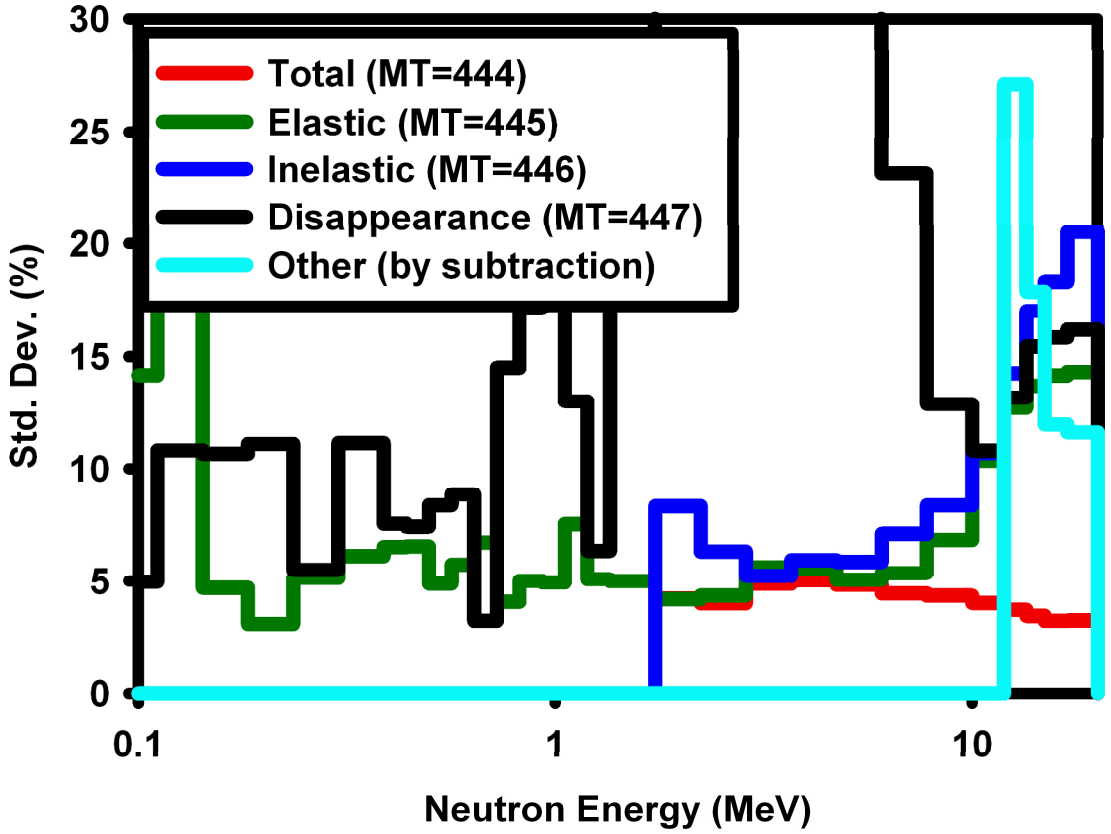
Note, total component, shown clearly in red at high energy, merges with the green elastic component at mid energies and drops to the black disappearance component at thermal energies.

Uncertainty of TENDL-2015 ^{28}Si Displacement Kerma Components (mid-energy region)



Note, total component, shown clearly in red at high energy, merges with the green elastic component at mid energies and drops to the black disappearance component at thermal energies.

Uncertainty of TENDL-2015 ^{28}Si Displacement Kerma Components high-energy region)



Note, total component, shown clearly in red at high energy, merges with the green elastic component at mid energies and drops to the black disappearance component at thermal energies.

There is a Strong Correlation between the Displacement Kerma Components → Low Uncertainty in Total Displacement Kerma

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Random Draw	Elastic (MT=445)	Inelastic (MT=446)	Disappearance (MT=447)	Other (subtraction)	Total (MT=444)
1	5.3399E4	1.8665E4	4.1531E4	6.586E+04	1.7945E5
2	5.6563E4	1.9536E4	3.8885E4	6.927E+04	1.8425E5
5	5.4363E4	1.9645E4	4.0004E4	6.919E+04	1.8320E5
27	5.0997E4	1.9562E4	3.3828E4	7.537E+04	1.7976E5
35	5.9361E4	2.0923E4	3.1675E4	6.880E+04	1.8076E5
44	5.1916E4	2.0239E4	3.5901E4	7.229E+04	1.8035E5
56	5.5910E4	1.9676E4	3.7919E4	6.733E+04	1.8083E5
75	5.8726E4	2.1422E4	3.6283E4	6.908E+04	1.8551E5
99	5.1472E4	2.0428E4	3.4034E4	7.515E+04	1.8108E5
Std. Dev. from anal./table	5.82% / 5.65%	7.20% / 4.16%	10.38% / 8.73%	--- / 4.72%	1.45% / 1.17%

Data for 16.9 – 20 MeV energy bin for ^{28}Si TENDL-2013 random library

Observation

- **TMC approach seen to be crucial in propagating uncertainty into the non-linear displacement kerma**
  - **TMC results show there is a high correlation at high energy**
  - **that means we cannot treat the displacement kerma components as independent.**

TOPIC:
UNCERTAINTY

Type ⇨ Damage Partition Function ⇨
Electronic and Nuclear Scattering Potential

Treatment ⇨ Sensitivity

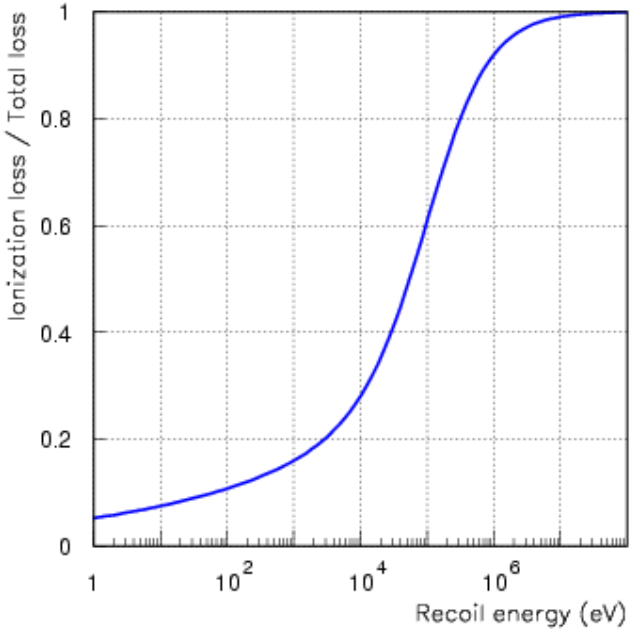
Robinson Partition Function

- **Fit to Lindhard Partition Function**

$$Q = 1/[1 + k_L\, g(\varepsilon)],$$

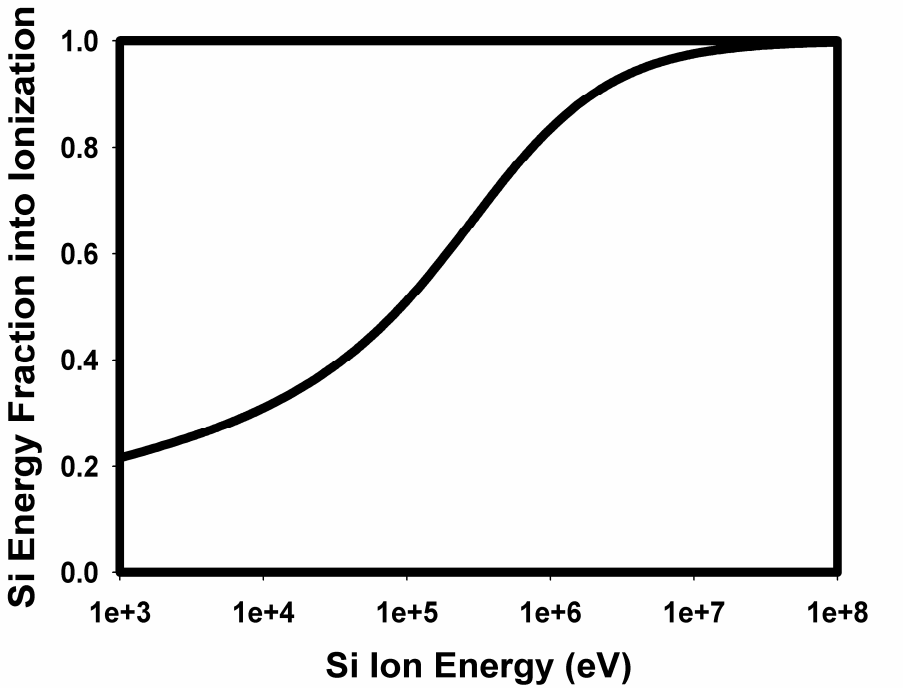
$$k_L = 0.0794 \frac{Z^{2/3} Z_1^{1/2} (A + A_1)^{3/2}}{(Z^{2/3} + Z_1^{2/3})^{3/4} A^{3/2} A_1^{1/2}}.$$

$$g(\varepsilon) = \varepsilon + 0.40244\, \varepsilon^{3/4} + 3.4008\, \varepsilon^{1/6}.$$

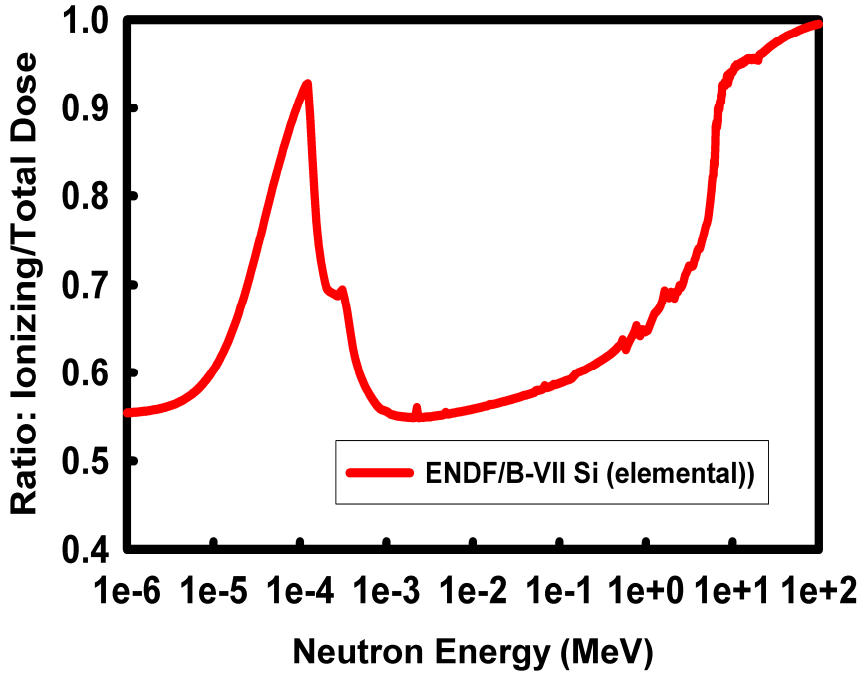


- **A/Z: atomic mass and number for incident ion**
- **A_l/Z_l: atomic mass and number for lattice atoms**

Neutron Damage Partition Function can be Derived from the Recoil Ion Energy Partition



Si Ion Ionization Fraction



Neutron on Si Ionization Fraction

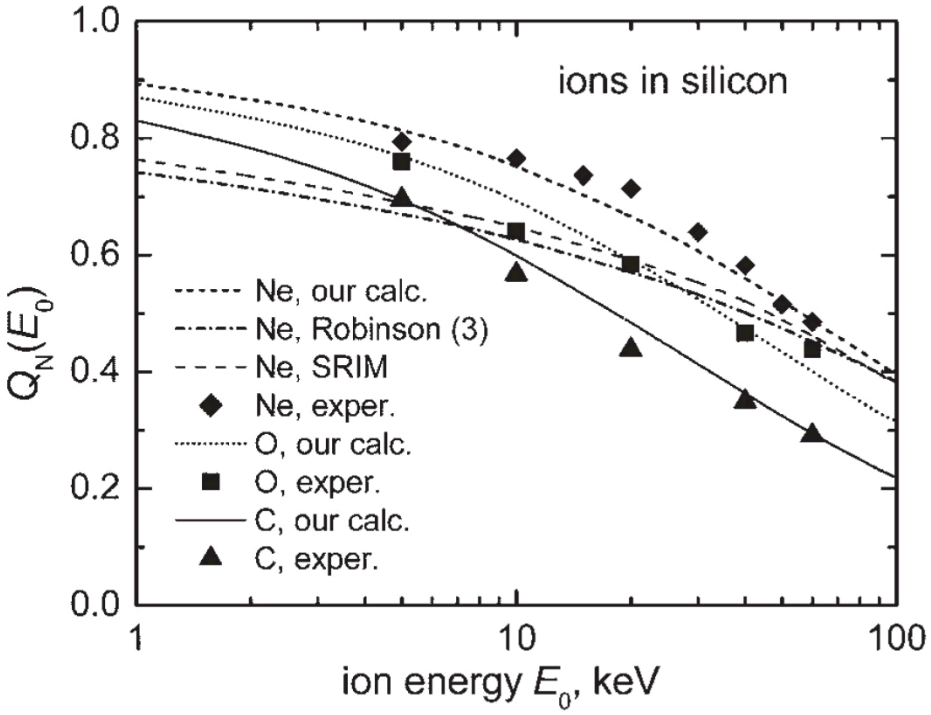
- **Ionization partition function based on Robinson fit to LSS partition**

Energy Partitioning: Akkerman

- 2006 Akkerman update using same functional form as Robinson but for Si only
  - Elastic: screen Coulomb using ZBL potential
  - Inelastic: combination of local (impact parameter dependent) and nonlocal models for electronic scattering
  - Changes up to 15% from LSS
  - Excellent agreement with experimental data

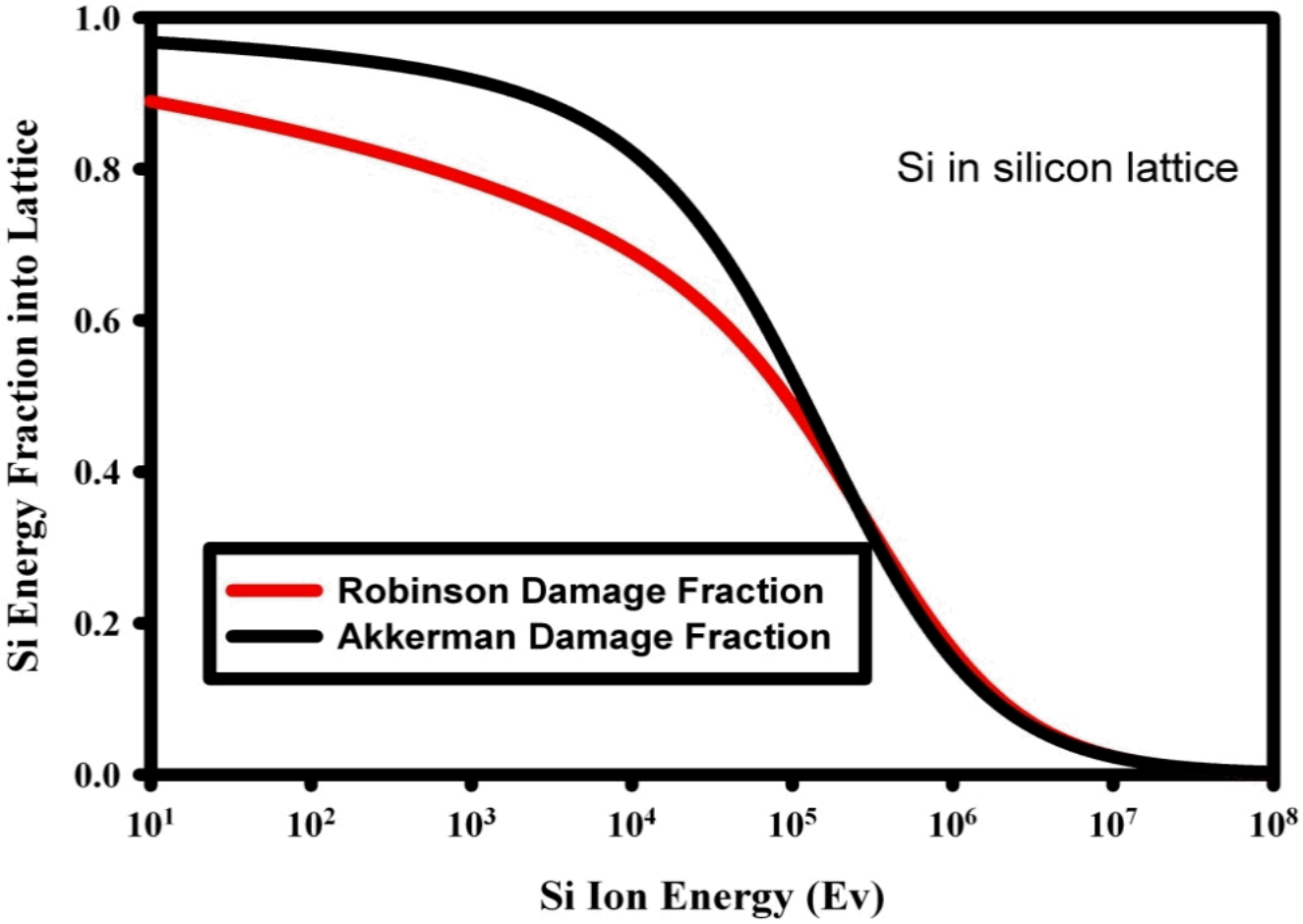
Partition: Robinson vs. Akkerman Eqn. for Si

- **Robinson fit for Si in Si**
  - $g(\varepsilon) = 0.227073\varepsilon + 0.40244\varepsilon^{3/4} + 3.4008\varepsilon^{1/6}$
- **Akkerman fit (2006)**
  - $g(\varepsilon) = 0.74422\varepsilon + 2.6812\varepsilon^{3/4} + 0.90565\varepsilon^{1/6}$



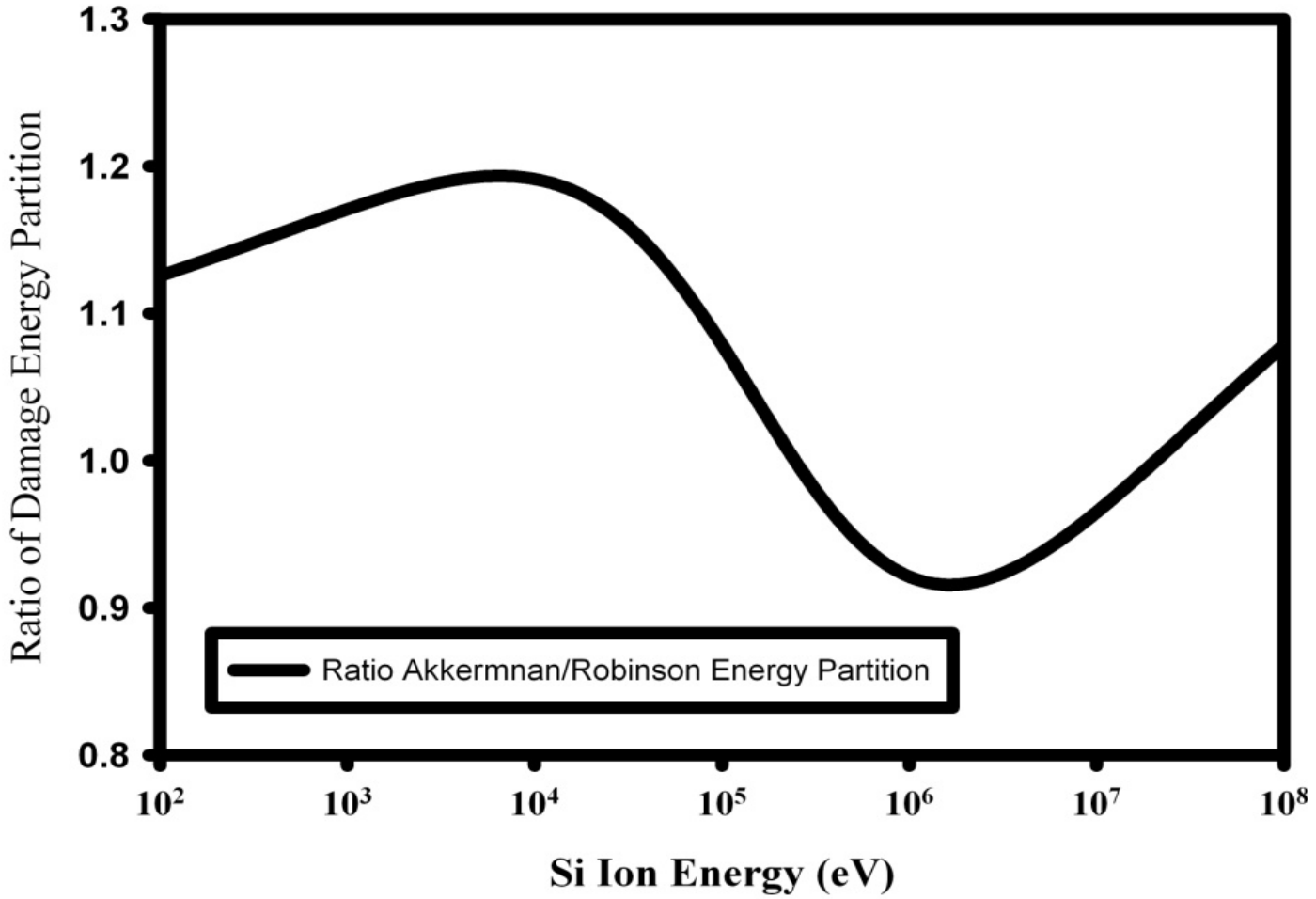
Akkerman vs. Robinson vs. SRIM for Ne/O/C ions in Si

Comparison of Robinson and Akkerman ^{28}Si Damage Partition Function

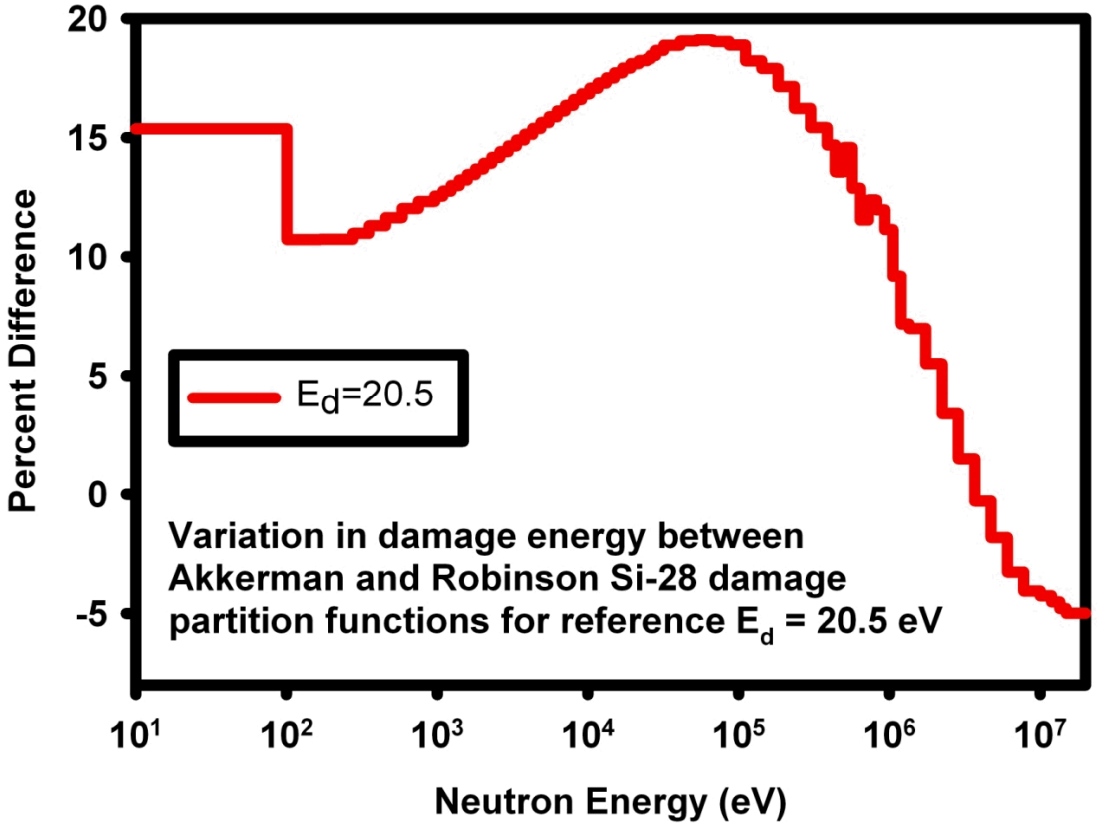


Ratio of Robinson and Akkerman ^{28}Si Damage Partition Function

Damage partition function shows a ~+20/-10% variation and a smooth correlation with energy.



Difference in Neutron Damage Energy in Silicon between Robinson and Akkerman Potentials



- Very little effect is seen at high neutron energies.
- Maximum difference of ~20%

Interatomic Potential Affects the Damage Partition

Si Ion Energy (keV)	MARLOWE BCA Code Using:		Robinson (LSS)
	Moliere Potential	ZBL Potential	
30 keV	29.1	32.9	38.5
50 keV	35.1	38.9	43.3
100 keV	44.0	47.8	52.
500 keV	72.0	72.9	74.5
1 MeV	82.7	82.7	83.5
10 MeV	94.7	95.0	97.6

The variation is large (30%) for low energy and small (3%) for high energy silicon ions. For dpa-relevant silicon recoil ion energies of 50 – 100 keV, the variation is ~15% .

BCA-based Damage Functions

- MARLOWE BCA code can be used to vary the interaction potential and examine the damage partition
- Potentials studies:
  - Ion electronic interactions:
    - LSS Lindhard, Scharff, Schiot
    - ZBL Zeigler, Biersack, Littmark
  - Ion lattice atom interaction:
    - Moliere
    - Exponential
    - Lenz-Jensen

Damage Energy from MARLOWE Code

- **BCA-based MARLOWE damage energy includes:**
  - **Kinetic energy transferred in quasielastic collisions to target atoms which are not displaced (each contribution < E_d).**
  - **Energy expended by displaced particles in overcoming binding (each contribution = E_b = binding energy).**
  - **Final kinetic energy of each recoil which stops within the target (each contribution < E_c = cut-off energy for ion tracking.**

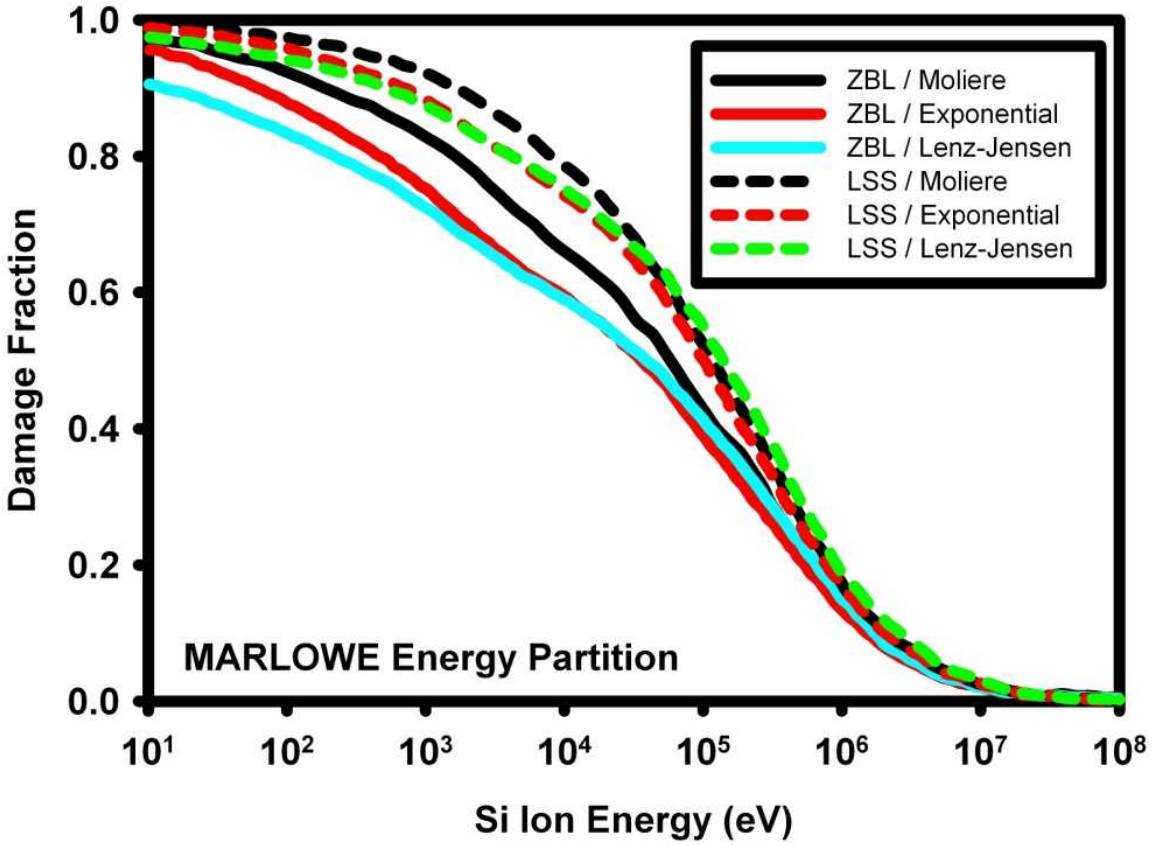
  - **E_b = 4.7 eV; E_c = 2.32 eV for Silicon**

Energy Deposition Metrics Reported by MARLOWE

Sandia National Laboratories

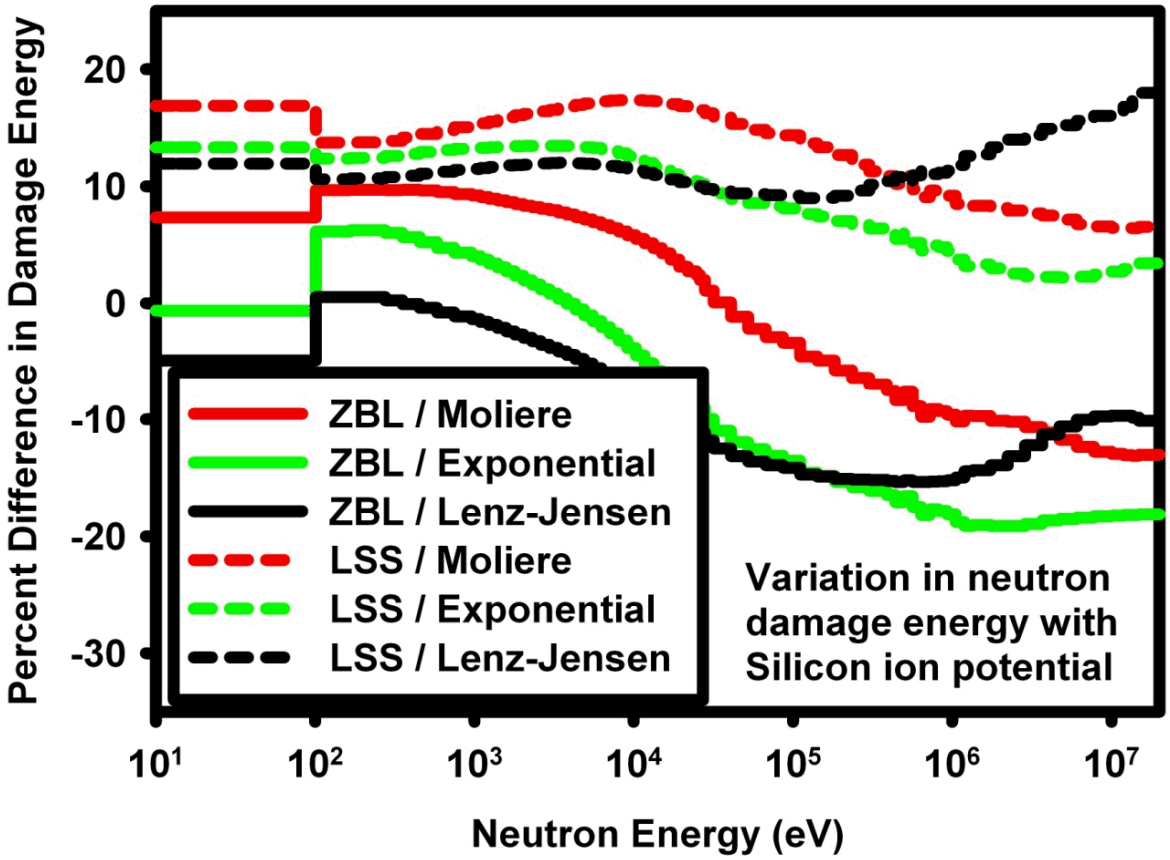
- Inelastic energy loss
- Binding loss (displacements)
- Binding loss (replacement)
- Binding loss (non-lattice)
- Sub-threshold loss (lattice)
- Sub-threshold Loss (non-lattice)
- Remaining kinetic energy
- In replacement sequences
- Carried by focusons
- Replacement threshold
- Focuson threshold
- Carried through front surface
- Binding loss (front surface)
- Remaining kinetic (front adatoms)

BCA-produced Damage Partition Functions for Various Potentials



- **A smooth variation is seen with energy, indicating the energy-dependent correlation must be considered.**

BCA-produced Variation in Neutron Damage Energy for Various Potentials



- **+20% / -20% variation seen in damage energy – similar to that from Robinson / Akkerman comparison**

TOPIC:
UNCERTAINTY

Type ⇨ Damage Partition Function ⇨
Electronic and Nuclear Scattering Potential

Treatment ⇨ Method of Characterization

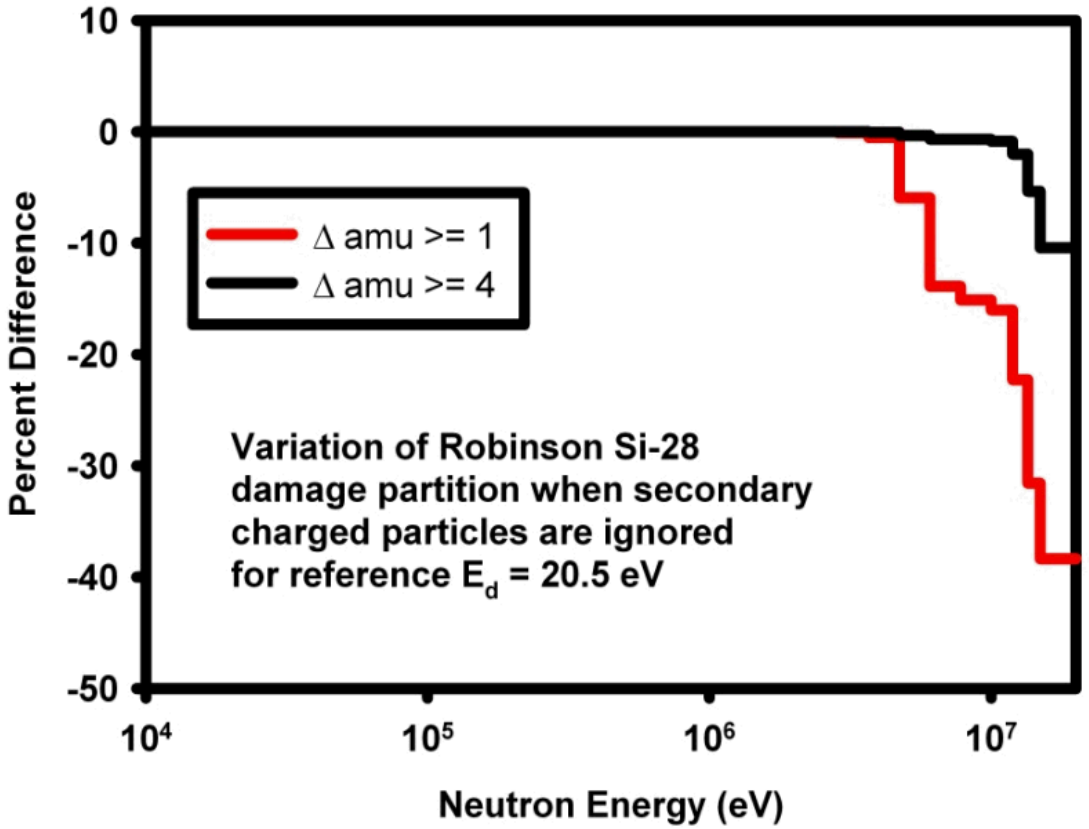
Methodology

- Characterize the uncertainty in the damage partition function
  - Use a covariance matrix derived from:
    1. inspection of variation in models to determine a covariance matrix
    2. Analytic model fit to observed variations with electronic and nuclear scattering potentials
- Modify NJOY-2012 to implement a user-input damage partition function
- Use a TMC approach to determine effect on damage energy

TMC Methodology

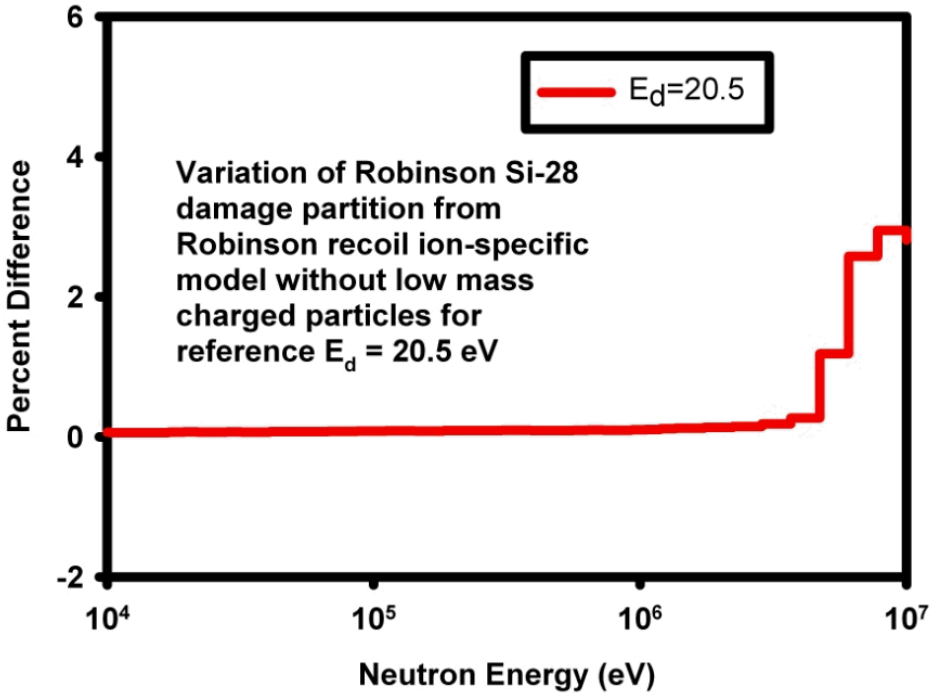
- Use a 66-point representation of damage partition function with log-linear interpolation between points
- Use a Cholesky decomposition of the covariance matrix to generate 750 samplings of the damage partition function
- Modify damage partition functions to enforce:
  - Range of 0 to 1 in partitioned damage energy
  - Monotonic decreasing shape
- Run NJOY 750 times with the various damage partition functions and extract a 89-group damage energy
- Direct statistical estimation of the resulting damage energy functions to extract a covariance matrix

Treatment of Damage Energy from Low Mass Recoil



- **If a static [mass insensitive] user-defined damage partition function is used, there can be a big effect for the high neutron energy damage energy.**

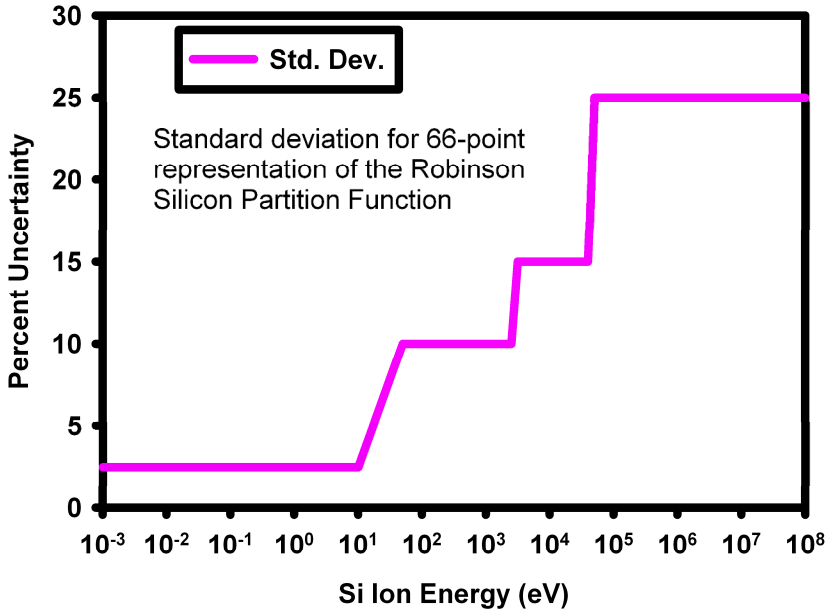
Treatment of Low Mass Recoil Particles in Exit Channel for User-defined damage partition functions



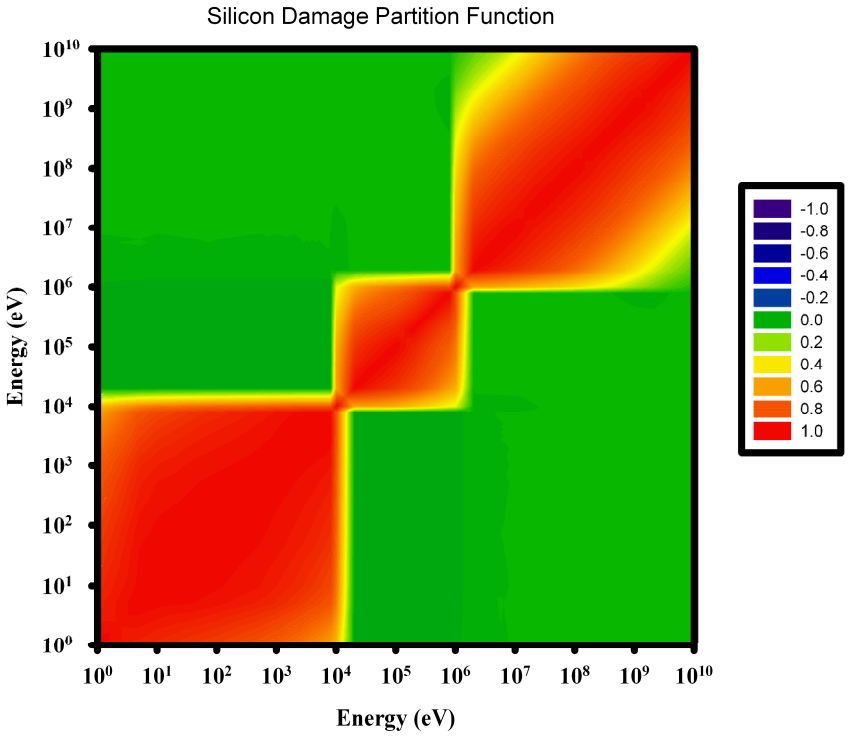
- When a user-defined damage partition function is used, what about the damage energy from outgoing alpha particles?
- The above figure shows that this is a minor contribution.
- Our analysis of the effect of the user-defined potential removes consideration of the alpha particles rather than treat them as a heavy ion PKA recoil.

Covariance Matrix for Silicon Partition Function

Standard Deviation

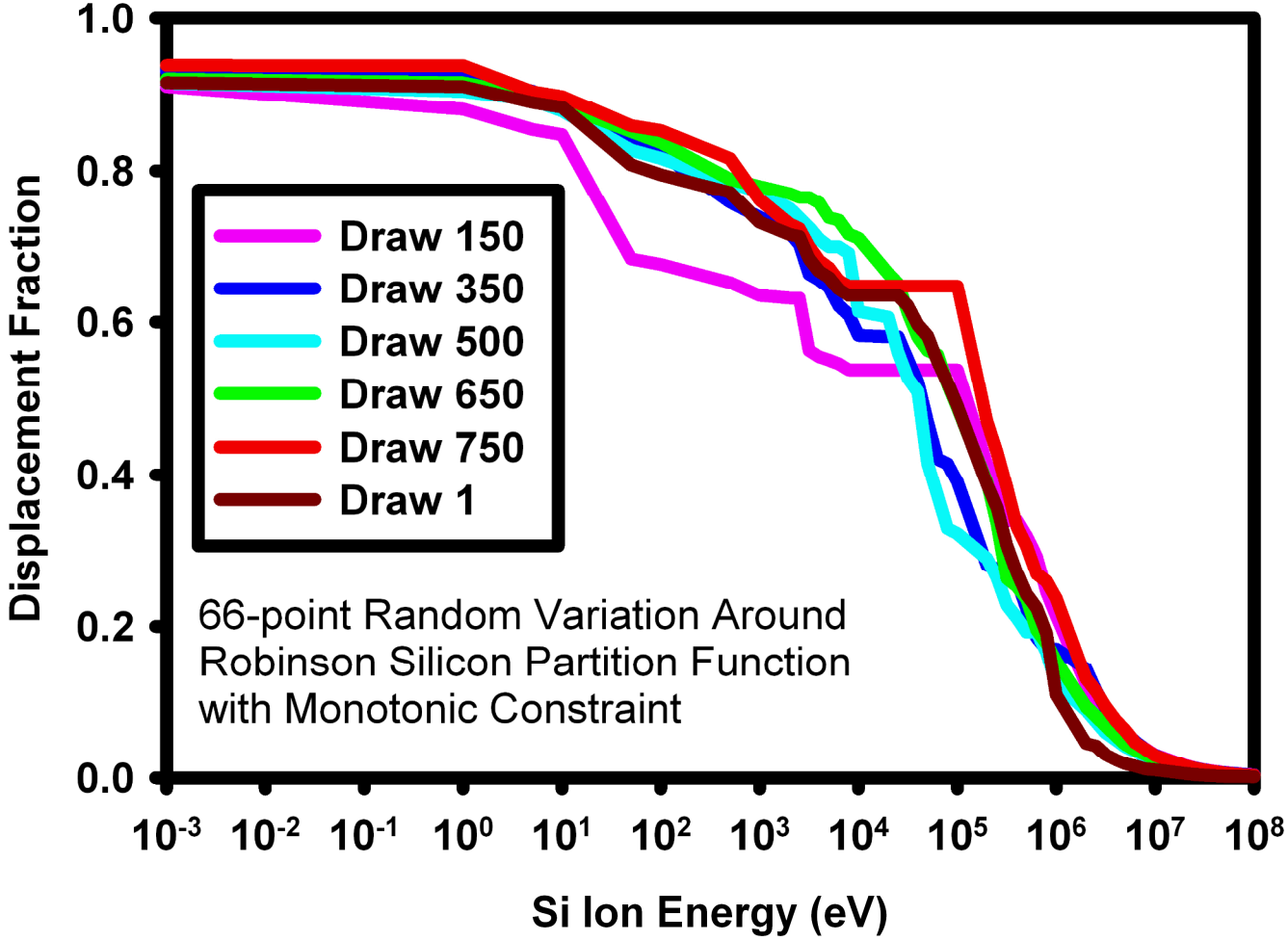


Correlation Matrix



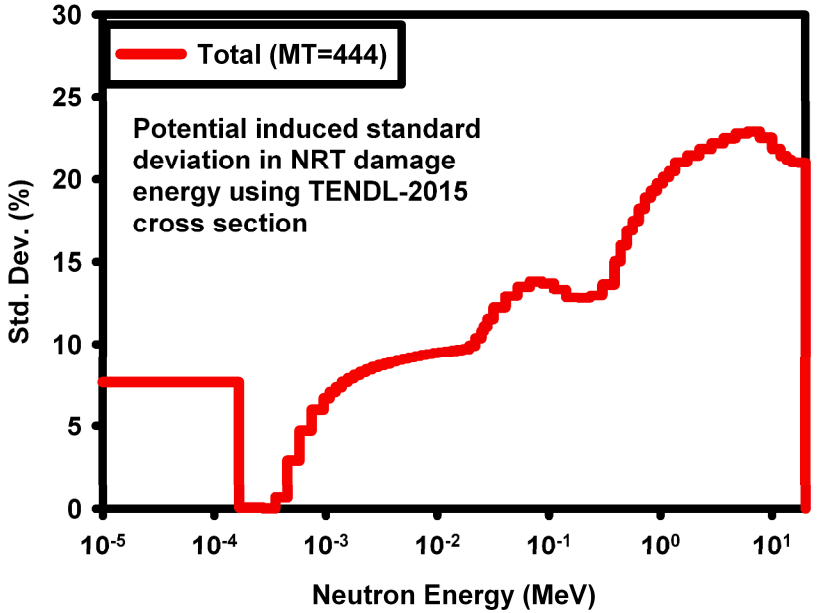
Sample Draws on Silicon Partition Function

Sampled from covariance matrix for a 66 point fixed representation and a log-linear interpolation applied.



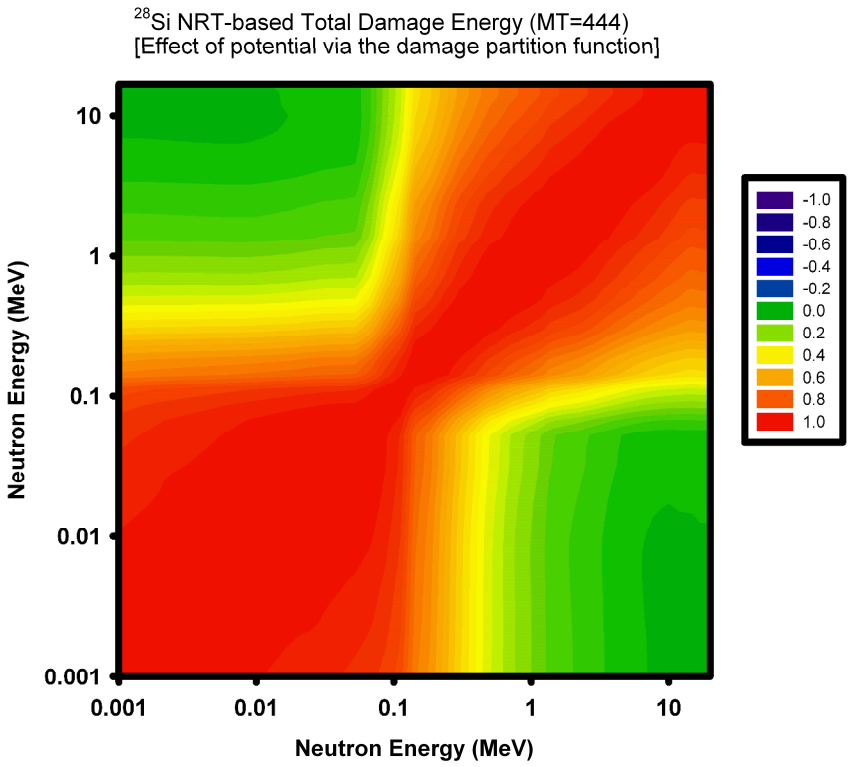
Covariance Matrix for ^{28}Si Total (MT=444) NRT-based Damage Energy from Partition Function

Standard Deviation



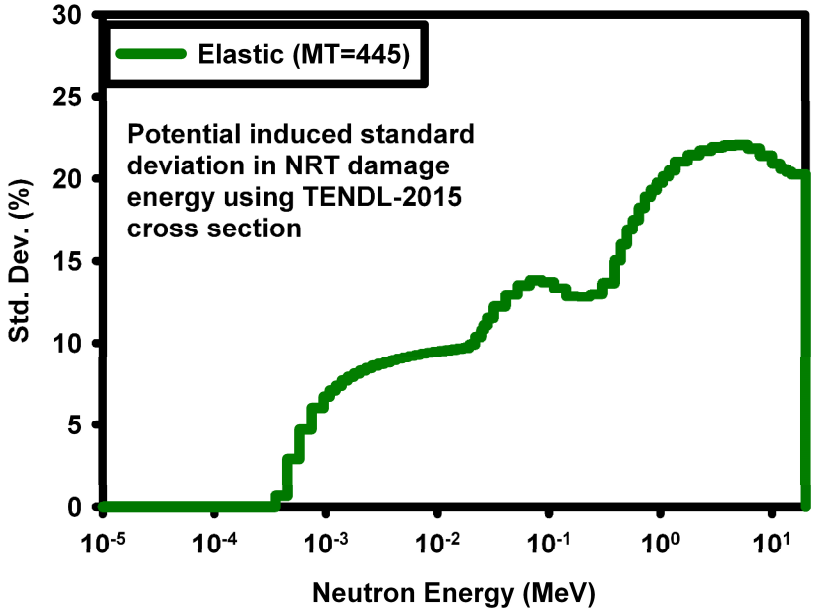
Note: total (red) curve merges with elastic (green) and then disappearance (black) curve

Correlation Matrix

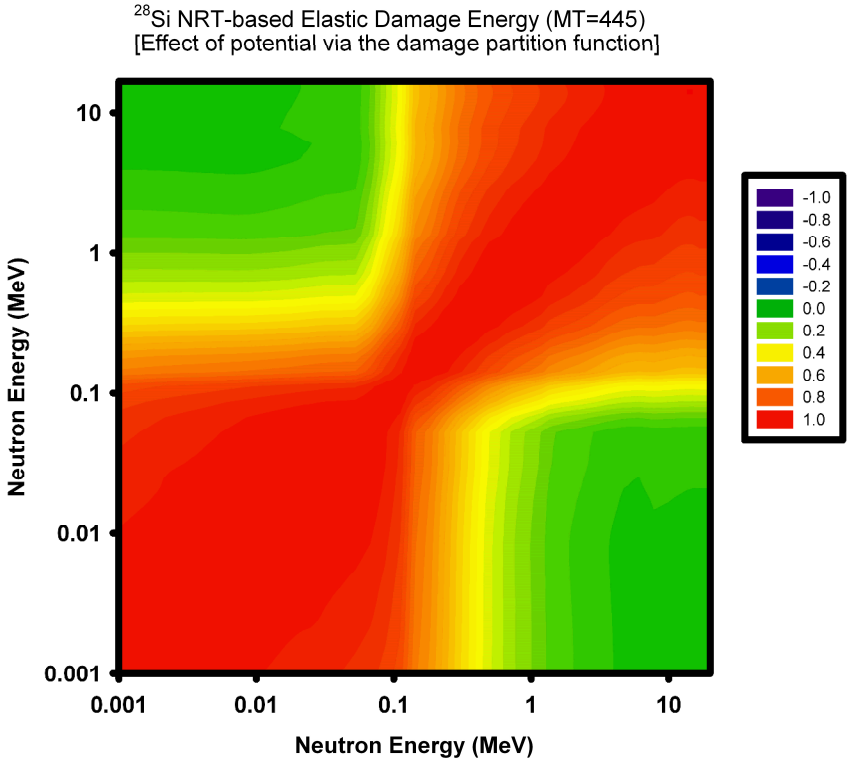


Covariance Matrix for ^{28}Si Elastic (MT=445) NRT-based Damage Energy from Partition Function

Standard Deviation

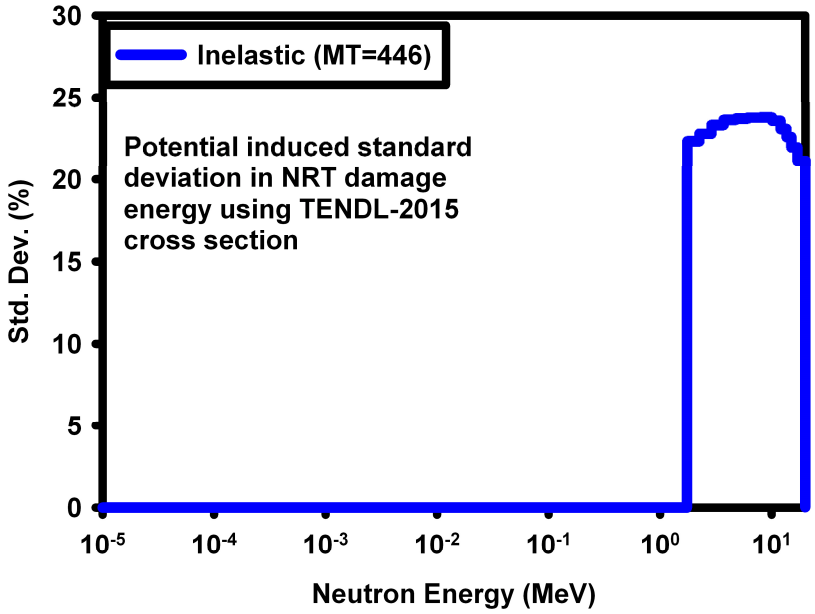


Correlation Matrix

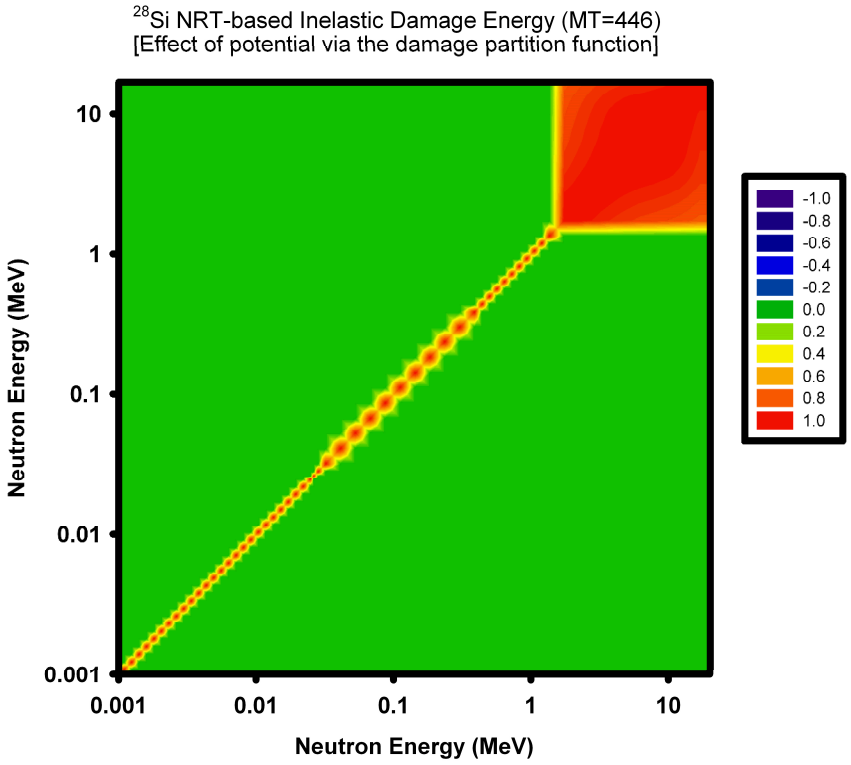


Covariance Matrix for ^{28}Si Inelastic (MT=446) NRT-based Damage Energy from Partition Function

Standard Deviation

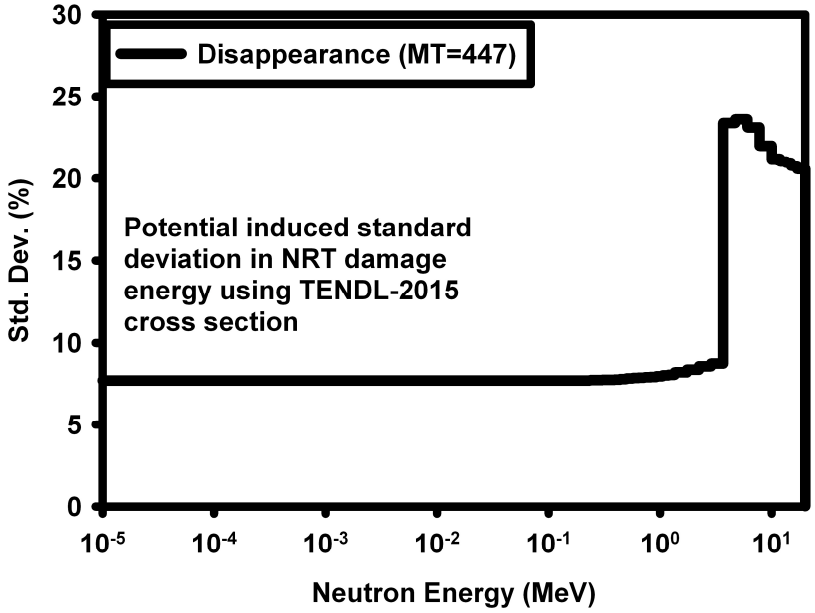


Correlation Matrix

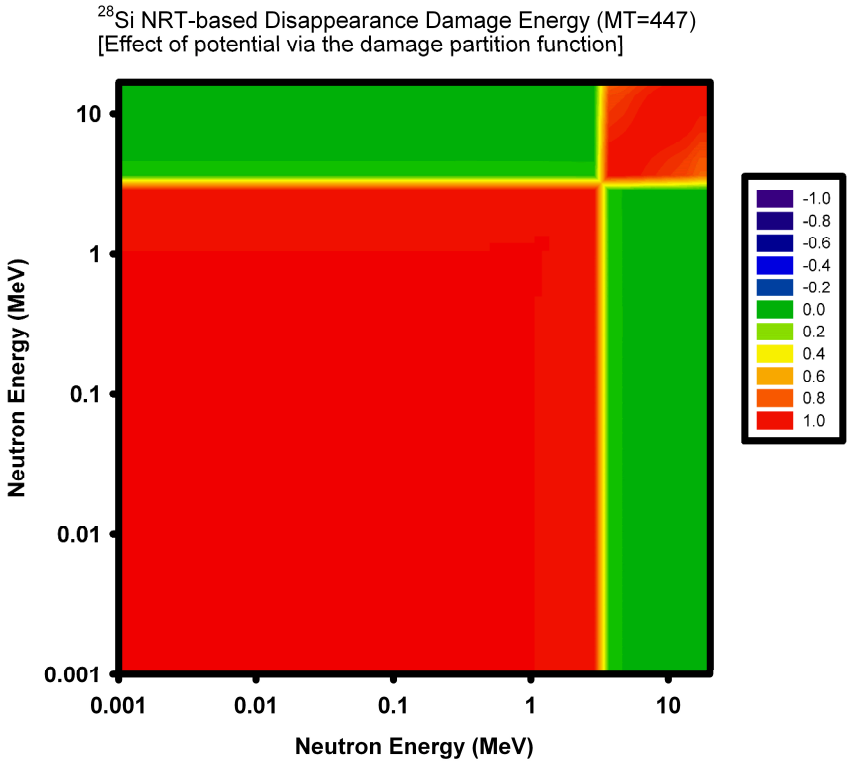


Covariance Matrix for ^{28}Si Disappearance (MT=447) NRT-based Damage Energy from Partition Function

Standard Deviation



Correlation Matrix



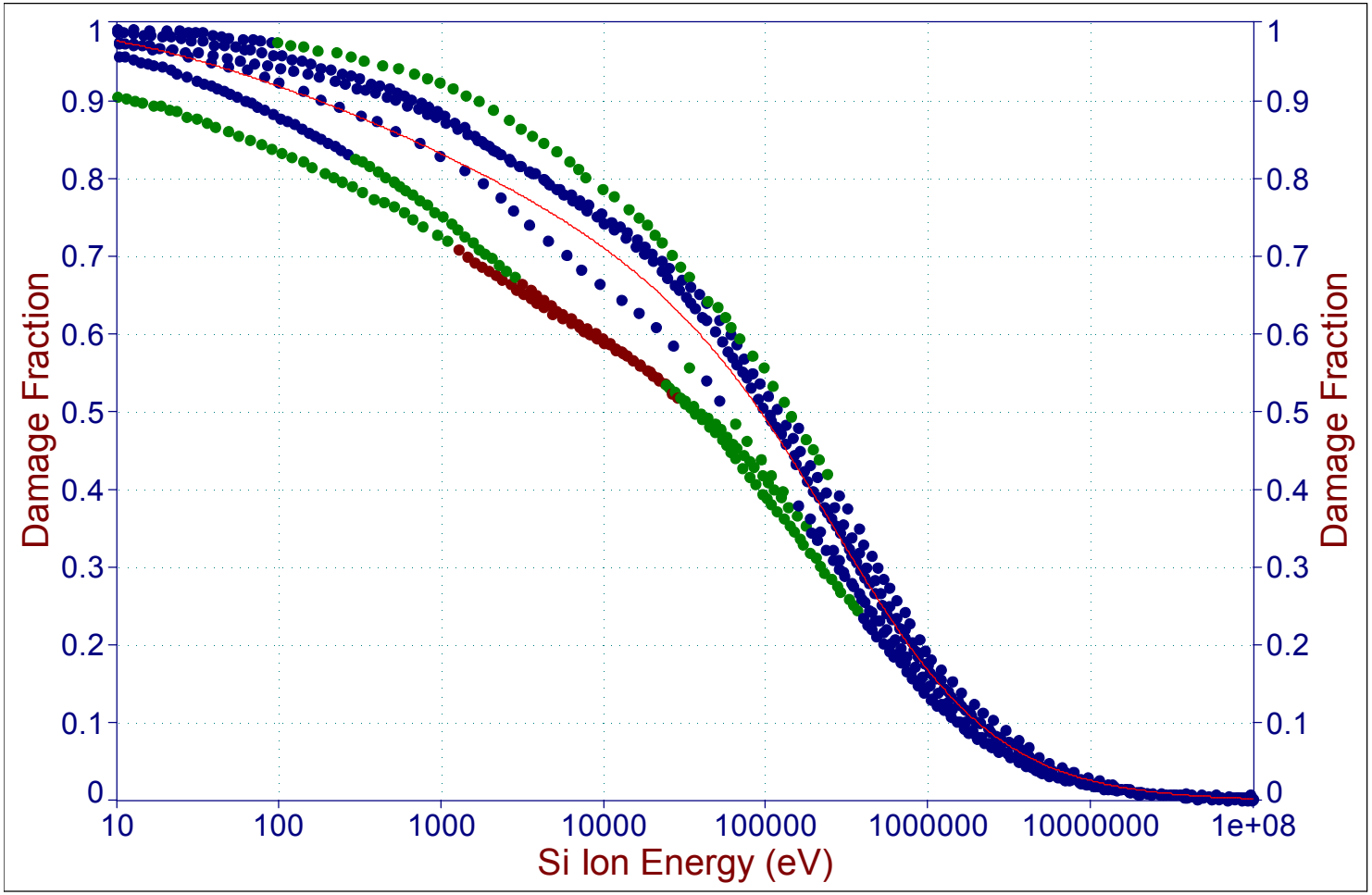
Use a Second Approach to Develop the Covariance Matrix for the Damage Partition Function

Sandia National Laboratories

- **The first approach uses the shape of the data and an energy-dependent data fit**
  - **And required post selection processing to assure proper constraints (bounds, monotonic)**

- **An alternate approach is to use an analytical functional fit that builds these constraints into the representation**

Analytic Functional Fit to Damage Energy from Various BCA Potential



Analytic Fit to Damage Partition Function

- 3-parameter fitting function
  - $y^{-1} = a + b*[\ln(x)]^2 + c*x/\ln(x)$
- Fit quality
  - R^2 Coef. Det. = 0.9748383511, proportion of variance predicted by fit
  - Fit Std. Error = 0.0545913887, least squared error of fit
  - F-value = 14548.0, extend eqn., represents data

Parameter	Value	Std. Dev. [%]	Confidence Interval	
a	1.002139873	0.667	0.989012765	1.015266981
b	0.004039061	3.94	0.003726505	0.004351616
c	5.8107E-5	3.538	5.50709e-5	6.21432e-5

Covariance Matrix for Fitting Parameters

- 3-parameter fitting function
  - $y^{-1} = a + b*[\ln(x)]^2 + c*x/\ln(x)$
- Diagonal of covariance matrix is square of std. dev.

Parameter	a	b	c
a	4.47137e-5	-8.35472e-7	4.87394e-9
b	-8.35472e-7	2.53488e-8	-1.94906e-10
c	4.87394e-9	-1.94906e-10	4.22689e-12

Correlation Matrix for Fitting Parameters

- 3-parameter fitting function
  - $y^{-1} = a + b*[\ln(x)]^2 + c*x/\ln(x)$
- Diagonal of correlation matrix is unity

Parameter	a	b	c
a	1.0	-0.78475	0.354527
b	-0.78475	1.0	-0.5954376
c	0.354527	-0.5954376	1.0

Damage Partition Form Fit for Various BCA Potentials

- 3-parameter fitting function
  - $y^{-1} = a + b*[\ln(x)]^2 + c*x/\ln(x)$

Elec. Pot.	Lattice Pot.	a	b	c	corr(b,c)
ZBL	Moliere	0.97965737	0.0050636486	7.0220873e-5	-0.5713
ZBL	Exponential	0.99122257	0.00711945	6.9402852e-5	-05732
ZBL	Lenz-Jensen	1.0619016	0.0066297817	5.6471389e-5	-0.5828
LSL	Moliere	0.97144559	0.0026607259	6.1747098e-5	-0.5276
LSL	Exponential	0.97436075	0.0034641813	6.1462263e-5	-0.6183
LSL	Lenz-Jensen	0.99740546	0.0031534558	4.8140408e-5	-0.5966

Analytic Fit for BCA-produced Damage Partition Functions

- 3-parameter fitting function
  - $y^{-1} = a + b*[\ln(x)]^2 + c*x/\ln(x)$

Parameter	Value	Std. Dev.	Confid. Interval
a	1.002139873	6%	[0.971 | 1.062]
b	0.004039061	78%	[0.0026 | 0.0071]
c	5.8107E-5	21%	[4.81e-5 | 7.02e-5]

- Select uniform rather than Gaussian sampling
- Consistent strong negative correlation is seen between b and c in individual fits, but not in baseline values. Thus we ignore this correlation is the statistical sampling.

Work in Progress

- A TMC approach using the sampled damage partition functions is in progress.
- The analysis will mirror the previous case.

TOPIC:
UNCERTAINTY

Type ⇨ Displacement Threshold ⇨ E_d

Treatment ⇨ Sensitivity

Displacement Threshold Energy

- **Experimental Values**
  - **10 – 30 eV** **ref. [Ho08]**
  - **20.5 ± 1 eV** **ref. [Bo76]**
  - **13 eV in <111> dir.** **ref. [Co66]**
  - **20.5 ± 1 eV** **ref. [Bo76]**

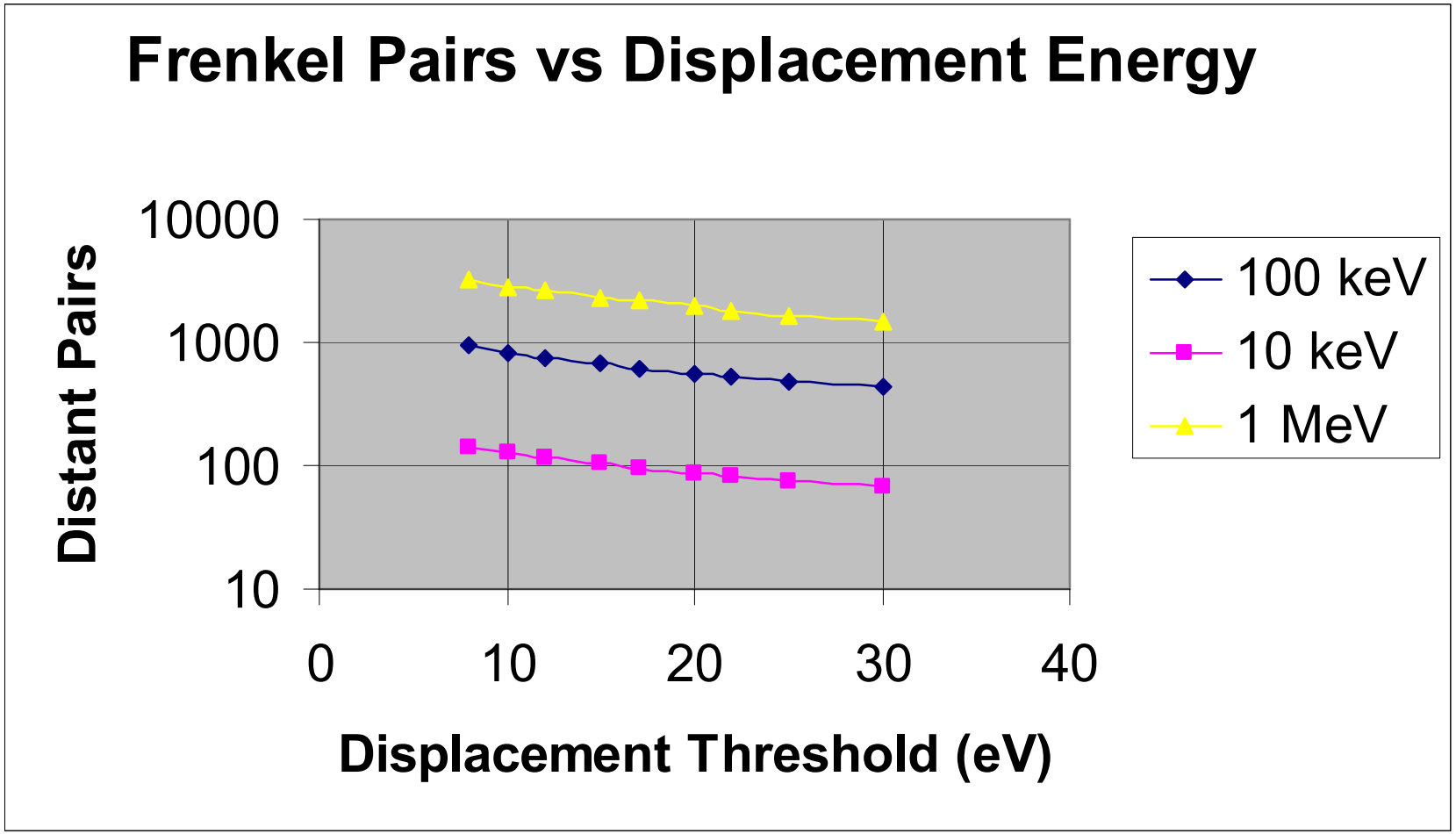
- **Result has a strong angle dependence**

Displacement Threshold

- Theoretical Values
  - 9 – 35 eV (BCA) ref. [Bu13]
  - 20 ± 2 eV in <100> dir. ref. [No97]
  - 12.5 ± 1.5 eV in <111> dir. ref. [No97]
  - 20 eV (rec. crystalline Si) ref. [Bu13]
  - 24 ± 2 eV (DFT-MD) ref. [Ho08]

- Result is strongly correlated over recoil energy

Silicon Displacement Energy Sensitivity

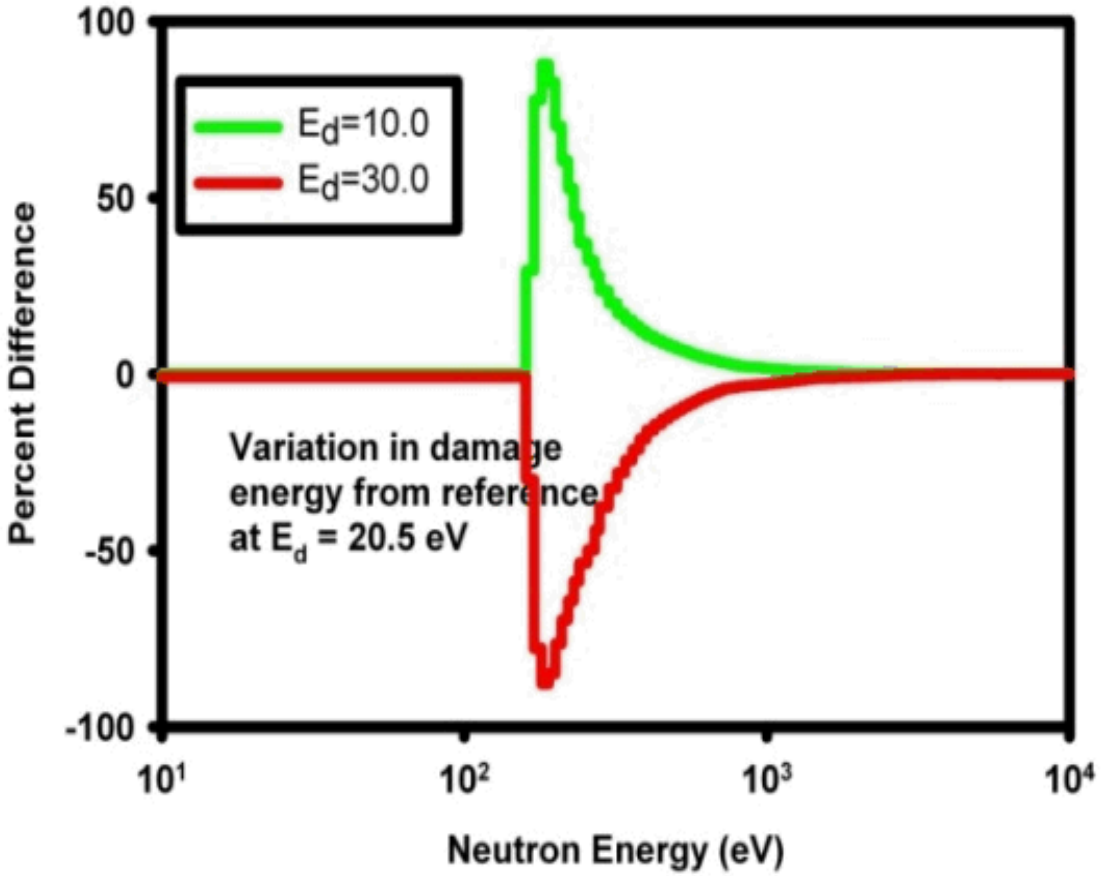


Displacement Threshold Energy from Standard Sources

- **ASTM recommended value:**
  - **E722-2015 20.5 eV using ^{nat}Si**
  - **E722-1994 25 eV using ^{28}Si**
    - **Difference is < 1% near 1-MeV**
    - **Difference is < 10% over all energies**

- **NJOY-2012 default value**
  - **25 eV**

Variation of NRT-based Damage Energy with E_d



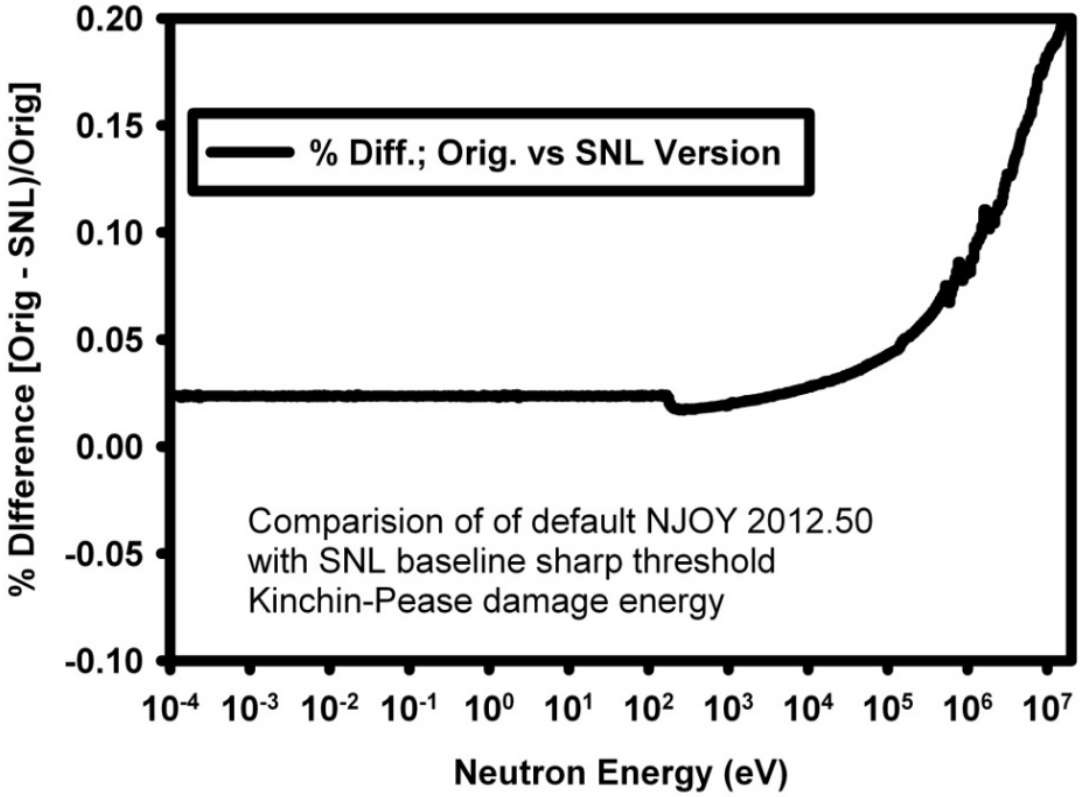
- 640-group comparison with reference is E_d = 20.5 eV

TOPIC:
UNCERTAINTY

Type ⇨ Displacement Threshold ⇨ Threshold Treatment

Treatment ⇨ Sensitivity

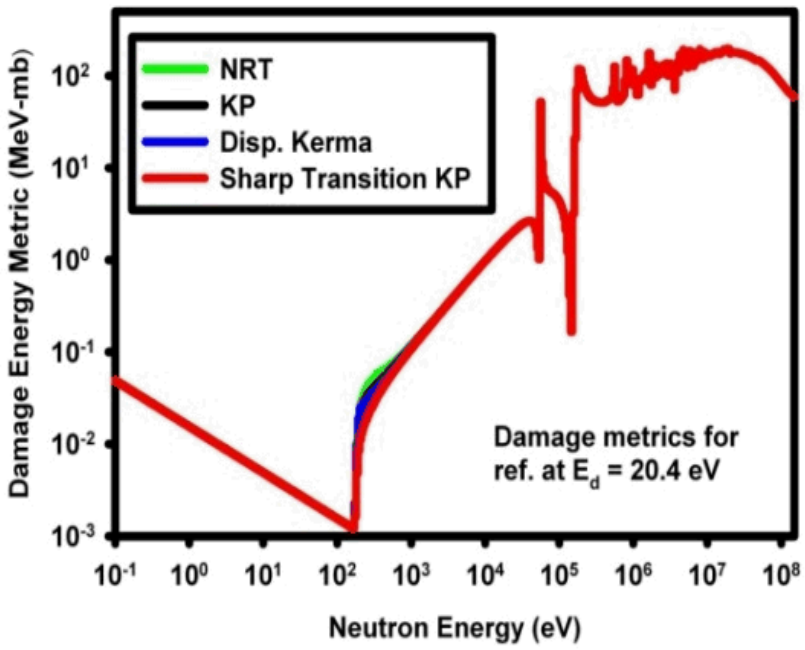
Effect of Using Lattice Atomic Weight Rather Than Isotopic Atomic Weight in Robinson Fit



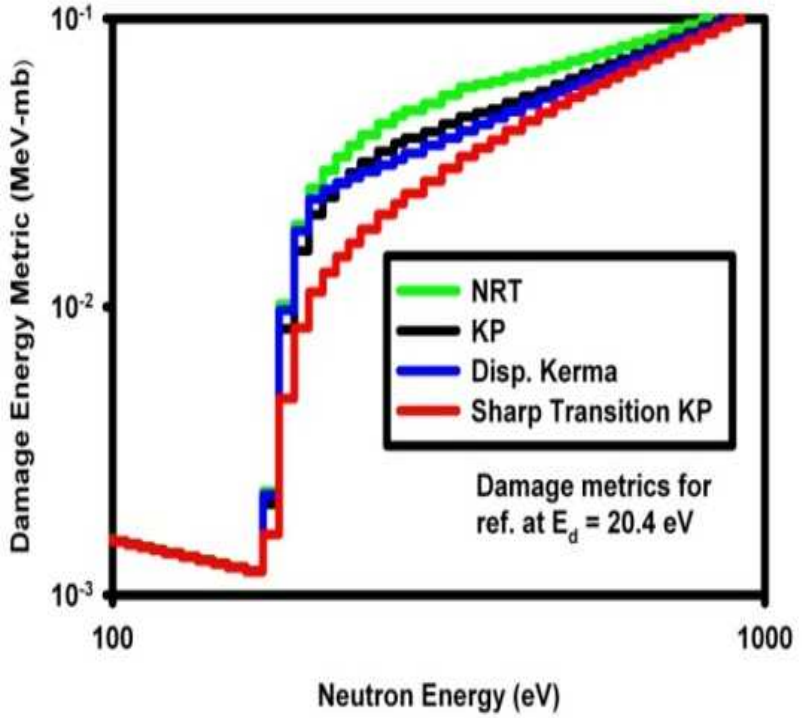
- Current analysis incorporates this aspect, but it has negligible effect
- Note, NJOY/ENDF uses atomic mass relative to neutron mass, not amu

Variation of Damage Energy Metric with Displacement Model

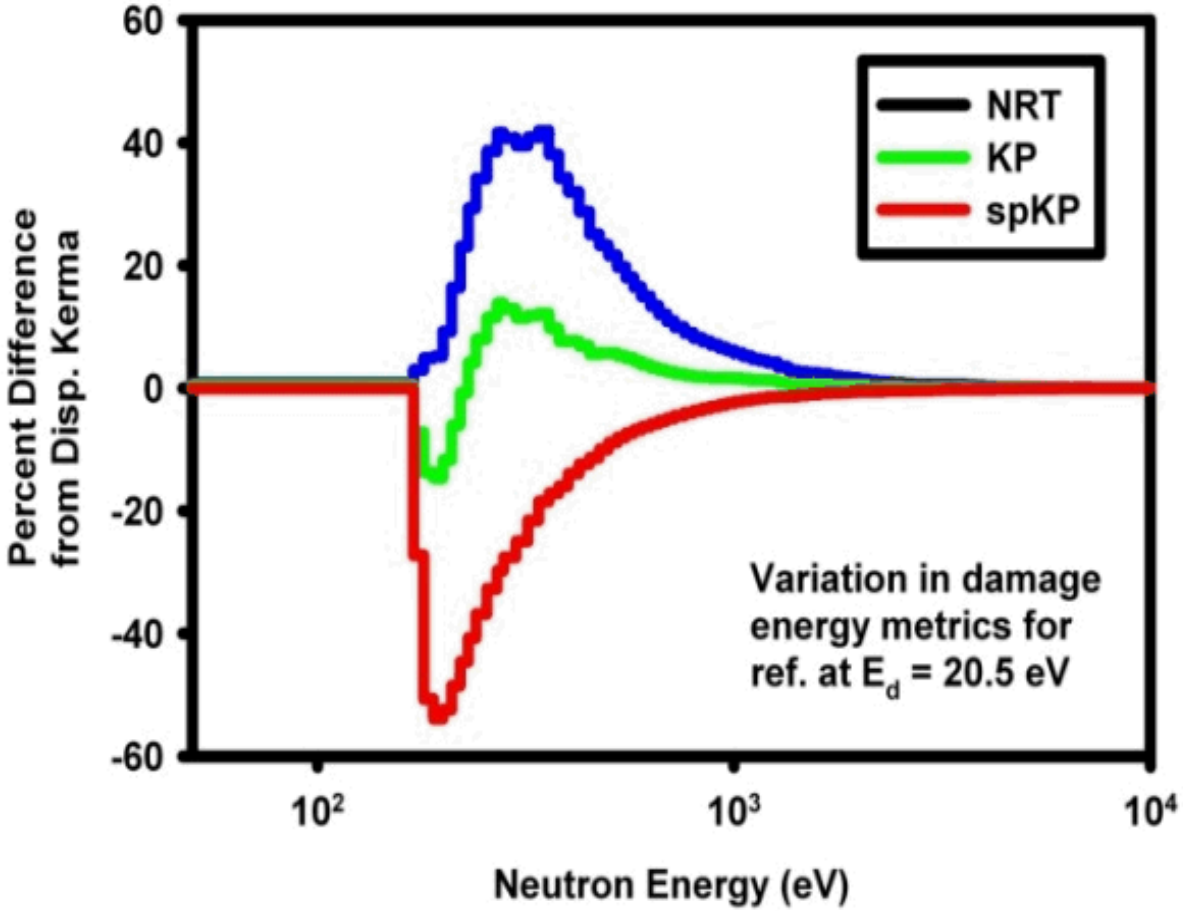
Total Neutron Energy Range



Expanded View



Effect of Displacement Model on Damage Energy



- **Difference between displacement kerma and various damage energy metrics**

TOPIC:
UNCERTAINTY

Type ⇨ Displacement Threshold ⇨ E_d & Threshold Treatment

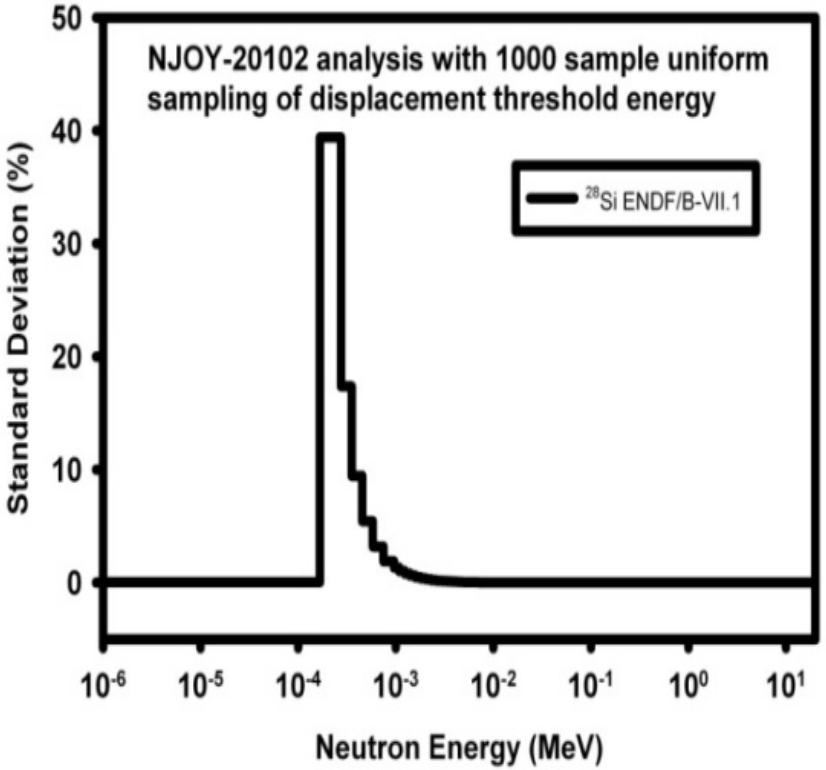
Treatment ⇨ Method of Characterization

Methodology

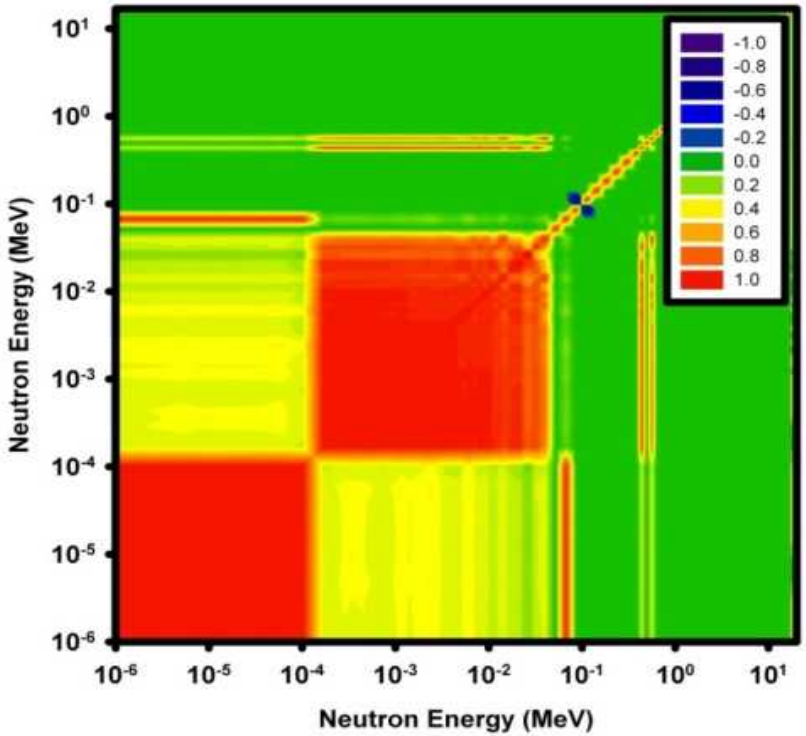
- **Set the displacement model to the NRT-based damage energy**
  - **This is the best representation of FP generation in Silicon**
  - **Comparisons of silicon transistor gain change with the NRT-based damage energy do not indicate a need for an arc-dpa model for neutron energies up to 20 MeV**
    - **Unlike silicon, an athermal recombination model is required to reproduce observed displacement damage in GaAs LEDs**
  - **Any residual uncertainty due to displacement threshold model will be included in the "model defect" comparison with observed damage**
- **Use TMC approach and NJOY-2012 processing**
  - **Use uniform sampling of E_d from 10 eV to 30 eV**

Covariance Matrix for ^{28}Si Total (MT=444) NRT-based Damage Energy from Displacement Threshold Energy

Standard Deviation



Correlation Matrix



TOPIC:
MODEL DEFECT

Model defect is the insensitivity of a calculation to some quantities that my affect the calculated attribute. If the model defect was understood, it would have led to a refined model. So, inclusion of its uncertainty is a challenge.

- Cross section models
- Recoil spectrum models
- Observed damage vs. calculated metric

Sources of Model Defect

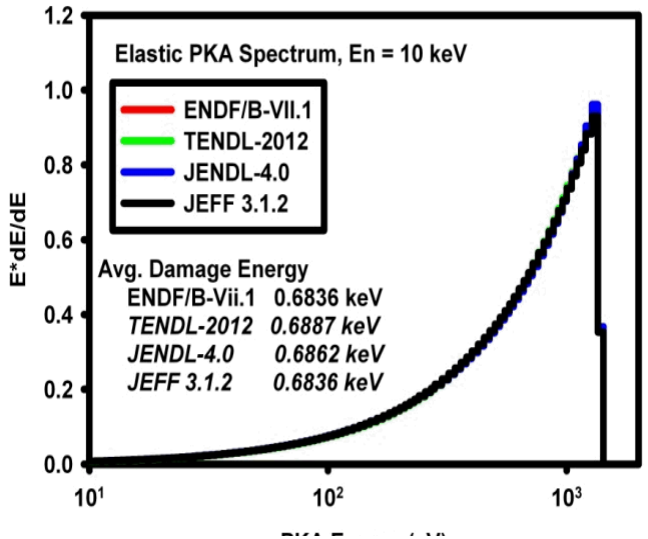
- Nuclear reaction models used in calculated cross sections (TENDL)
- Model-based recoil spectra (TENDL and ENDF/B-VII)
- Displacement threshold energy
  - Definition of a “distant” Frenkel pair that does not immediately recombine
  - Angle dependence
- Treatment of displacement threshold energy
- Difference between damage energy, number of initial defects, number of residual defects.
- All defect types do not have the same damage efficiency.

TOPIC:
UNCERTAINTY

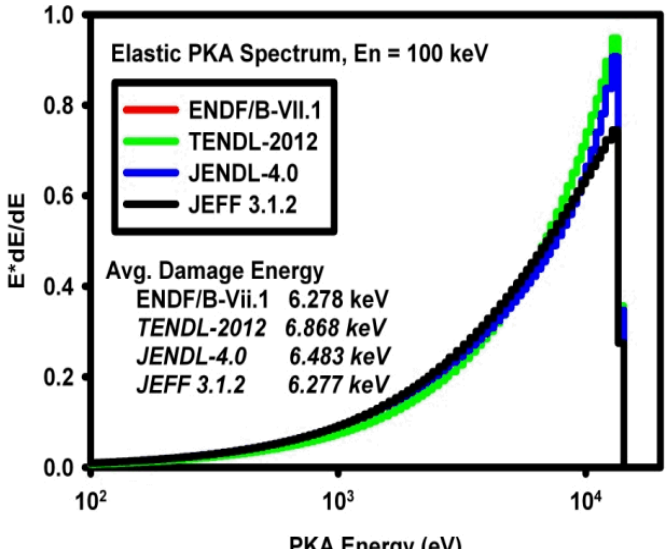
Type ⇨ Model Defect ⇨ Cross Section Model

Treatment ⇨ Sensitivity

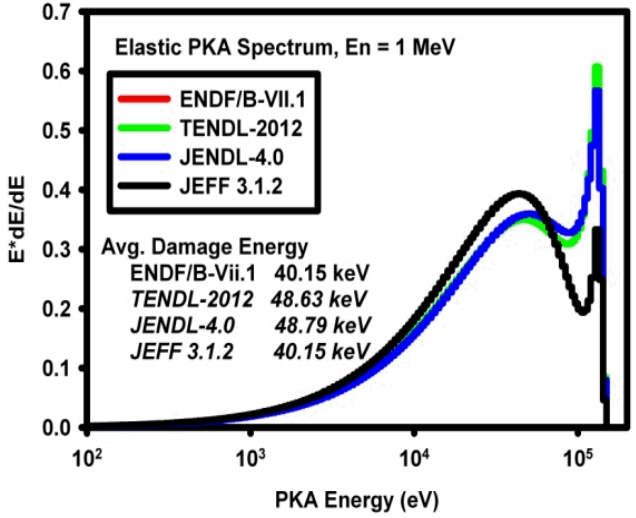
Variation in Elastic Recoil Spectrum



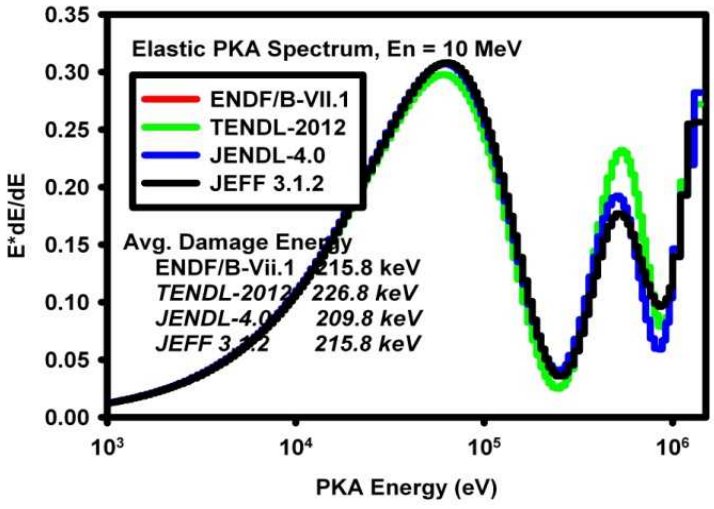
10 keV



100 keV

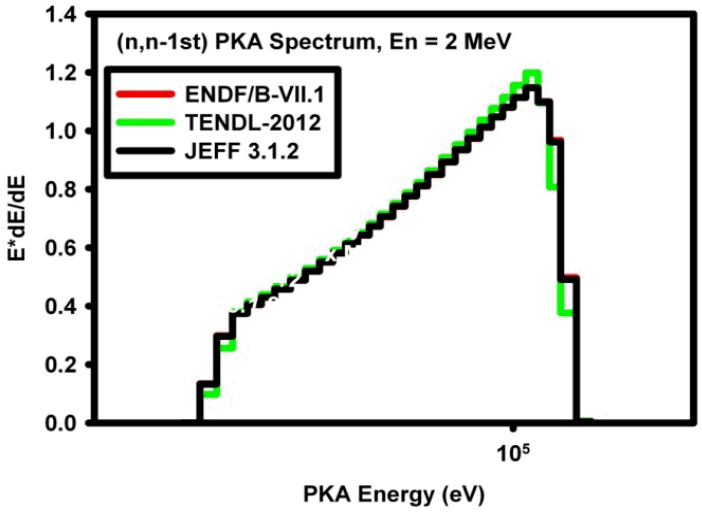


1 MeV

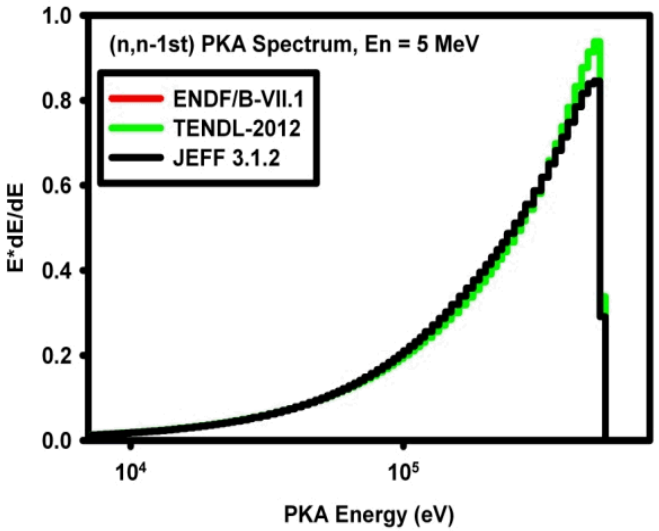


10 MeV

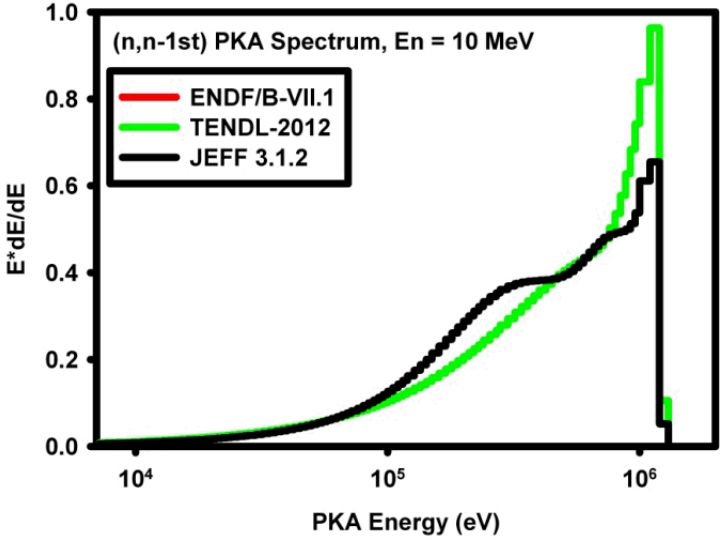
Variation in (n,1stn') Recoil Spectrum



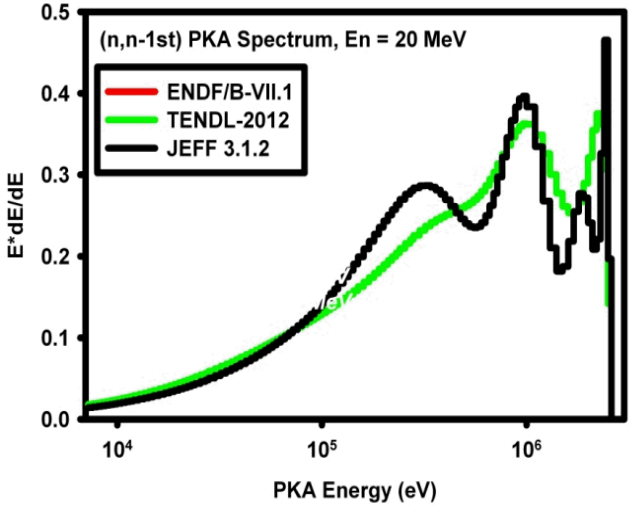
2 MeV



5 MeV

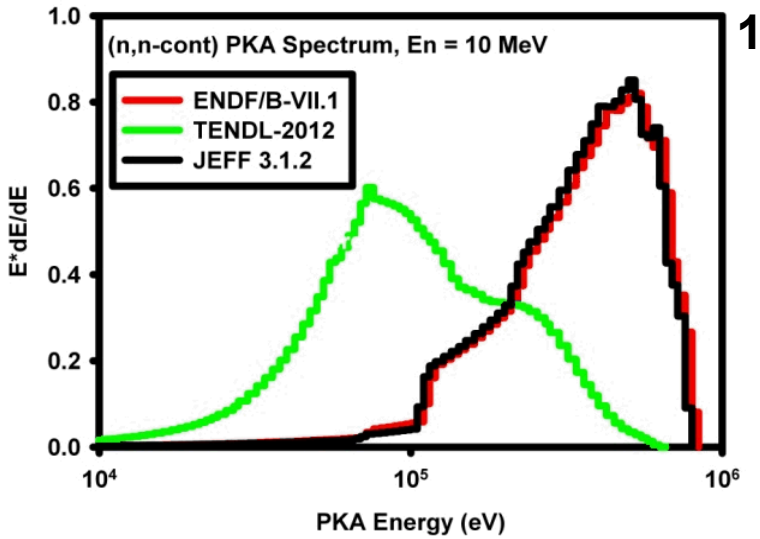


10 MeV

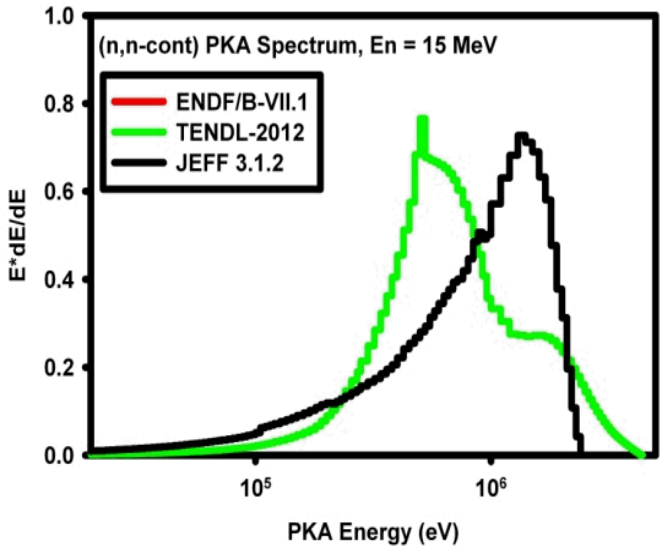


20 MeV

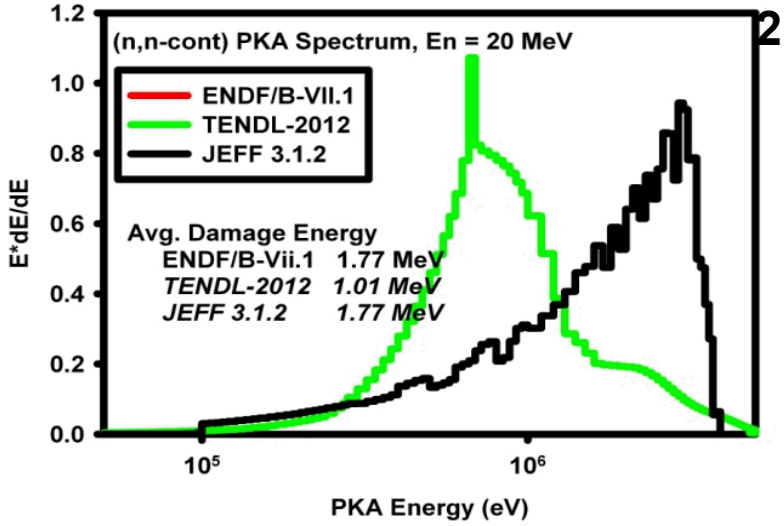
Variation in (n,n'-continuum) Recoil Spectrum



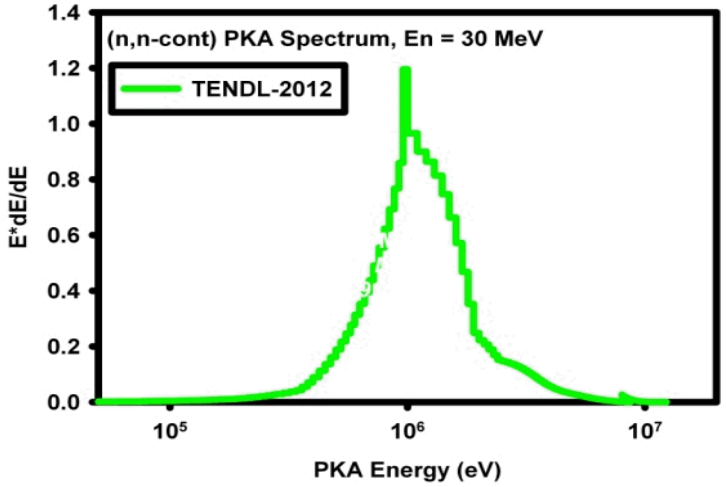
10 MeV



15 MeV

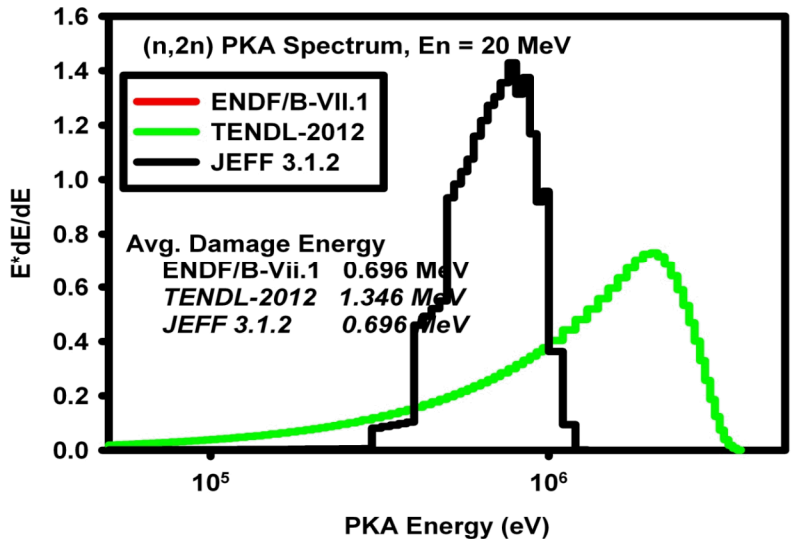


20 MeV



30 MeV

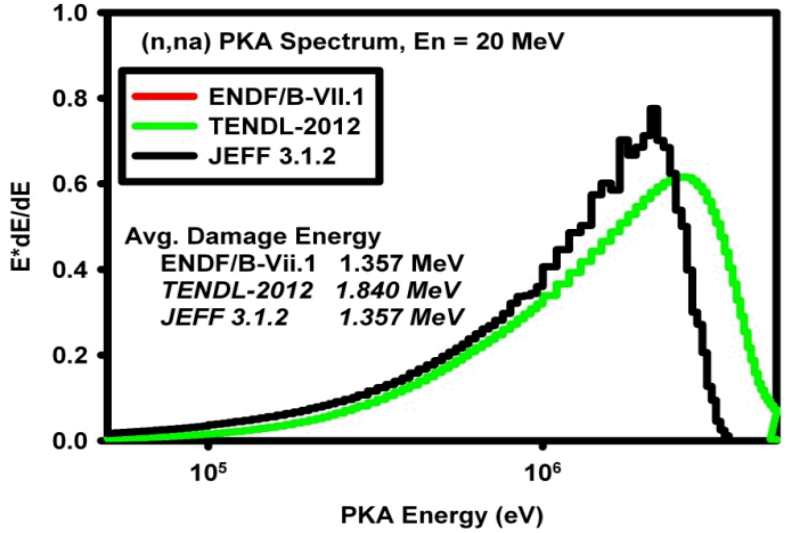
Variation in (n,2n) Recoil Spectrum and Other Reactions Near 20-MeV



(n,2n) 20 MeV

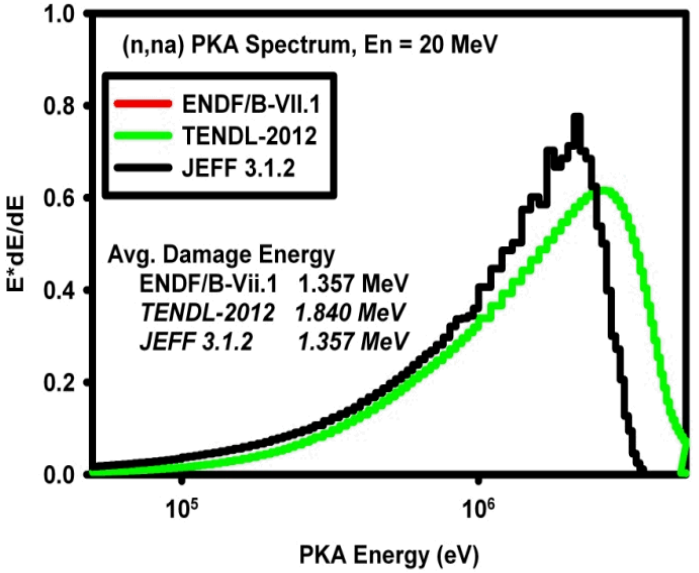
Large (n,2n) recoil spectrum variation seen at 20 MeV. But this is similar to other reactions near the reaction threshold energy.

E_{th} = 17.799 MeV

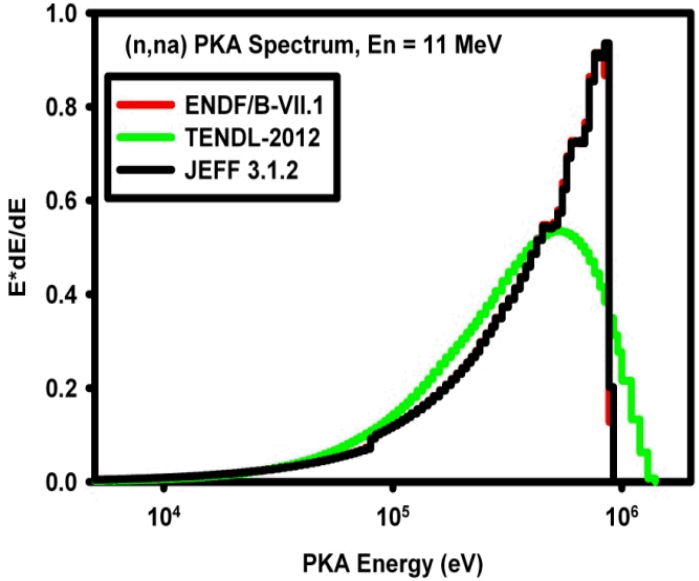


(n,nα) 20 MeV

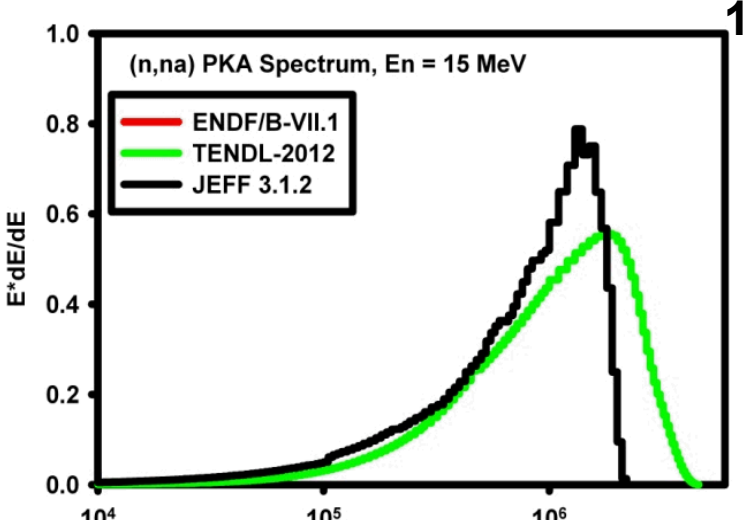
(n,np) 20 MeV



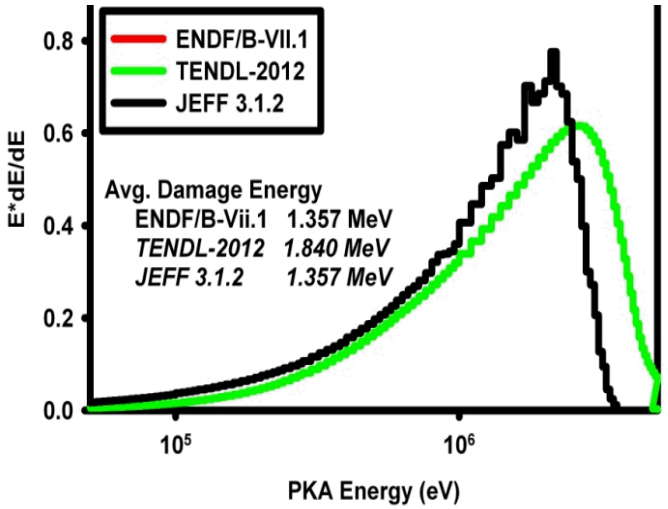
Variation in (n,nα) Recoil Spectrum



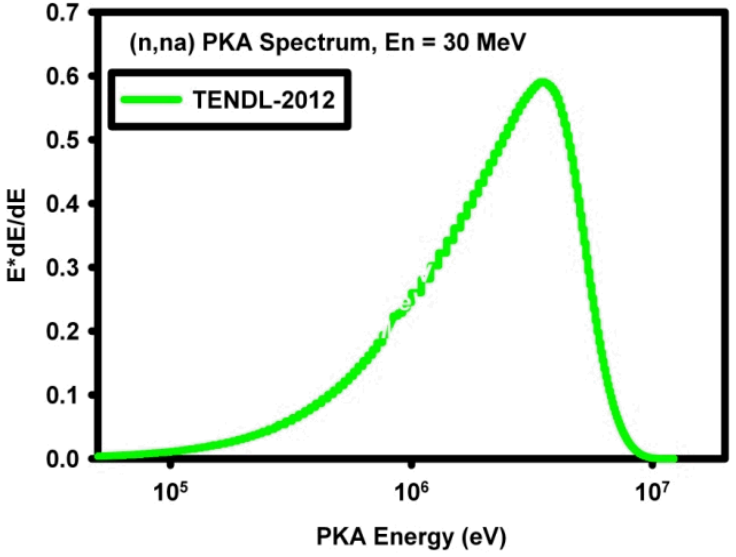
11 MeV



15 MeV

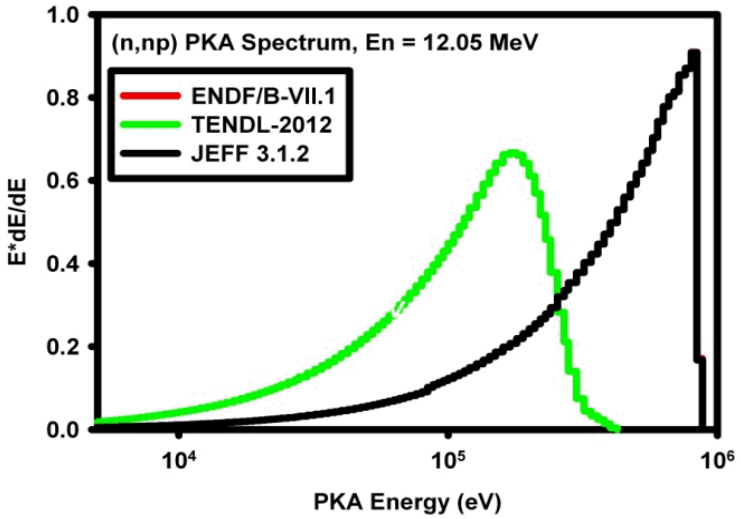


20 MeV

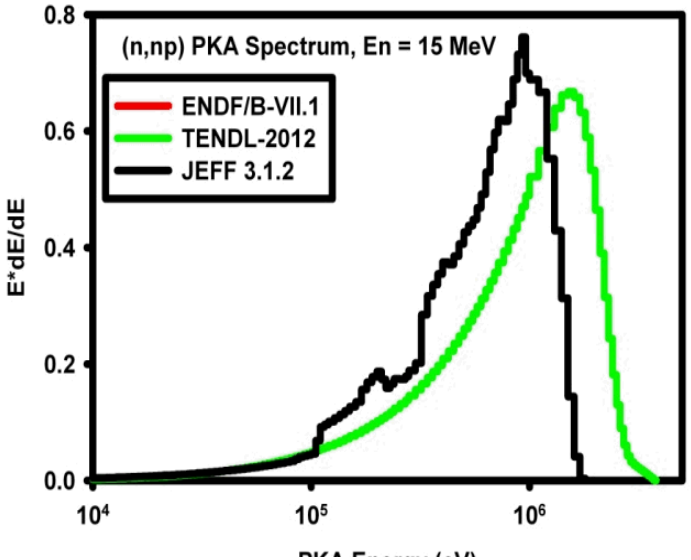


30 MeV

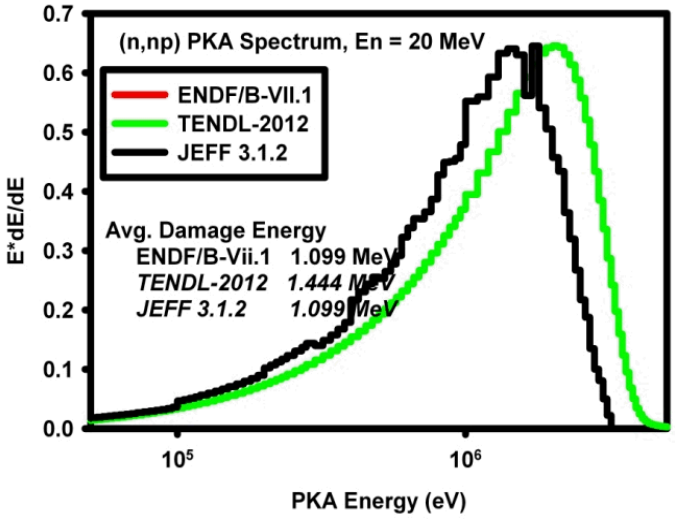
Variation in (n,np) Recoil Spectrum



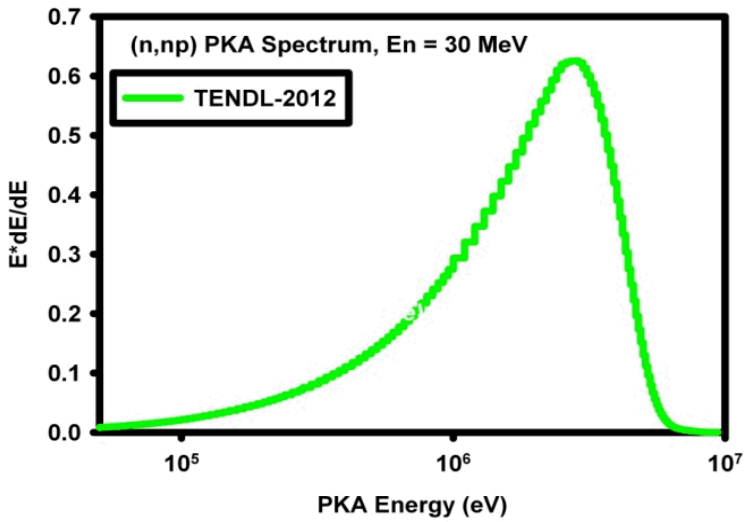
12.05 MeV



15 MeV

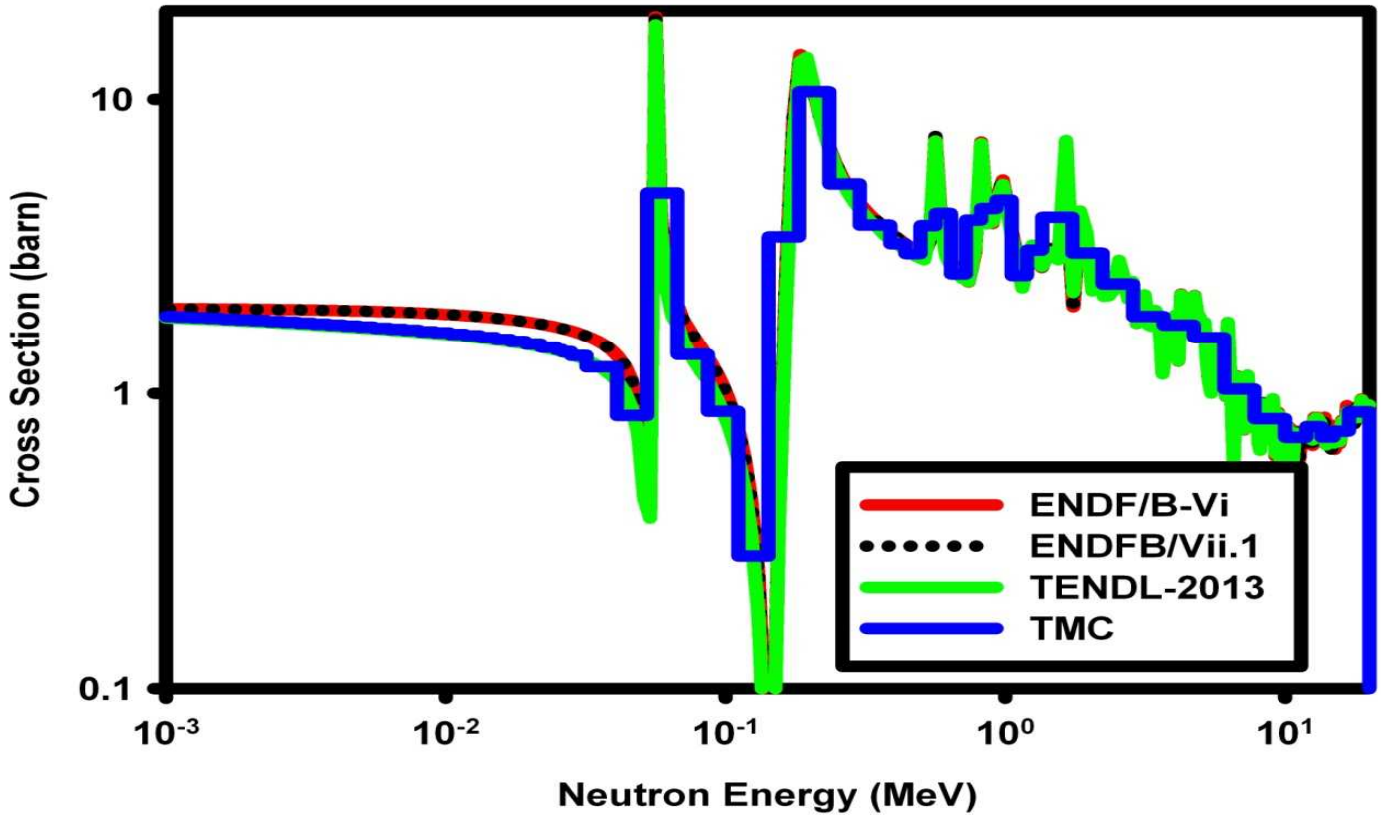


20 MeV



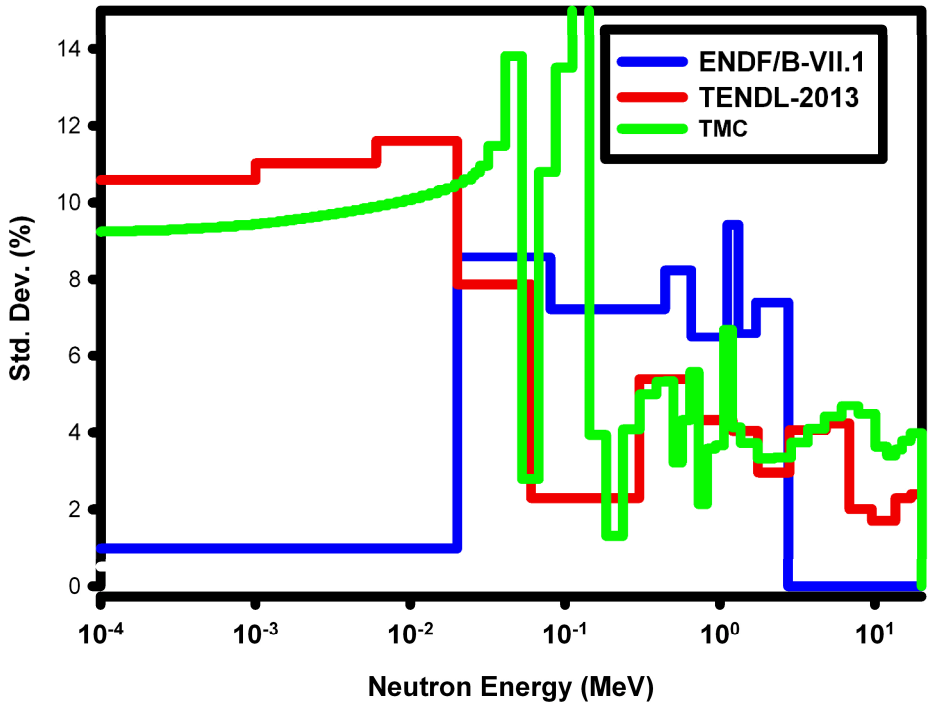
30 MeV

Variation in Elastic Cross Sections



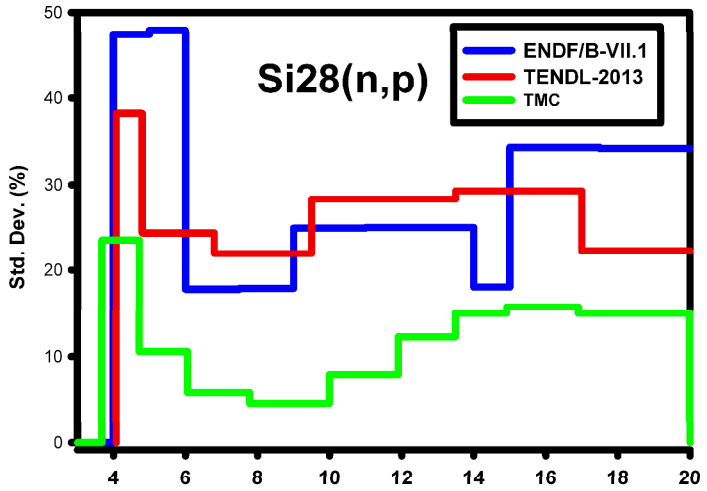
Variation between evaluations based on evaluation methodology and weighting of experimental data.

Variation in Uncertainty for Elastic Cross Section

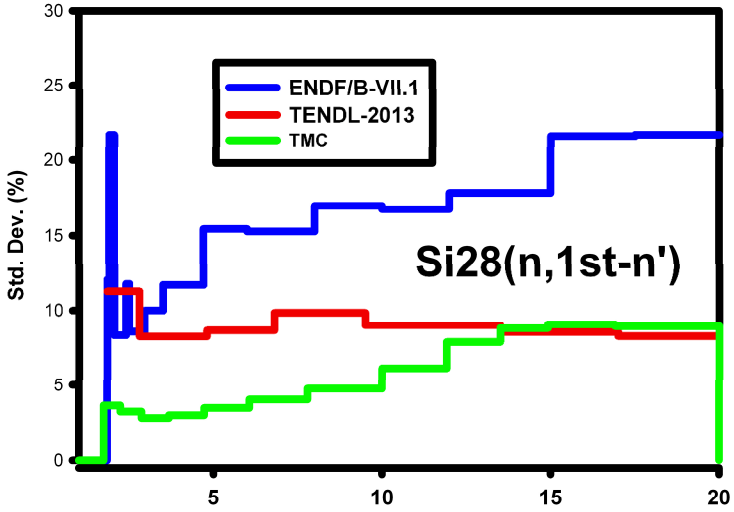


- Variation between evaluations based on evaluation methodology
- Some TENDL/TMC variation based affected by energy group structure.
- Note, ENDF/B-VII.1 only contained File 33 covariance data, i.e. no File 32 resonance data, even though the resonance contribution dominates the low energy cross section. ENDF/B-VII.1 high energy covariance is also missing, but it is found in ENDFB-VI.

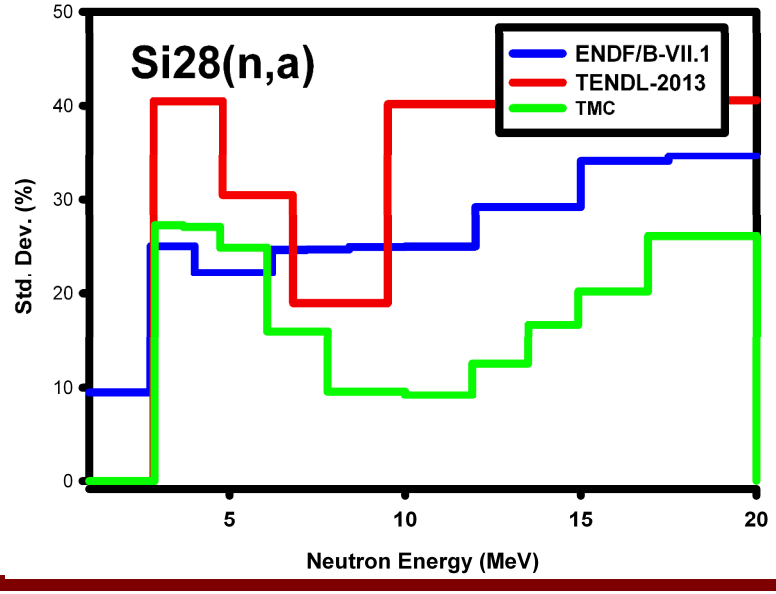
Uncertainty in Reaction-specific Cross Sections



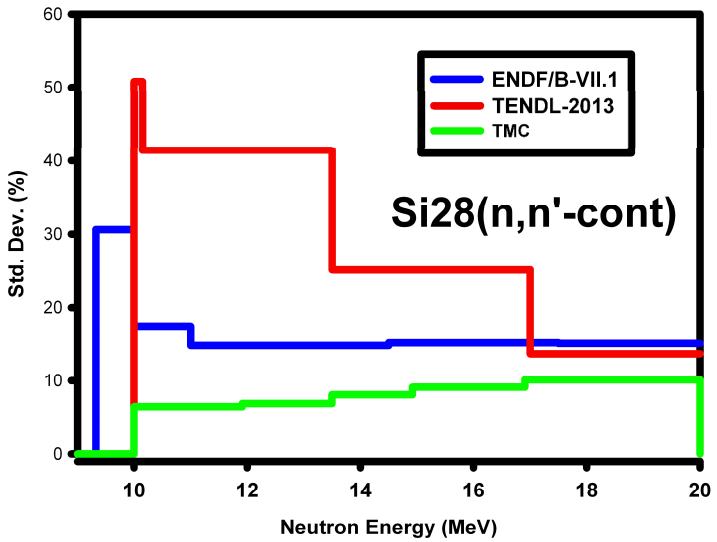
(n,p)



(n,1st n')

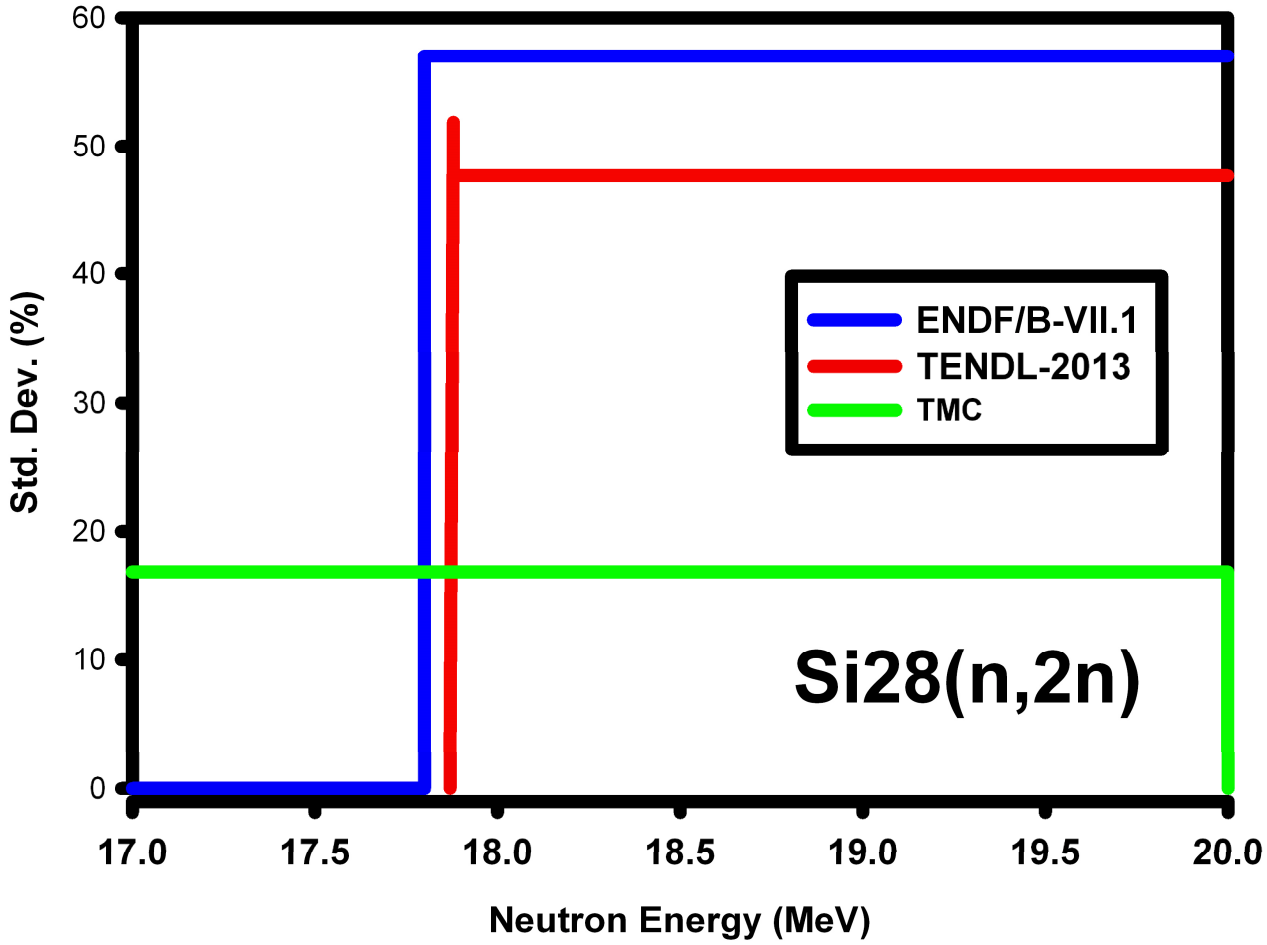


(n,a)



(n,n'-cont)

Uncertainty in Reaction-specific Cross Sections



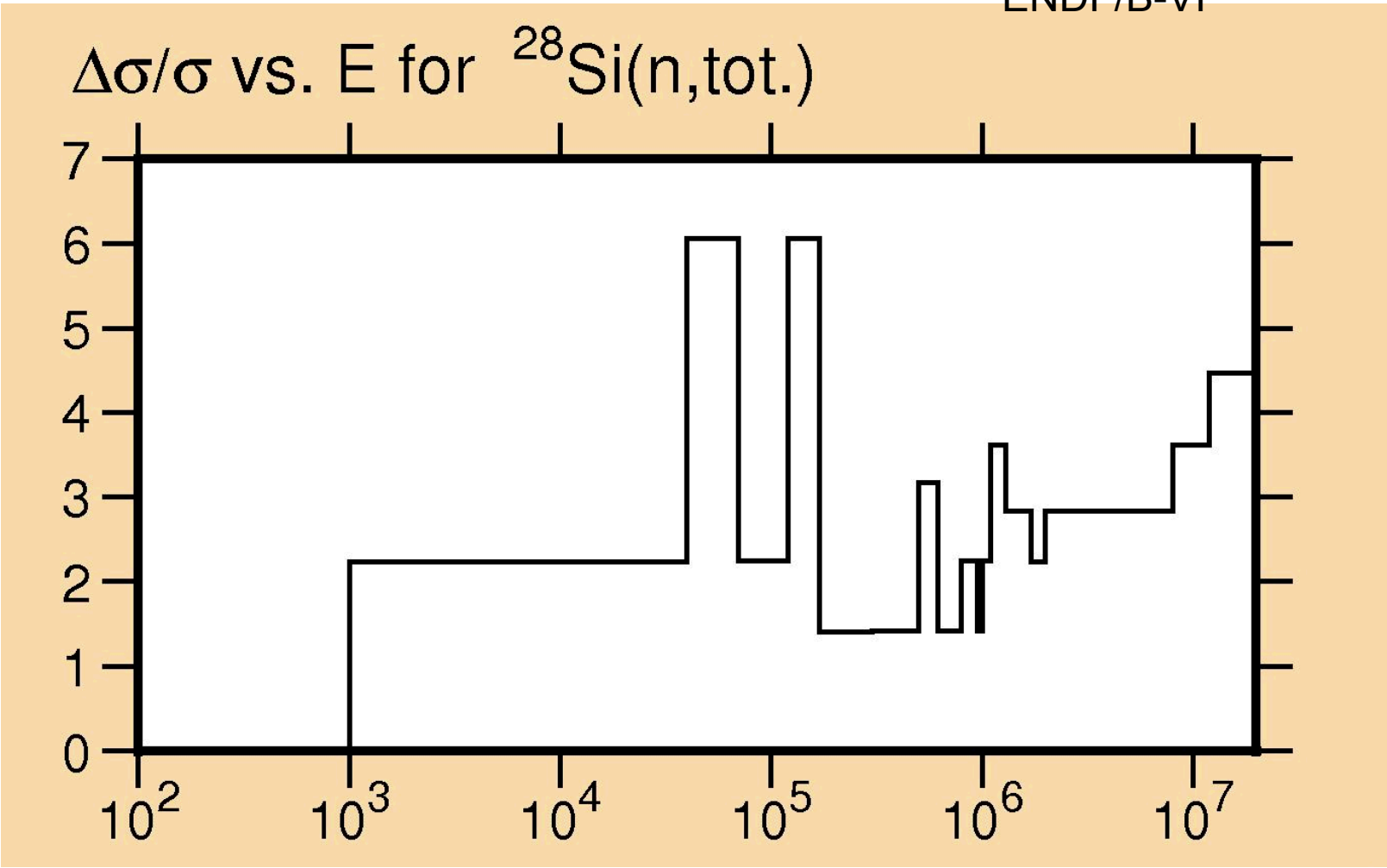
(n,2n)

Pending Investigation

- A comparison of the variation seen in the TENDL-2015 sampling and that the seen between ENDF/B-VII.1 would be one indicator of a “model defect”.
- The strong correlation seen in the displacement kerma components suggests that a variation in the individual cross section components is not informative of any “model defect”. Only a comparison of the total cross section would have merit.

Is this good agreement in total ^{28}Si total cross section warranted? Consistent with data?

ENDF/B-VI



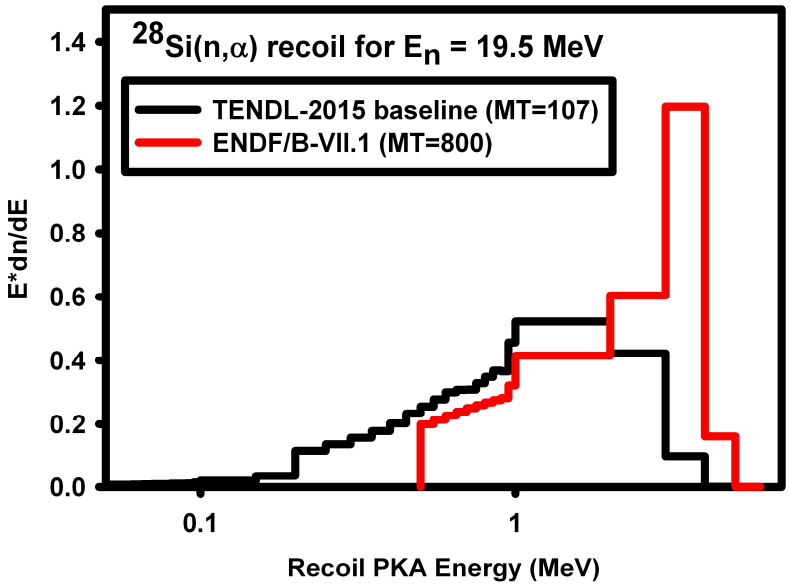
TOPIC:
UNCERTAINTY

Type ⇨ Model Defect ⇨ Recoil Spectrum Model

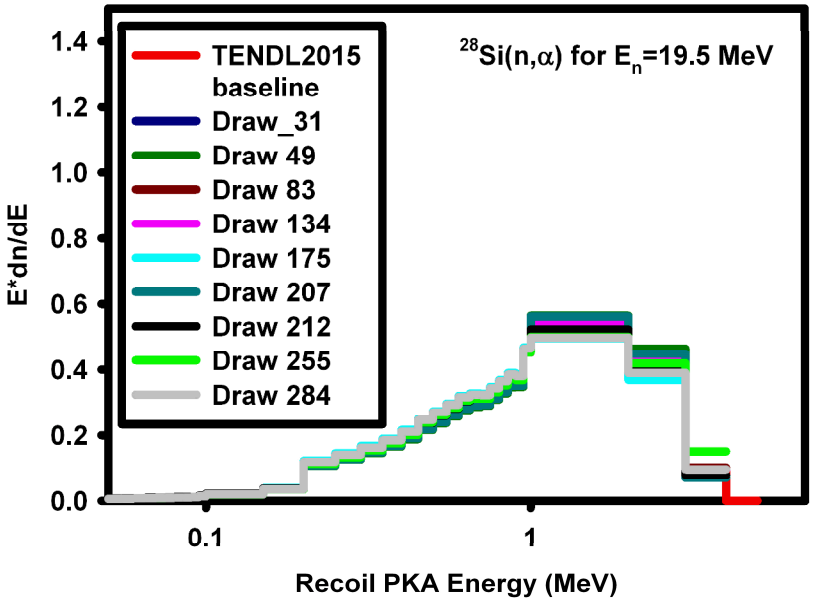
Treatment ⇨ Sensitivity

^{28}Si(n,α) PKA recoil spectrum: E_n=19.5 MeV

Comparison of baseline values



TENDL-2015 random draws



Comparison of Variation in ^{28}Si Recoil Spectra (1/3)

Reaction	Neutron Energy (MeV)	Percent Damage Energy from PKA		
		TENDL-2015 Random Sample	TENDL-2015 Baseline	ENDF/B-VII.1 / [Diff.]
Elastic	0.0125	6.8007 ± 0.007%	6.801	6.743 [1%]
	0.125	6.1318 ± 0.477%	6.112	5.548 [10%]
	1.5	4.6274 ± 2.791%	4.560	4.660 [2%]
	10.5	2.4360 ± 14.34%	2.388	2.262 [6%]
	19.5	1.3679 ± 17.791%	1.419	1.328 [7%]
1st Inelastic	2.5	4.401 ± 0.428%	4.395	4.337 [1%]
	5.5	5.5502 ± 0.204%	5.549	5.401 [3%]
	10.5	6.2711 ± 1.202%	6.316	5.414 [17%]
	14.5	4.8633 ± 5.937%	4.980	4.308 [16%]
Continuum Inelastic	10.5	2.2027 ± 2.02%	2.206	4.026 [45%\
	13.5	2.8293 ± 10.48%	2.922	5.814 [49%]
	17.5	2.0506 ± 14.8%	2.173	7.968 [73%]
	19.5	1.6964 ± 14.29%	1.856	8.820 [79%]

Comparison of Variation in ^{28}Si Recoil Spectra (2/3)

Reaction	Neutron Energy (MeV)	Percent Damage Energy from PKA		
		TENDL-2015 Random Sample	TENDL-2015 Baseline	ENDF/B-VII.1 [Diff.]
(n,p)	4.5	3.9973 ± 0.188%	3.998	4.151 [4%]
	5.5	4.3046 ± 0.37%	4.325	4.439 [3%]
	10.5	4.7562 ± 1.75%	4.784	5.833 [18%]
	14.5	5.0490 ± 2.11%	5.029	6.230 [19%]
	19.5	4.7962 ± 4.67%	4.736	6.229 [24%]
(n,a)	3.5	6.9561 ± 0.835%	6.928	7.1 [3%]
	5.5	9.9629 ± 0.241%	9.975	10.89 [9%]
	10.5	10.5656 ± 1.971%	10.62	13.31 [20%]
	14.5	9.1474 ± 4.052%	9.266	14.01 [34%]
	19.5	8.6840 ± 2.560%	8.706	14.42 [40%]
(n,2n)	18.5	1.2456 ± 0.66%	1.243	3.802 [67%]
	19.5	2.7754 ± 1.46%	2.766	3.651 [40%]

Comparison of Variation in ^{28}Si Recoil Spectra (3/3)

Reaction	Neutron Energy (MeV)	Percent Damage Energy from PKA		
		TENDL-2015 Random Sample	TENDL-2015 Baseline	ENDF/B-VII.1
(n,na)	10.5	---	---	3.925 [--%]
	14.5	5.857 ± 0.70%	5.859	6.301 [7%]
	17.5	6.644 ± 1.9%	6.576	6.971 [6%]
	19.5	6.575 ± 1.5%	6.654	6.985 [5%]
(n,np)	12.5	2.105 ± 0.57%	2.102	3.690 [43%]
	14.5	3.880 ± 2.2%	3.834	4.867 [21%]
	17.5	4.187 ± 2.65%	4.175	5.592 [25%]
	19.5	4.315 ± 2.97%	4.326	5.711 [24%]

Observation

- **Variation between {TENDL-2015 and ENDF/B-VI.1 recoil spectra} vs. {TENDL-2015 random draws}**
  - **high energy disappearance channels:**
    - **TMC variation seriously fails to capture variation seen in evaluations**
  - **Elastic channel:**
    - **TMC consistent with variation seen in evaluations**
  - **Inelastic channel:**
    - **1st Inelastic channel: serious differences**
    - **Continuum inelastic channel: differences, but comparison may not be valid since evaluations define continuum differently, i.e. model a different number of discrete inelastic states**
- **Need to include "model defect" uncertainty in capturing high energy PKA recoil spectra for transmutation reactions**

TOPIC:
UNCERTAINTY

Type ⇨ Model Defect ⇨ Observed Damage vs. Damage Metric

Treatment ⇨ Method of Characterization

Methodology

- **Compare ratios of measured damage response to calculated metric in varying benchmark neutron fields.**
- **Fields surveyed:**
  - **^{252}Cf (sf)**
  - **14-MeV from DT**
  - **2.45 MeV from DD**
  - **Fast fission from ^{235}U FBR**
  - **Moderated fission from pool-type reactors with various spectrum moderators**

Observations on Observed vs. Calculated Model Defect in Silicon

- **Significant issue for thermal neutron fields**
  - **Low displacement point defects behave different than clustered defects with respect to residual defects of interest, i.e. V-V and V-O versus isolated interstitials**
- **For fast neutrons, damage ratio data fits calculations to within measurement uncertainties, ~8%, see Precision and Bias Section of ASTM E1854.**
  - **Gain change in silicon bipolar transistor is the metric used for observed damage.**
  - **Other metrics, such as bulk resistivity, should be investigated.**

Conclusion

- This work has investigated the uncertainty contributions to primary radiation damage in Silicon.
- Most uncertainty contributors have been characterized with energy-dependent covariance matrices which can be combined for a total covariance.
- Reaction channel correlations were found to be important, and were handled in the recommended TMC process.
- Investigations on how much added uncertainty to add to account for “model defect” are on-going.

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Questions

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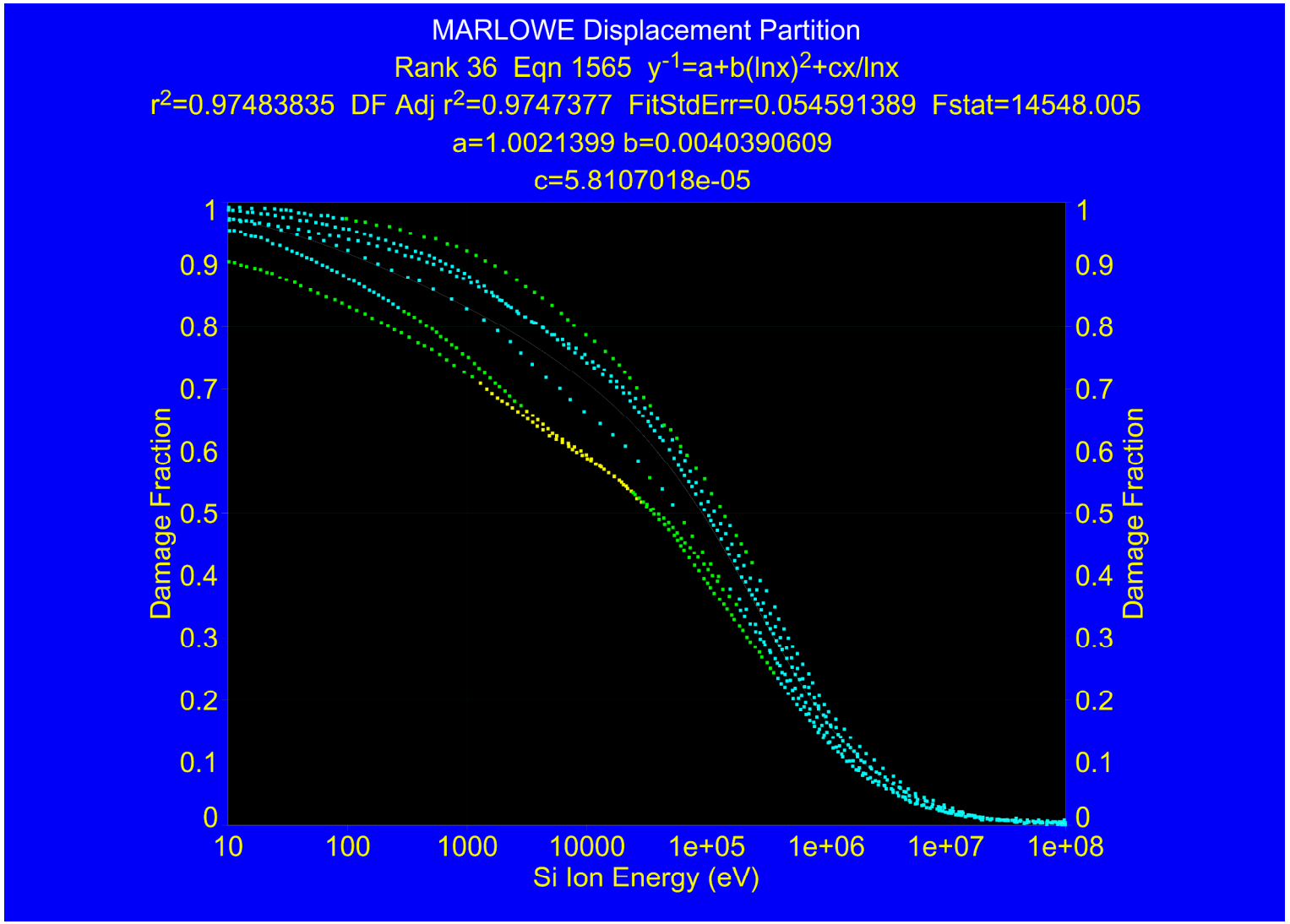
Back-up Material

Analytic Functional Fit to Damage Energy from Various BCA Potential



Validation Evidence

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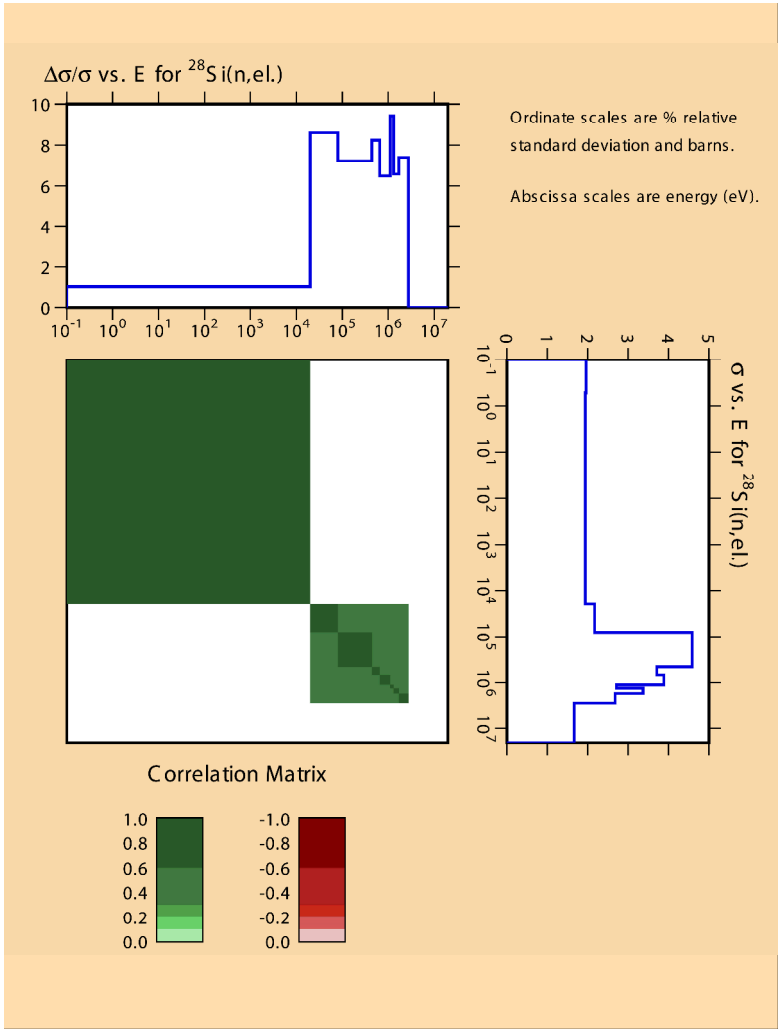
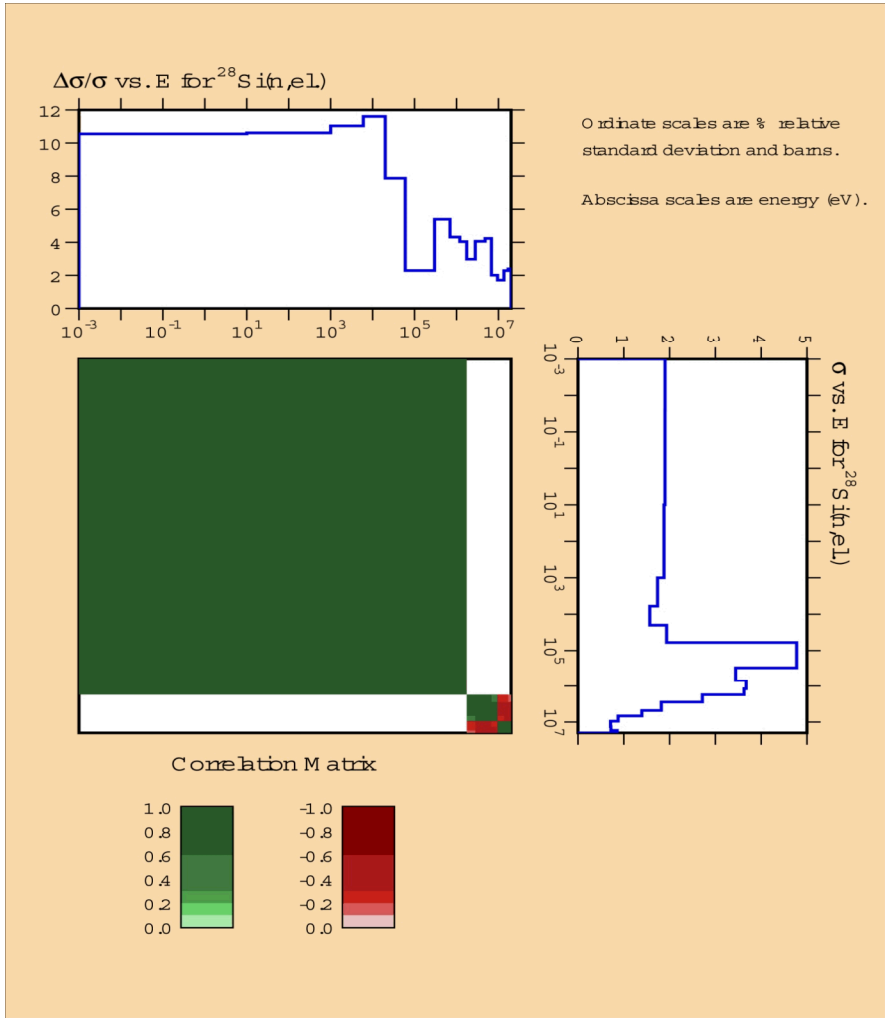
- **Silicon**
  - Evidence exists for silicon transistor gain degradation at 14-MeV (DT), 2.5 MeV (DD) and various fast and moderated fission reactor spectra (~ 1-MeV). References cited in ASTM E722.
  - Excellent correlation for displacement kerma and observed damage – except at thermal neutron energies.
- **GaAs**
  - Similar experimental evidence exists, but it indicates that the high energy neutron damage does NOT track with the displacement kerma. A thermal spike, i.e. defect recombination, has been proposed as the explanation. An empirical recoil energy efficiency has been adopted. This can be reformulated into the arc-dpa formalism.
- **Other**
  - Some work on SiC. No experimental work on GaN , InP or AlN or other III-V materials. No standard for energy-dependent response function.

Uncertainty/Variation in Elastic Cross Sections

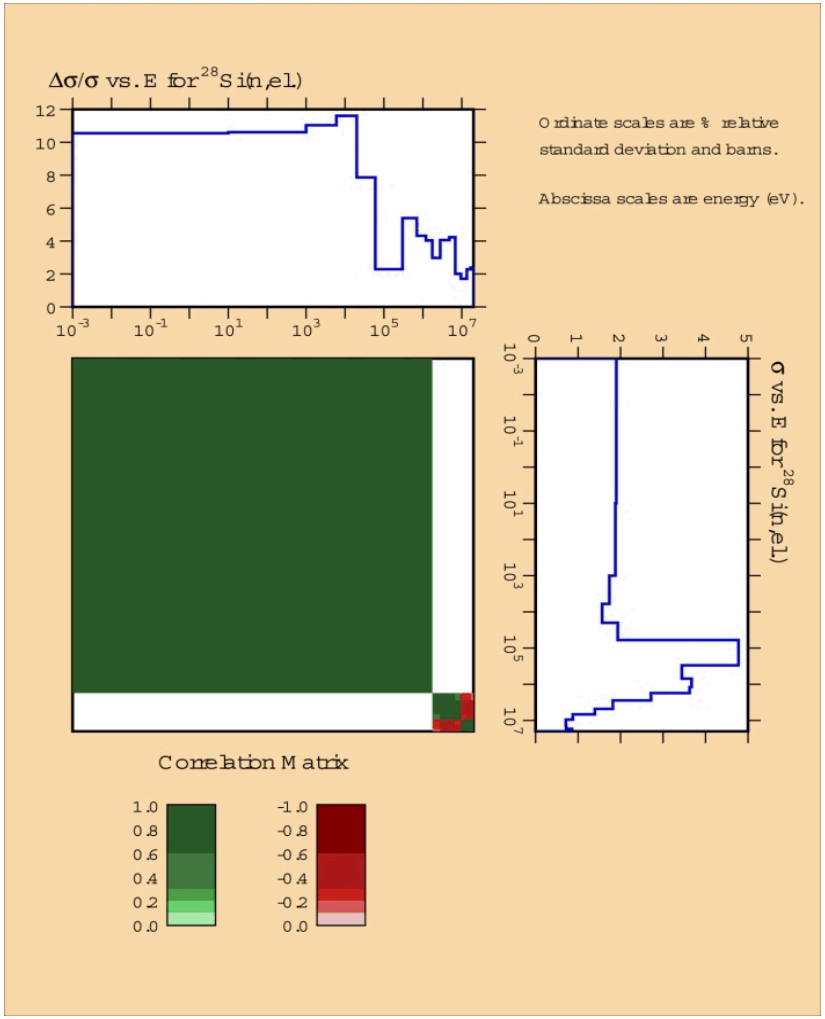


ENDF/B-VII.1

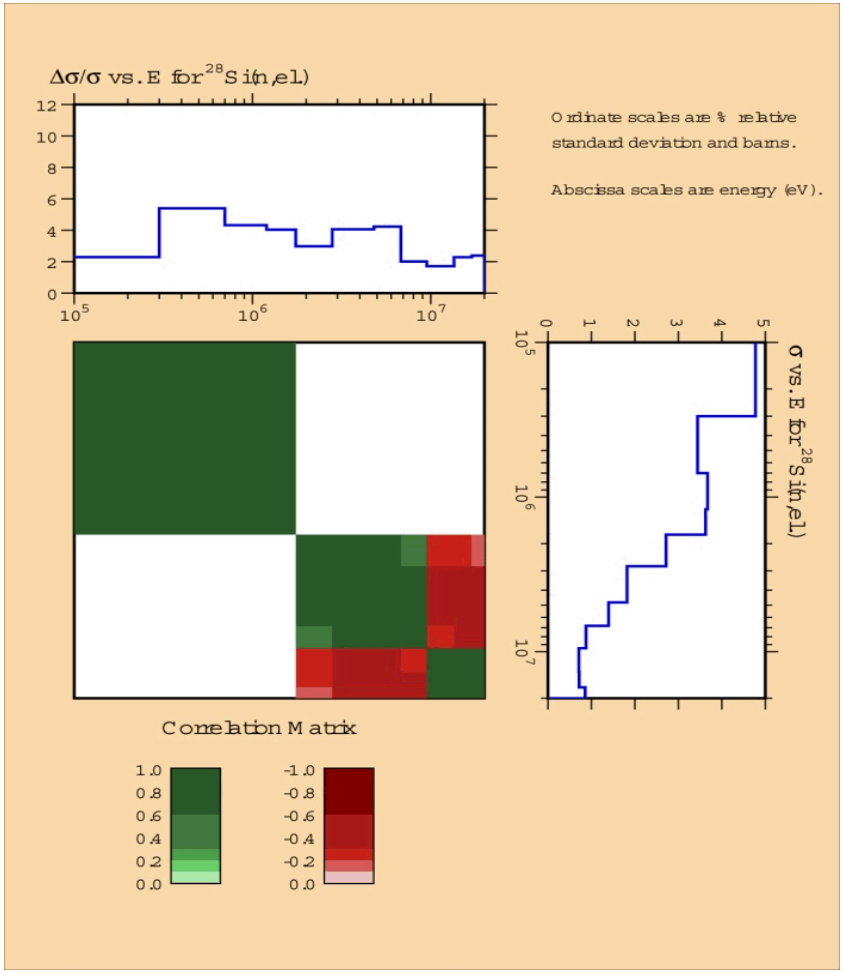


TENDL

Uncertainty/Variation in TENDL Elastic Cross Sections

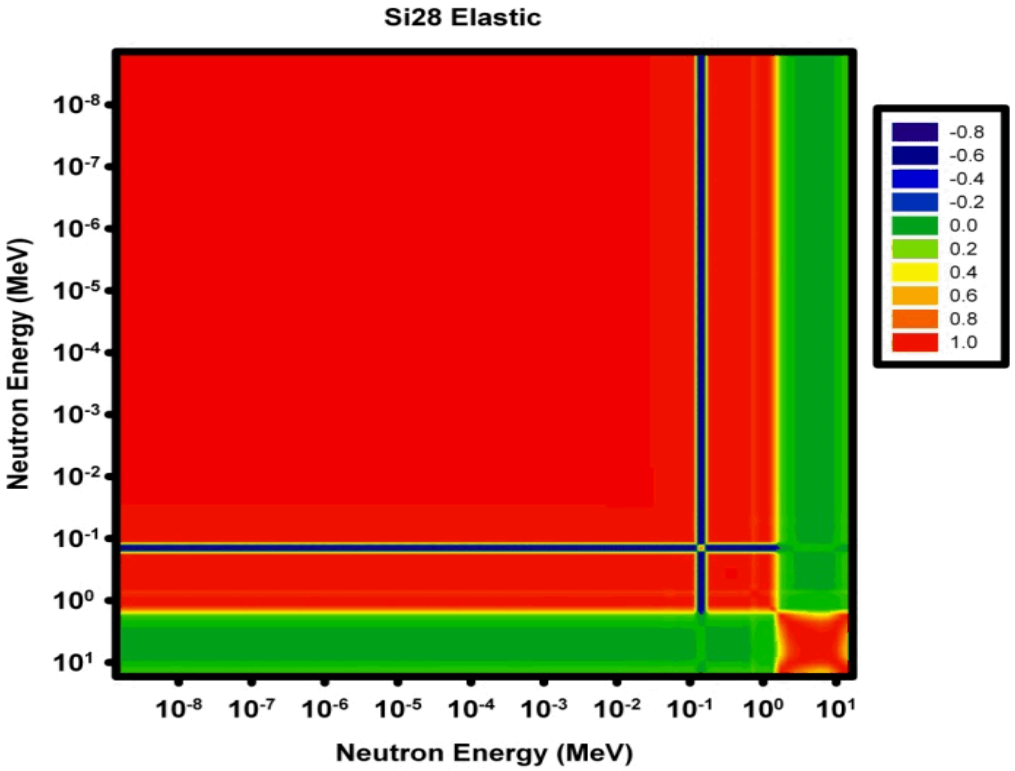


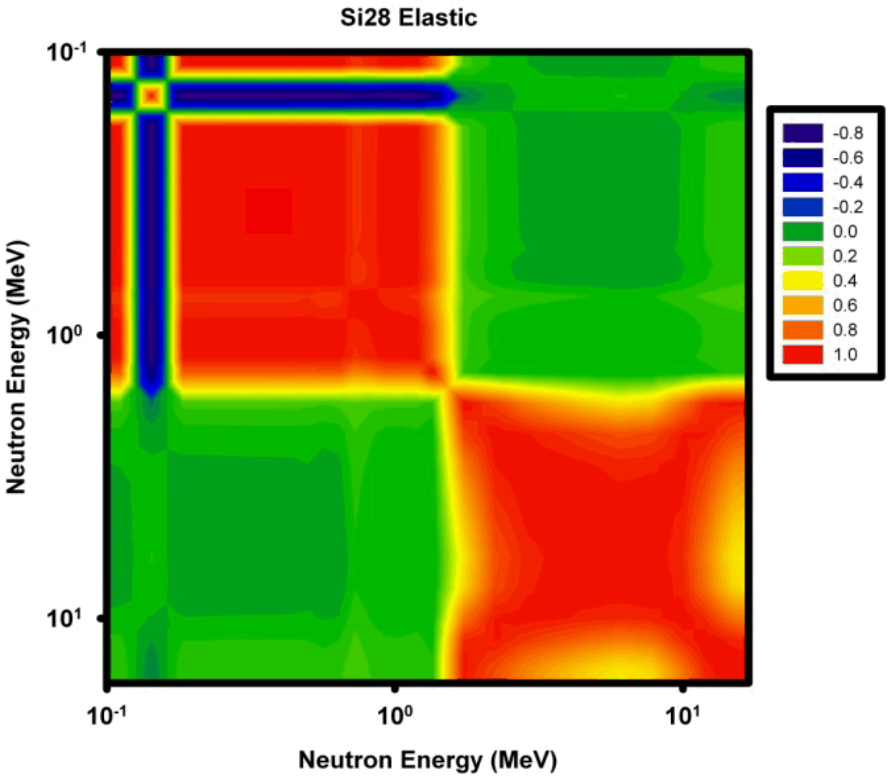
Wide Energy Range



High Energy range

Uncertainty/Variation in TENDL TMC Elastic Cross Sections



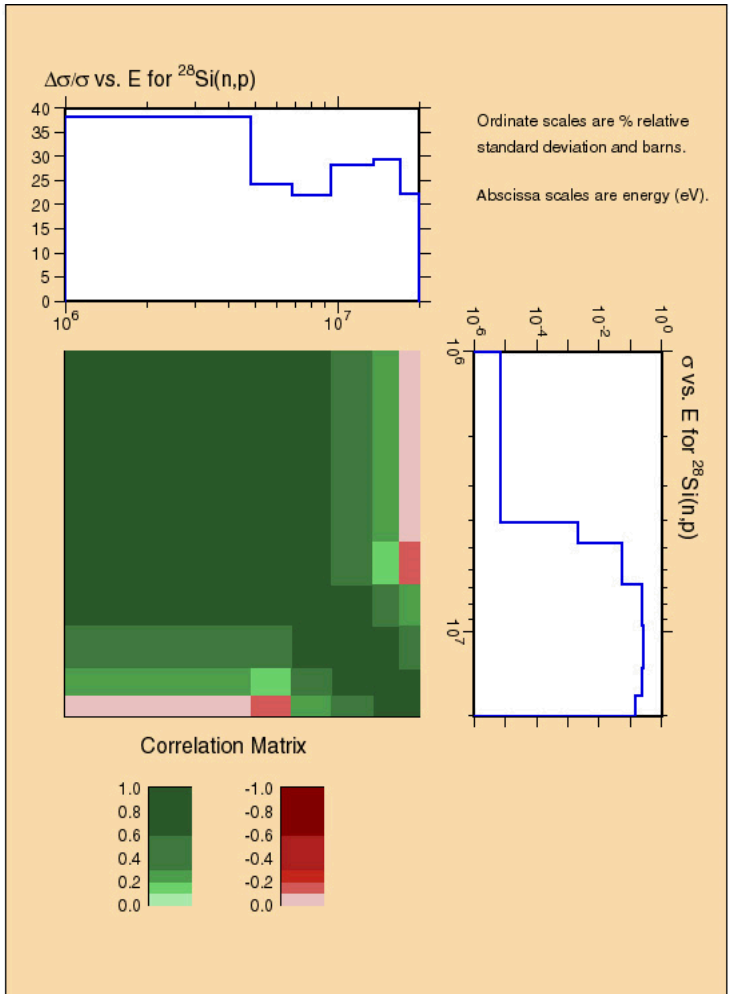


Wide Energy Range

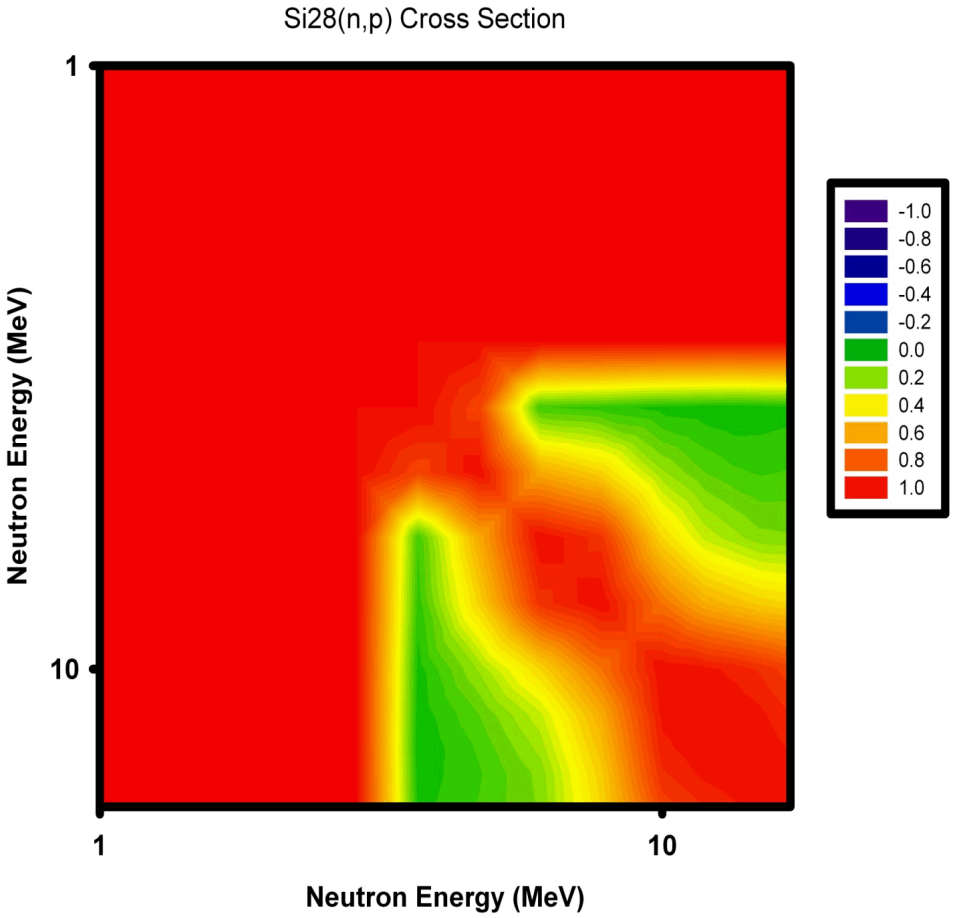
High Energy range

Narrow uncorrelated region probably due to 89-group energy structure and resonance strucutres.

Uncertainty/Variation in TENDL (n,p) Cross Sections

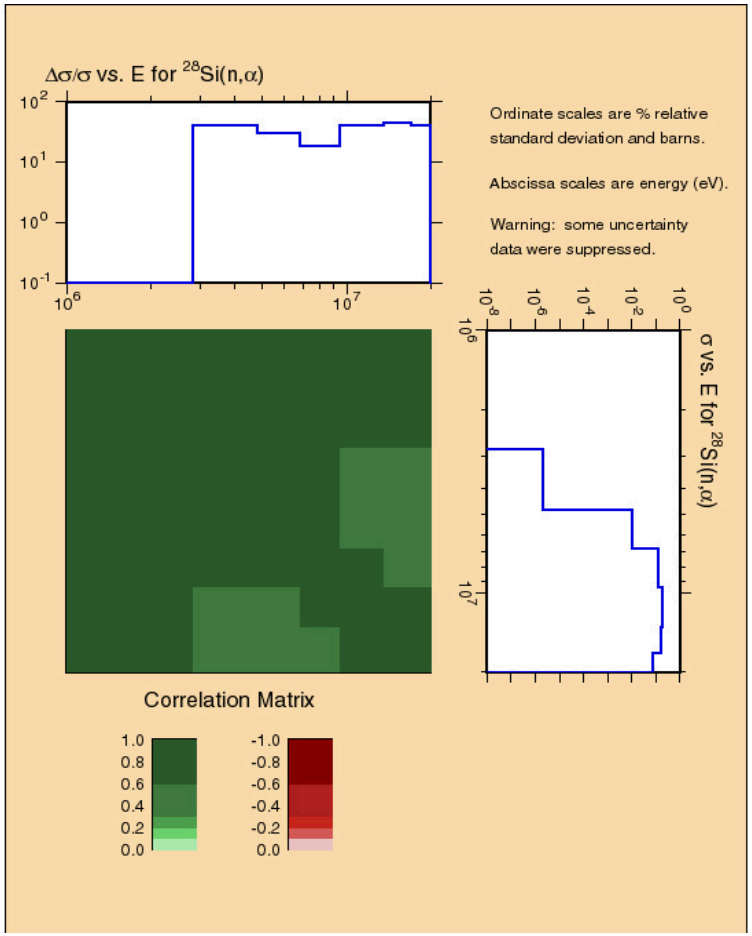


TENDL-2013

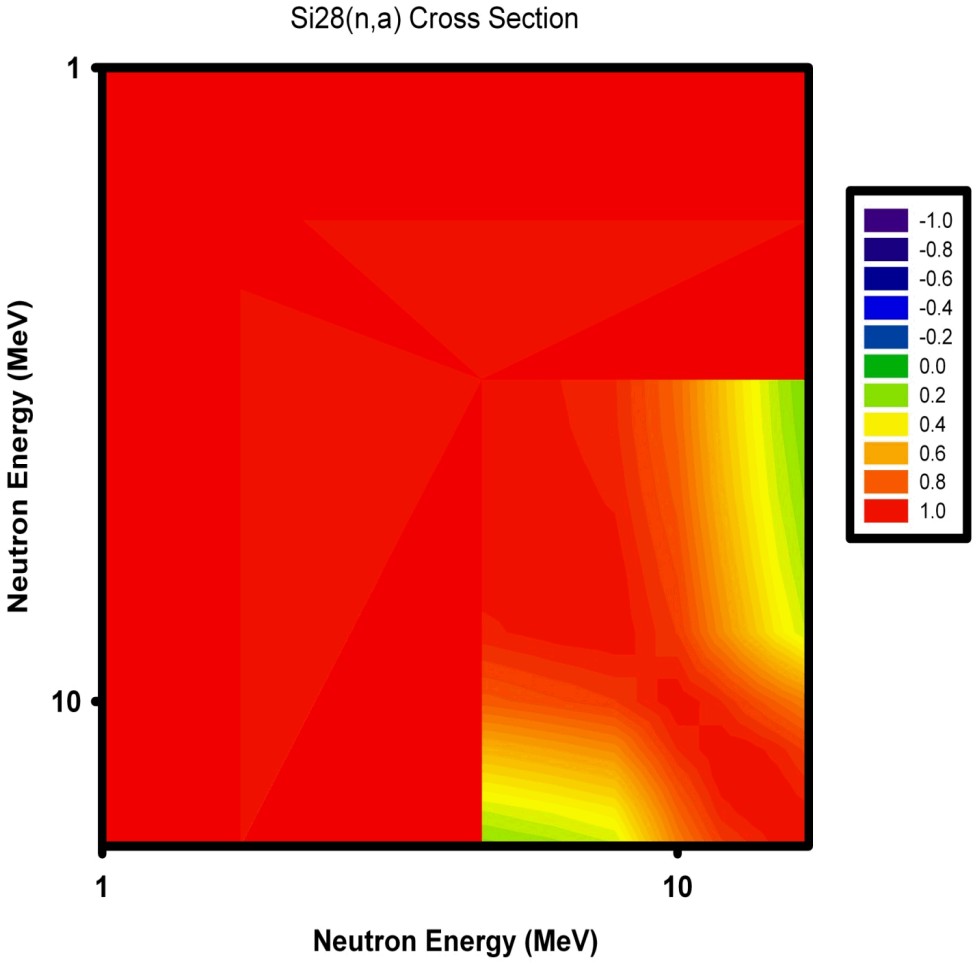


TENDL TMC

Uncertainty/Variation in TENDL (n,α) Cross Sections

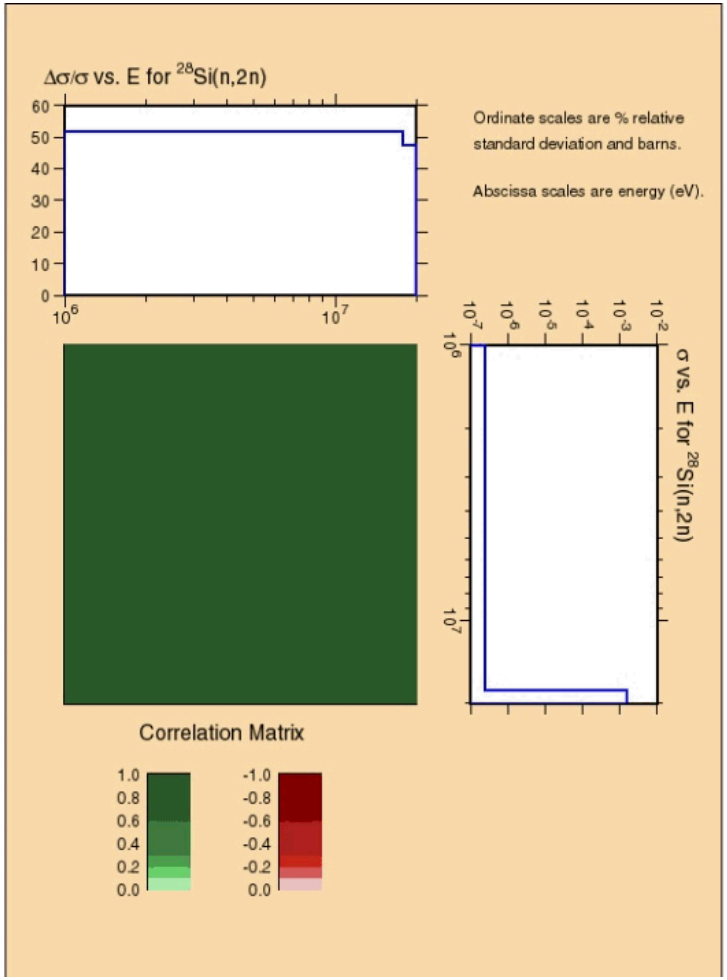


TENDL-2013

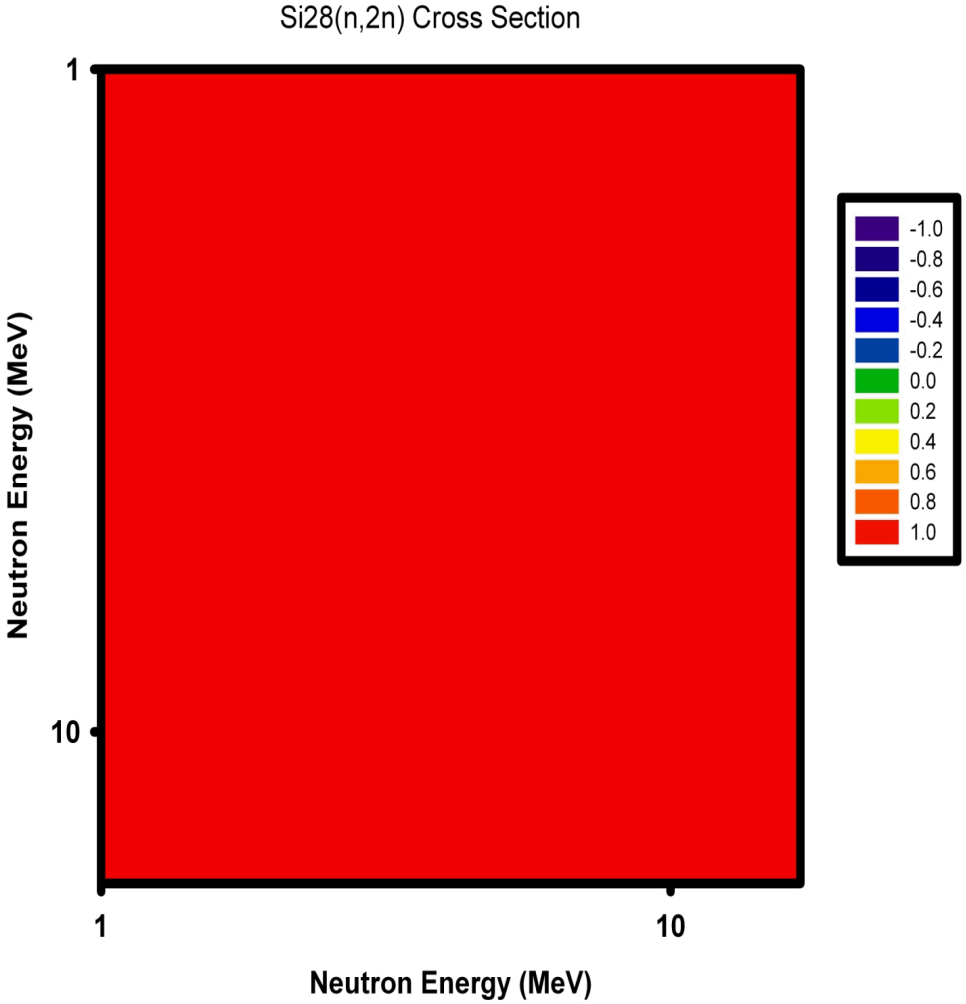


TENDL TMC

Uncertainty/Variation in TENDL (n,2n) Cross Sections

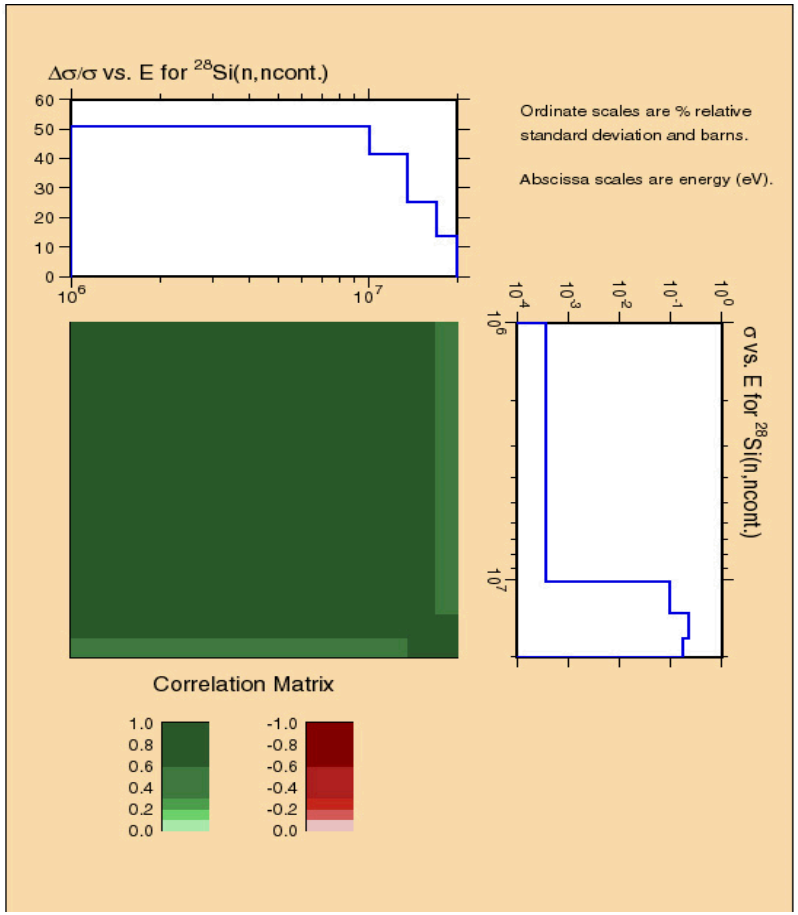


TENDL-2013

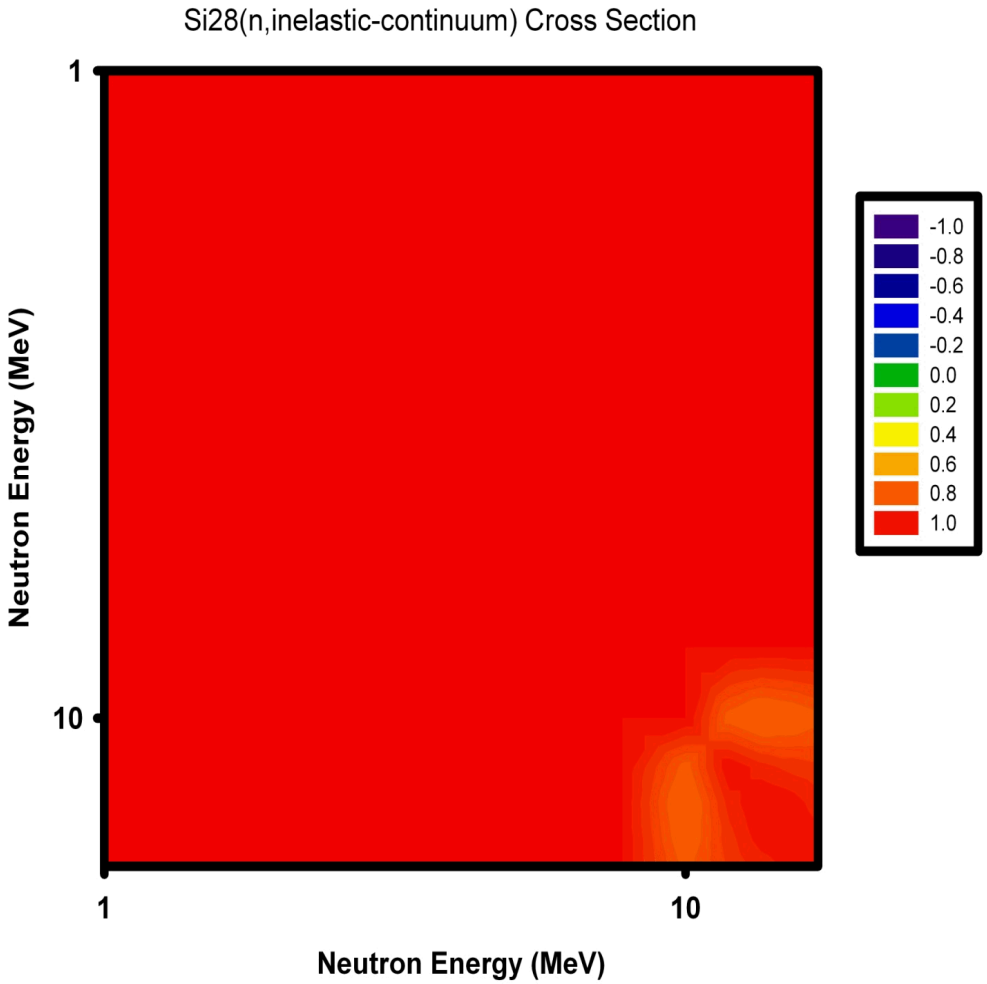


TENDL TMC

Cross Section Uncertainty/Variation for TENDL (n,n'-continuum)

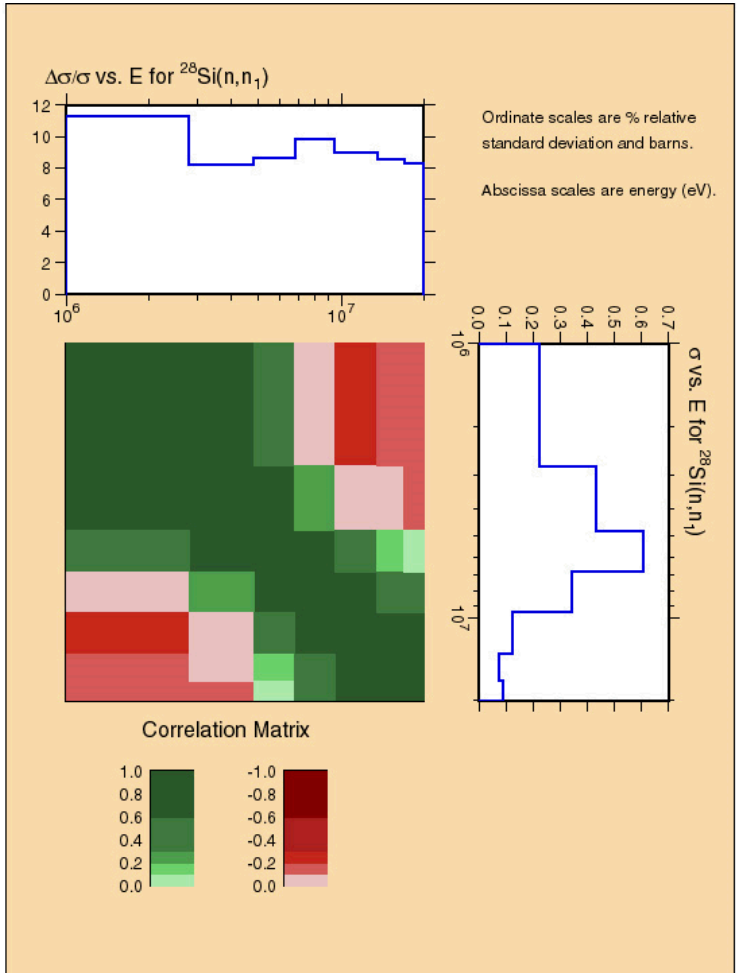


TENDL-2013

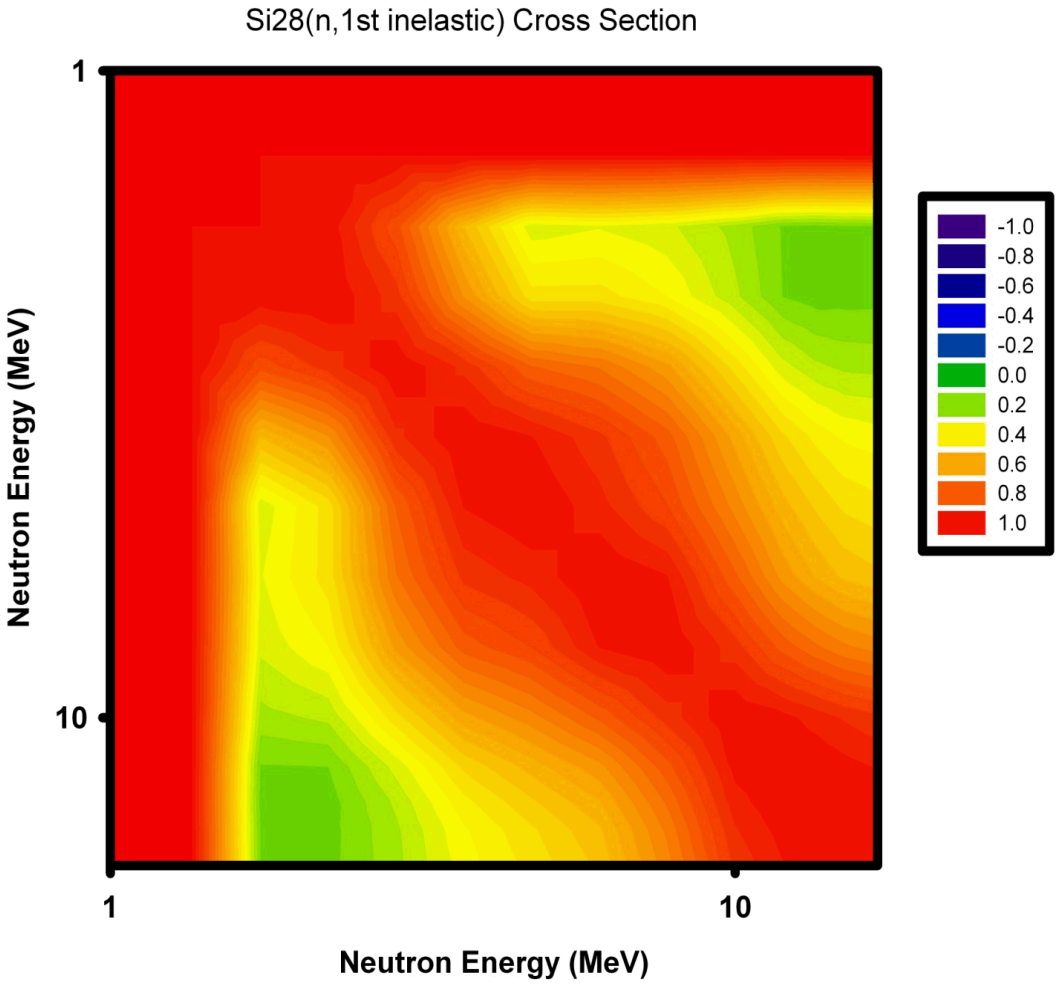


TENDL TMC

Cross Section Uncertainty/Variation for TENDL (n,1stn')



TENDL-2013

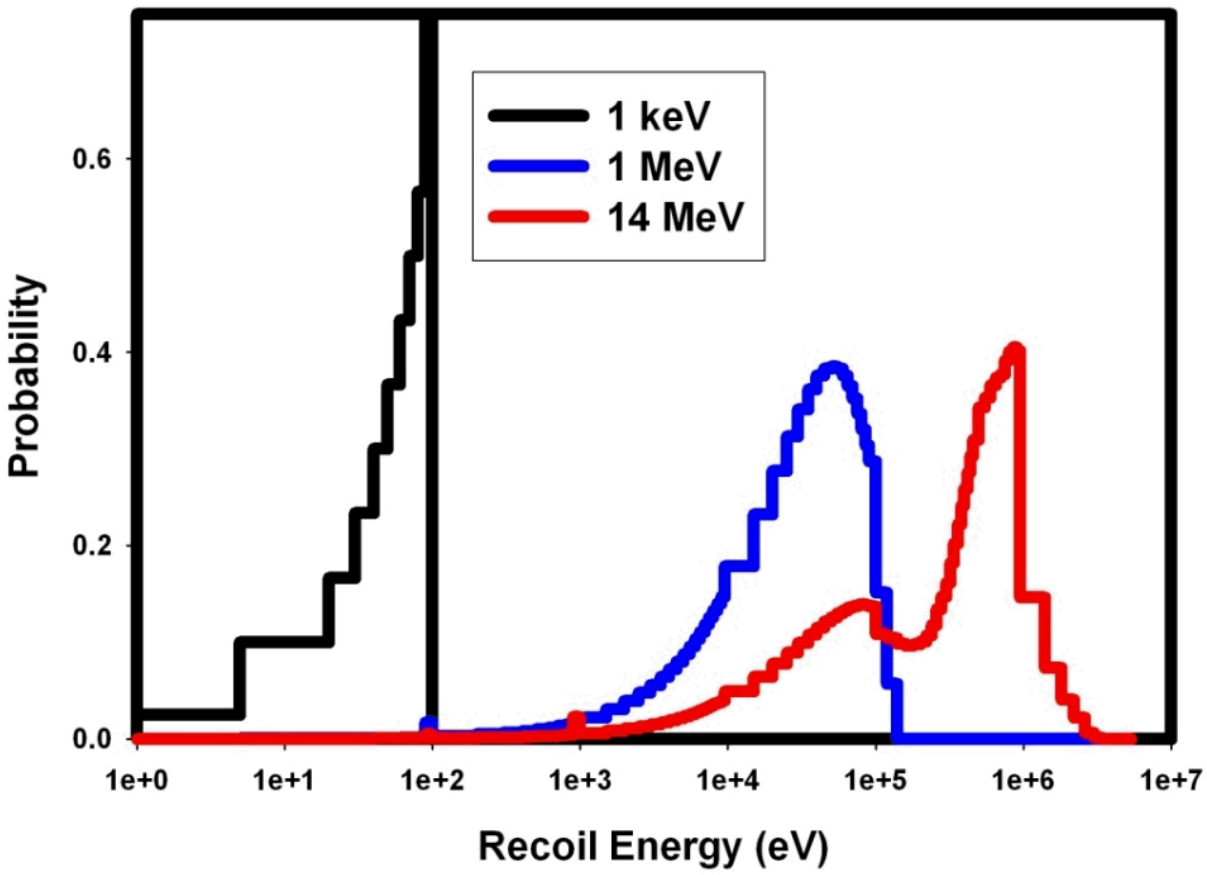


TENDL TMC

Neutron Spectra → Composite Recoil Spectra

Mono-energetic Neutron

Max. recoil ion energy for elastic reactions



Silicon recoil with EMPIRE module

Alternate Silicon Recoil Spectra Models

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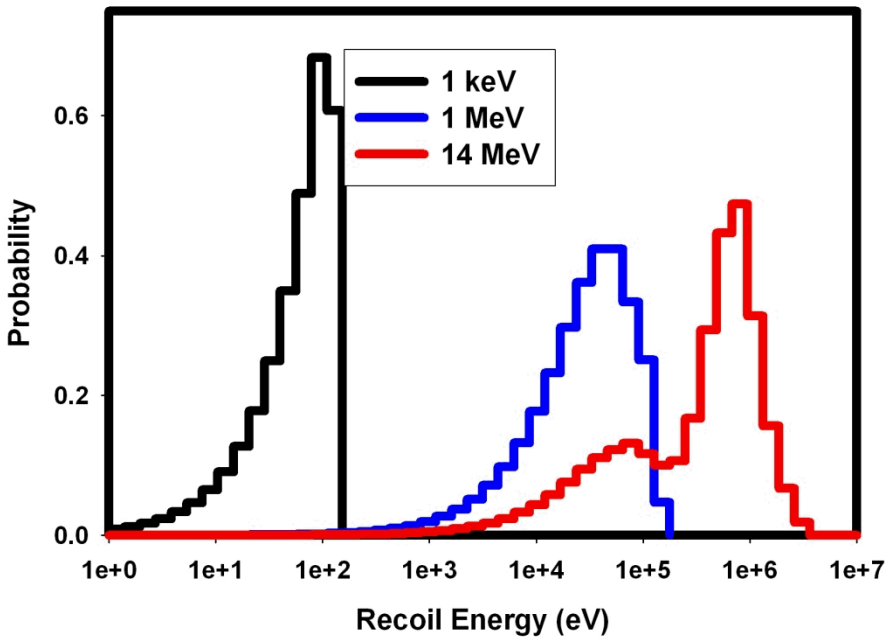
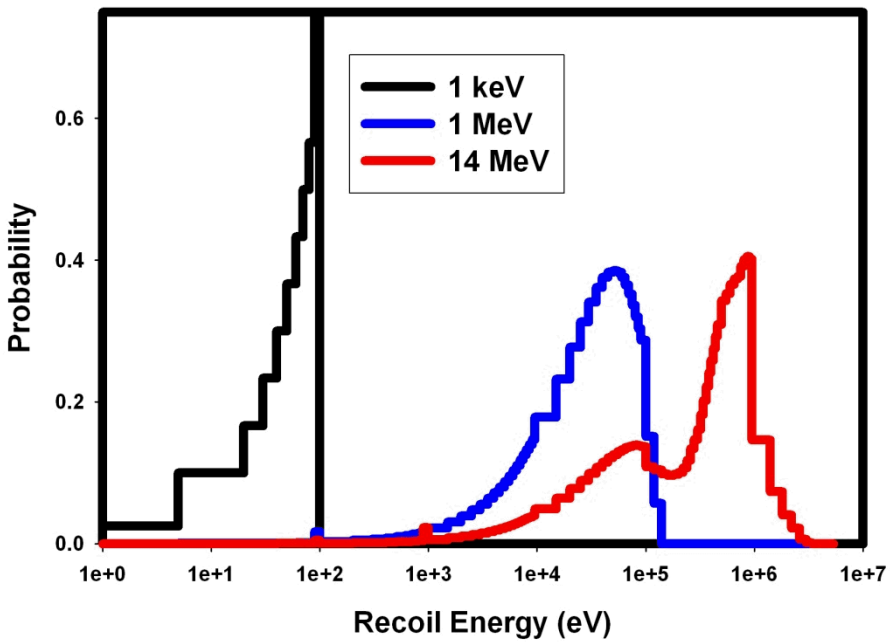
EMPIRE module



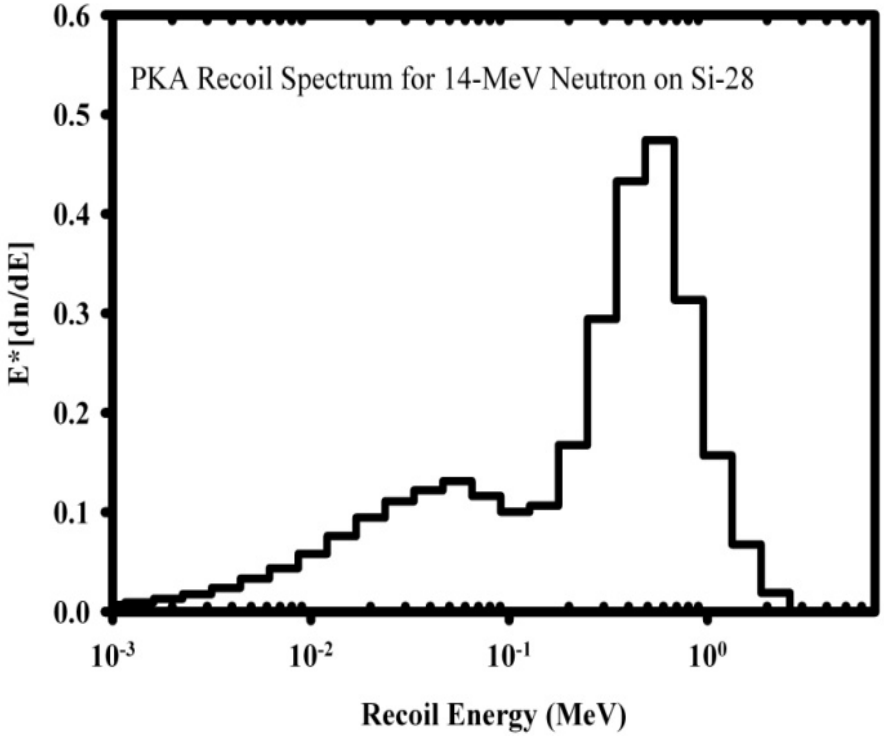
$\langle E \rangle_{1\text{-kev}}$ = 70 eV
$\langle E \rangle_{1\text{-Mev}}$ = 41 keV
$\langle E \rangle_{14\text{-Mev}}$ = 569 keV + 5.58 MeV α

SPECTER module

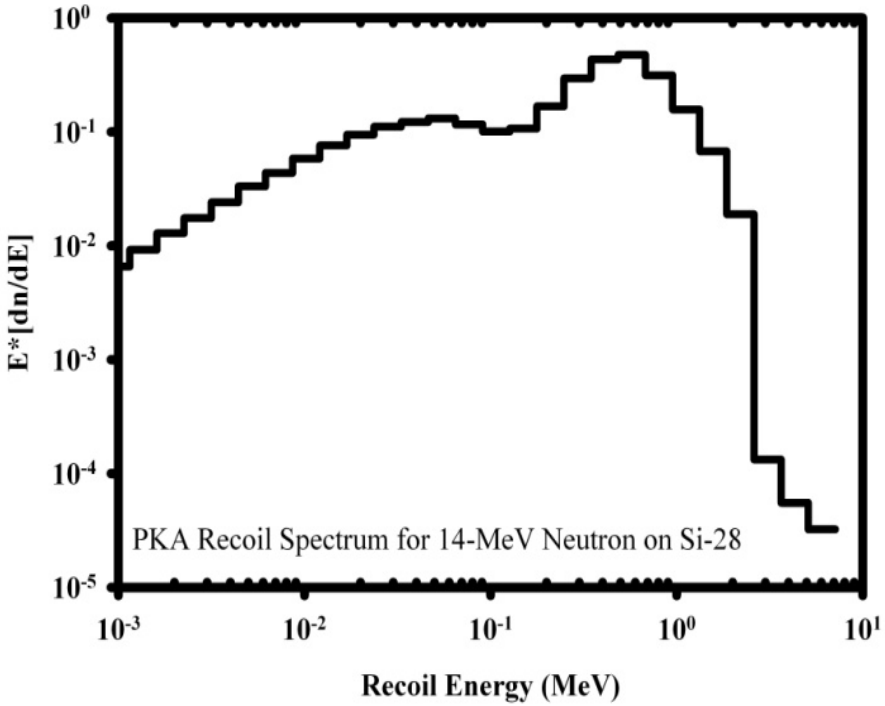


$\langle E \rangle_{1\text{-kev}}$ = 59 eV
$\langle E \rangle_{1\text{-Mev}}$ = 39 keV
$\langle E \rangle_{14\text{-Mev}}$ = 490 keV

PKA Recoil Spectrum: 14-MeV Neutron on ^{28}Si

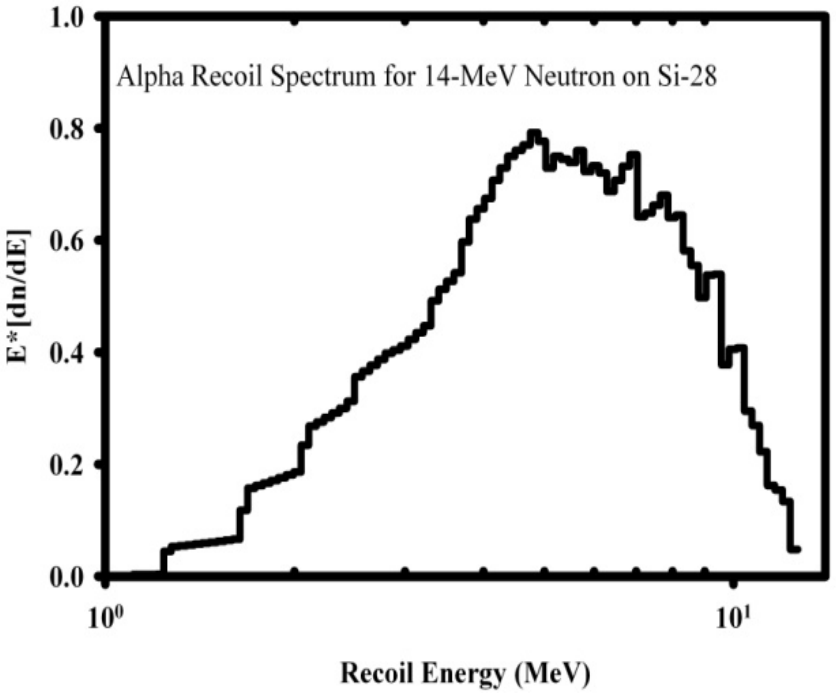


E*dn/dE Lethergy Plot

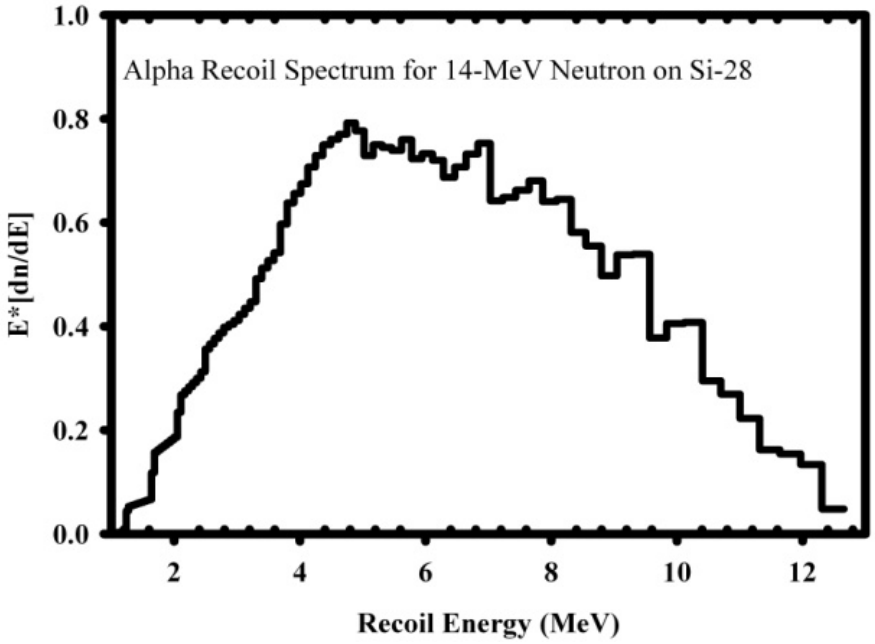


E*dn/dE Logarithmic Plot

Alpha Recoil Spectrum: 14-MeV Neutron on ^{28}Si

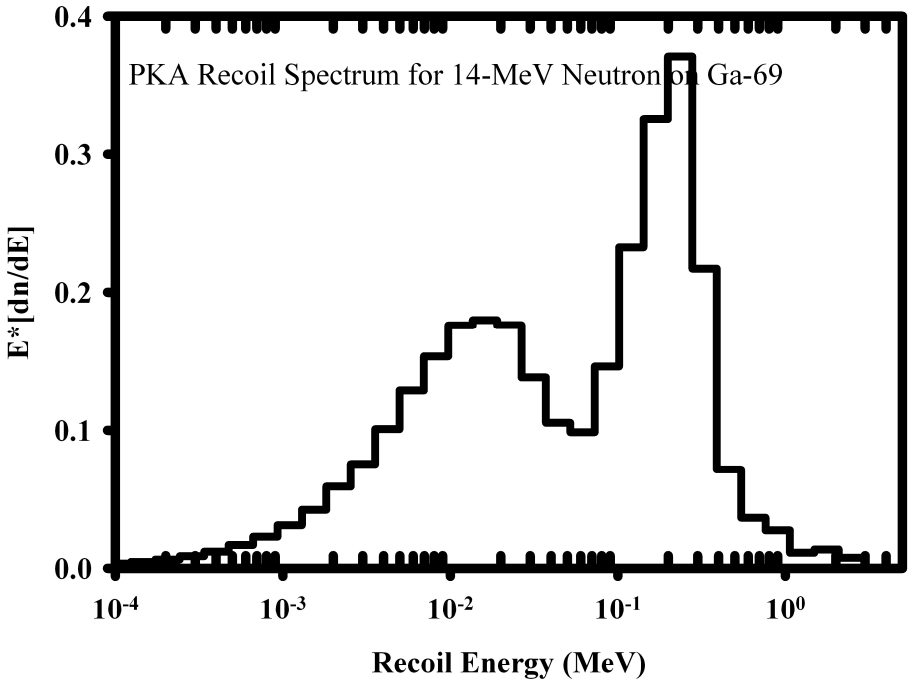


E*dn/dE Lethergy Plot

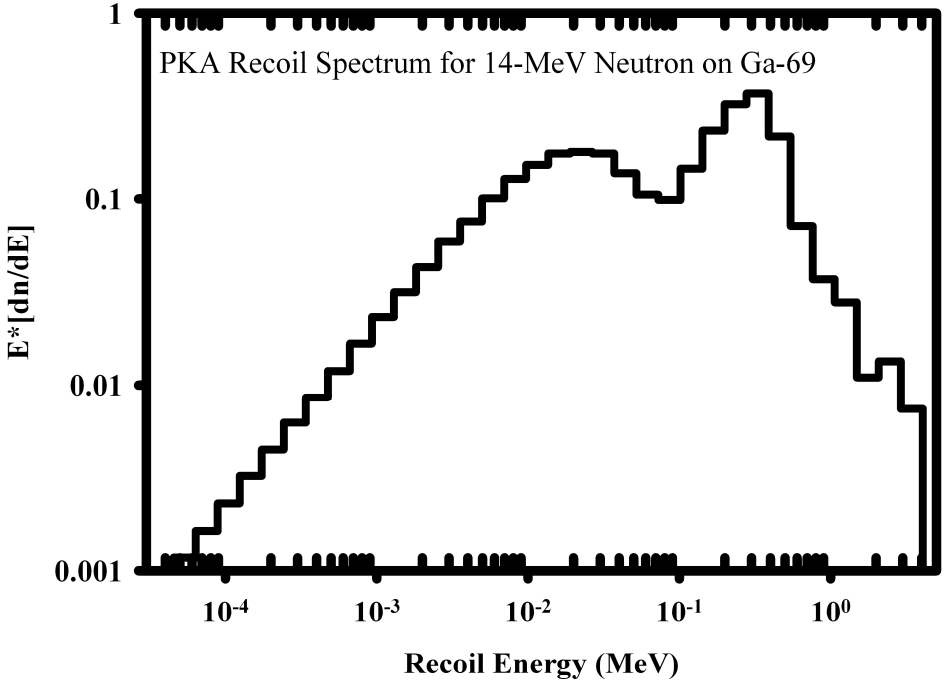


E*dn/dE Linear Plot

PKA Recoil Spectrum: 14-MeV Neutron on ^{69}Ga

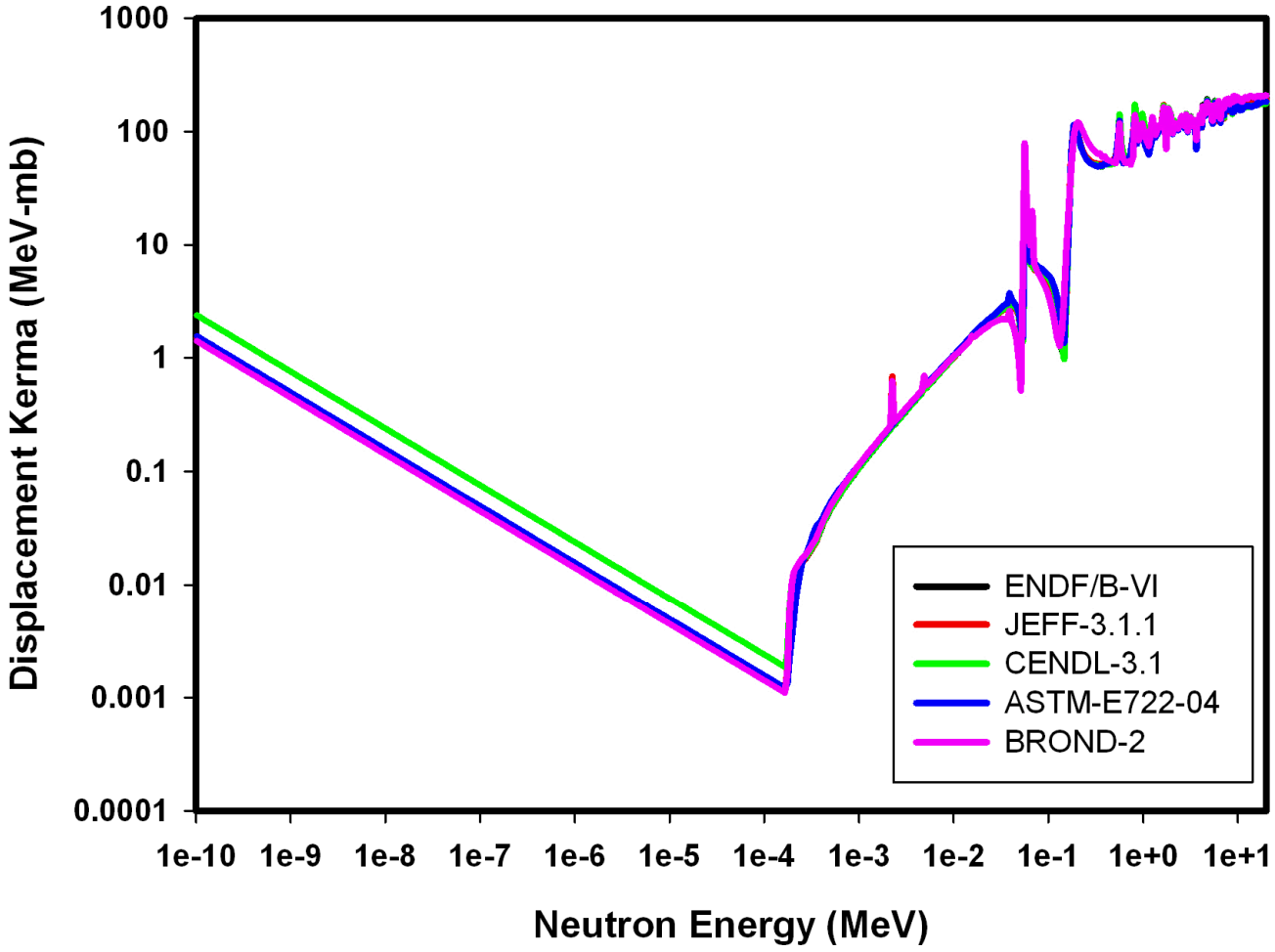


E*dn/dE Lethergy Plot

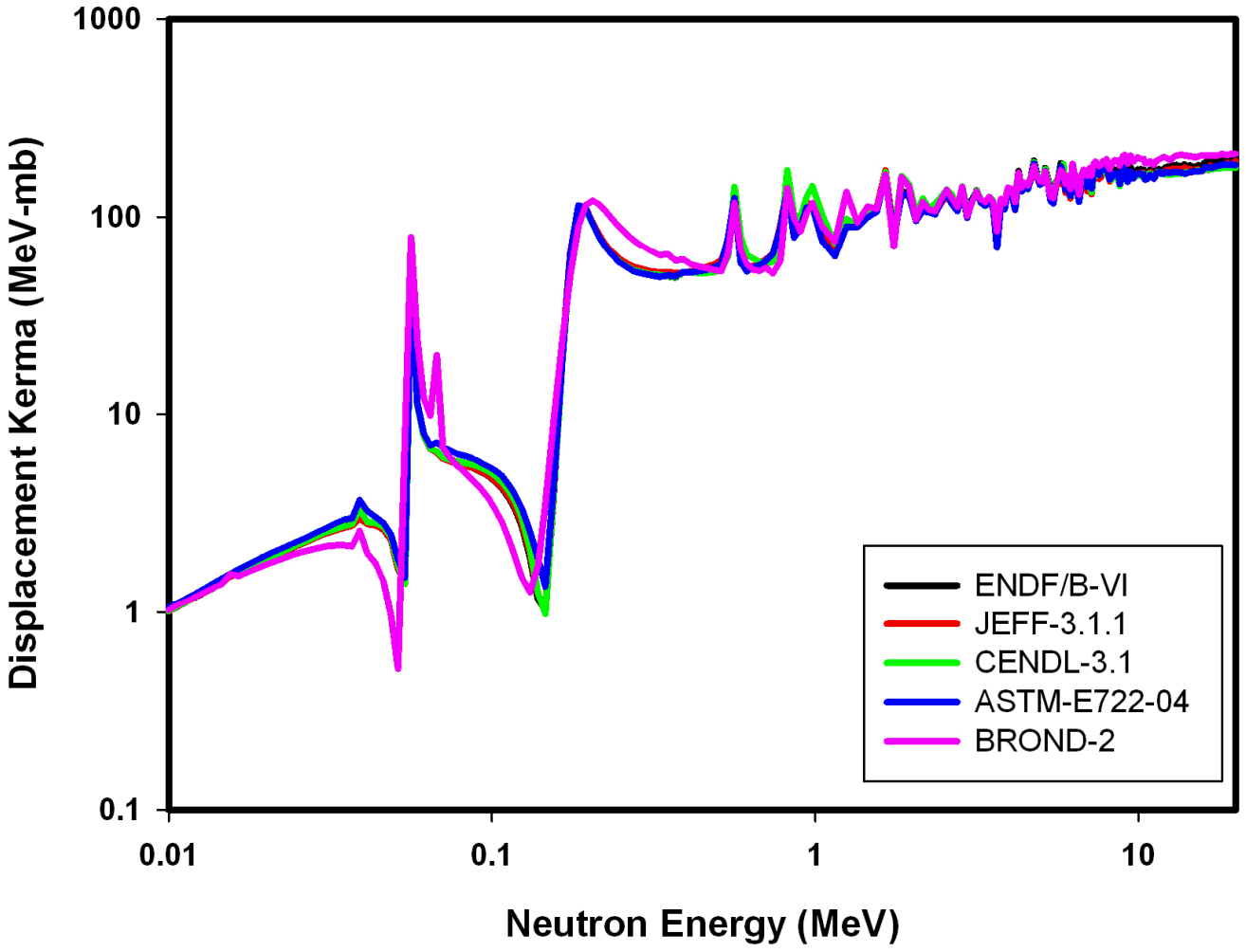


E*dn/dE Logarithmic Plot

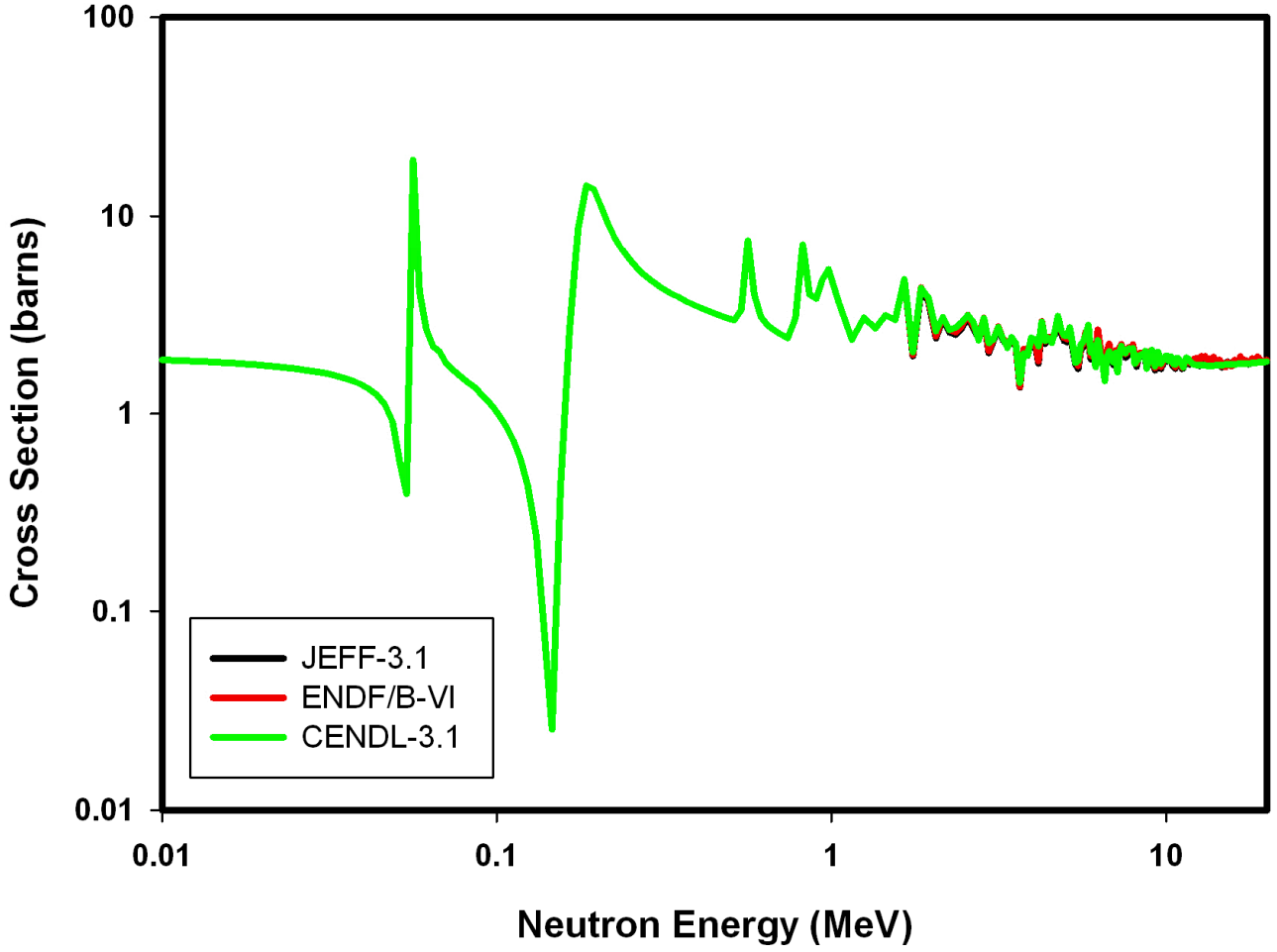
Comparisons of ^{nat}Si Damage Energy: ENDF/B-VI, JEFF-3.1.1, CENDL-3.1, BROND-2



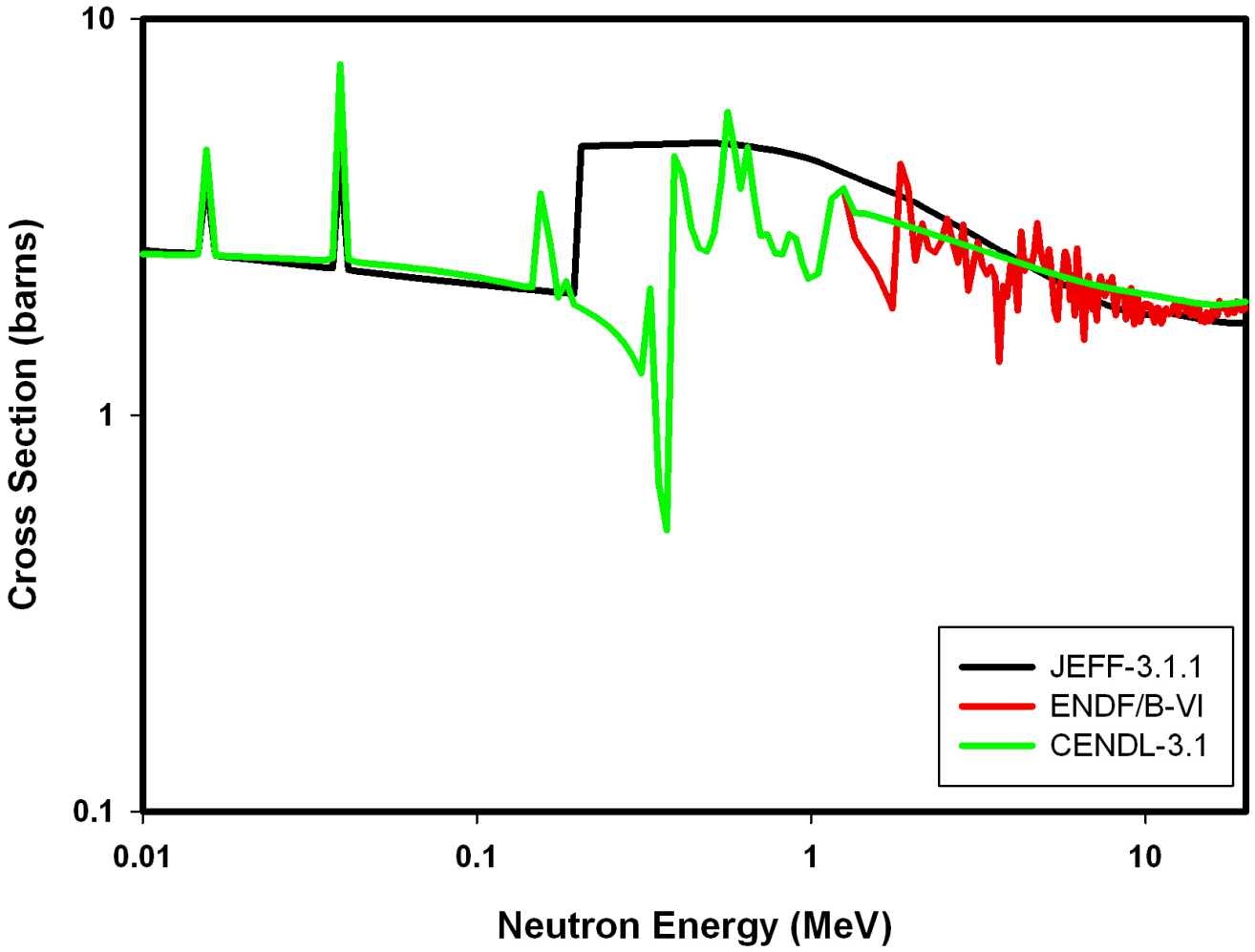
Comparisons of ^{nat}Si Displacement Kerma: ENDF/B-VI, JEFF-3.1.1, CENDL-3.1, BROND-2



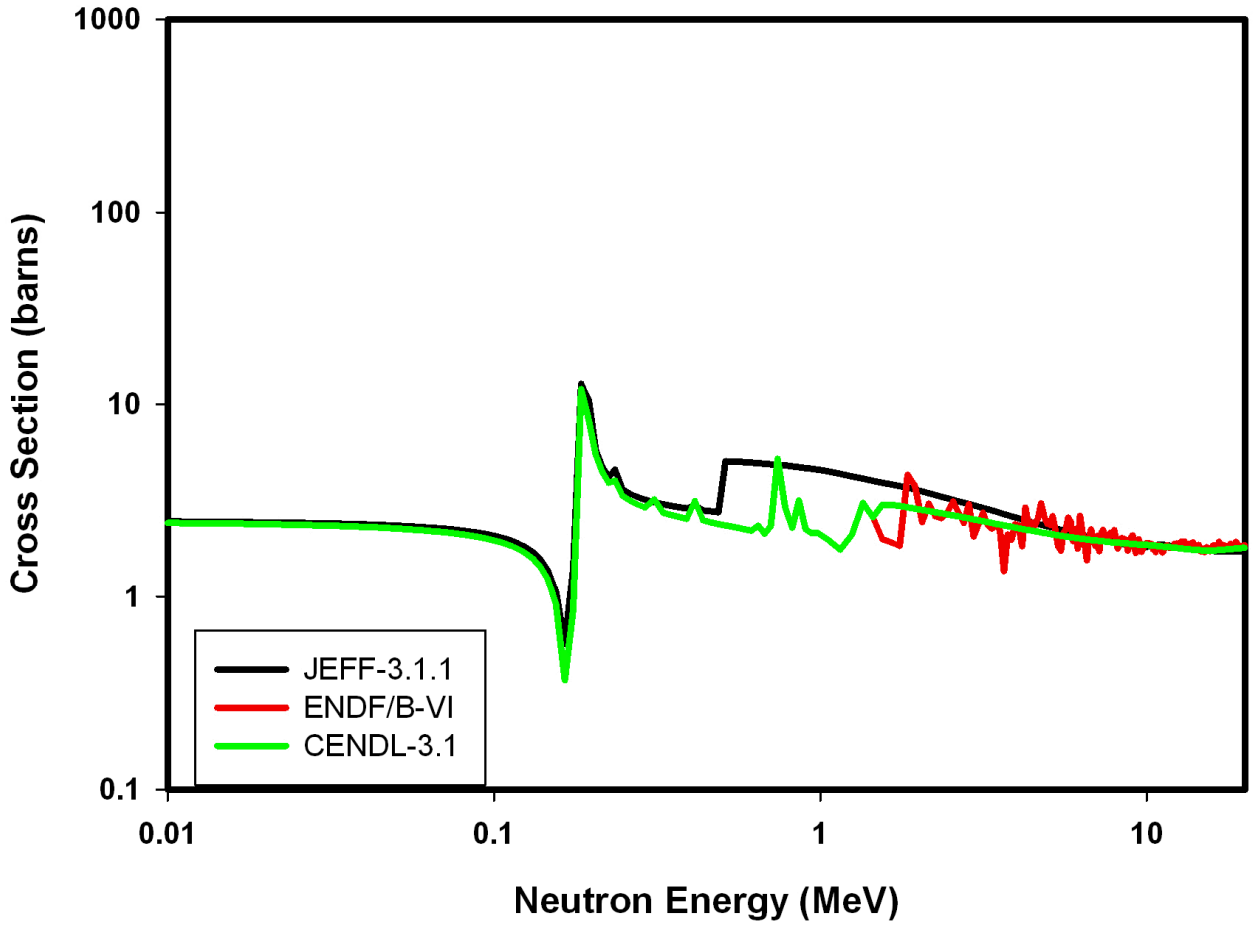
The good agreement is not a surprise since the total cross section for ^{28}Si is in agreement in data-driven evaluations.



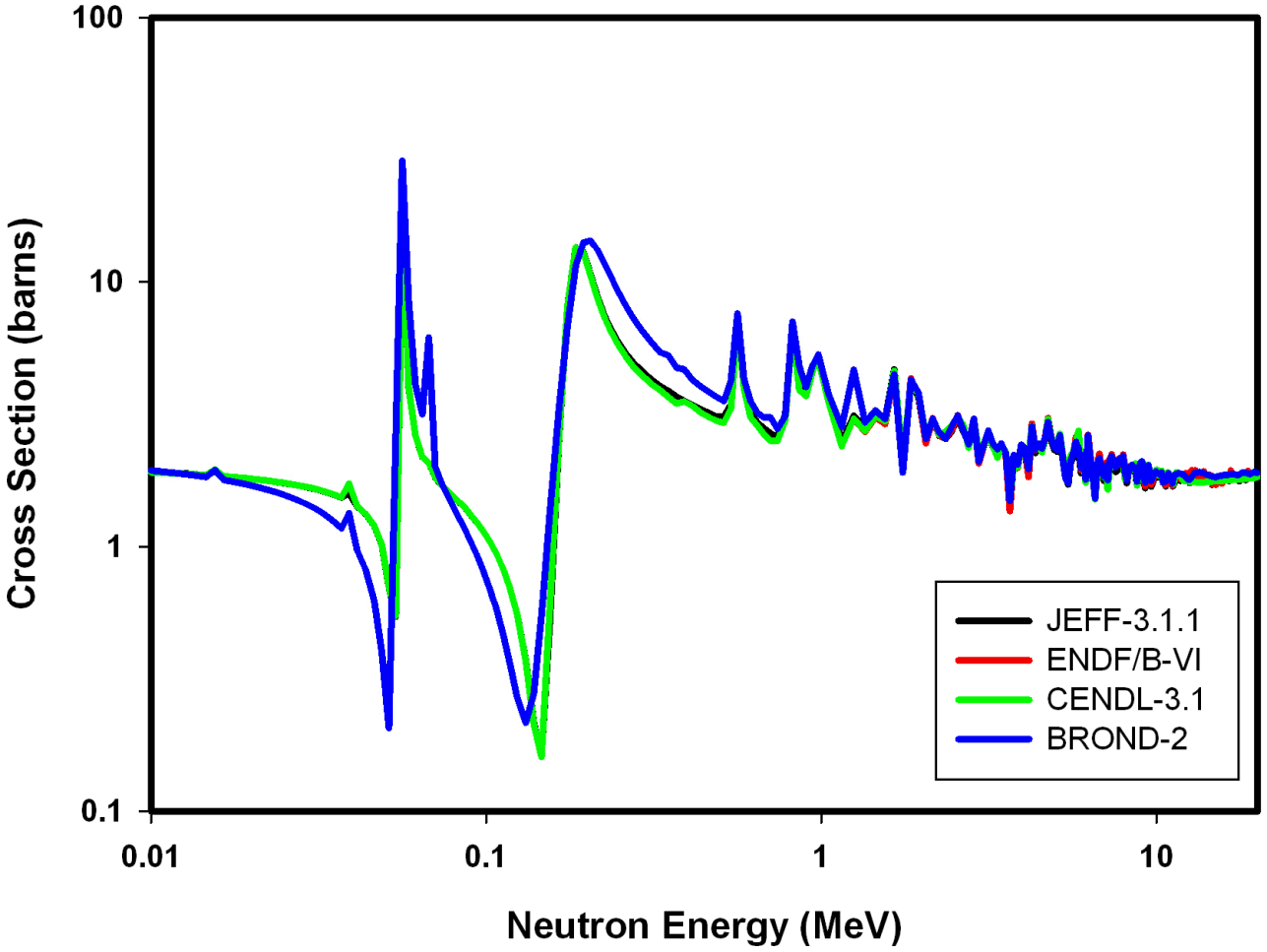
There is more variation in the ^{29}Si total cross section



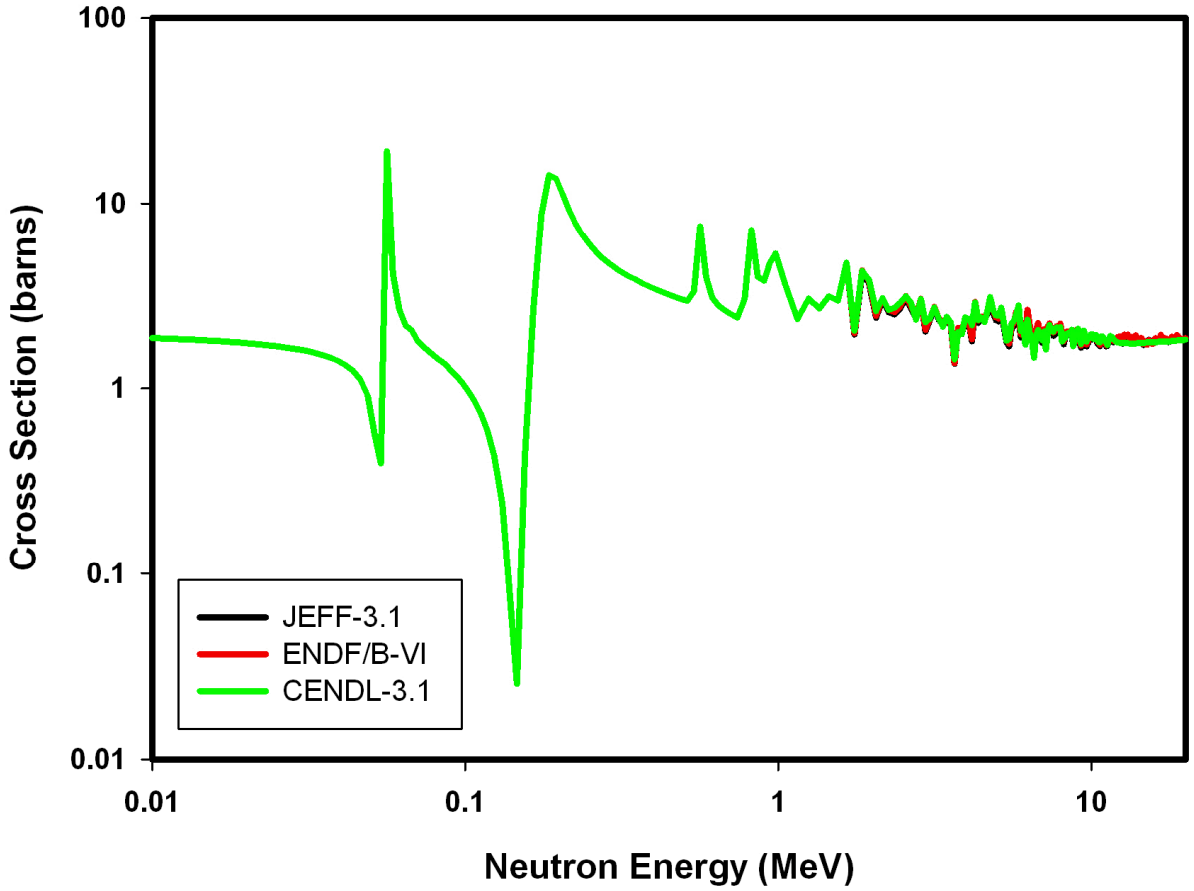
Similar agreement for ^{30}Si total cross section



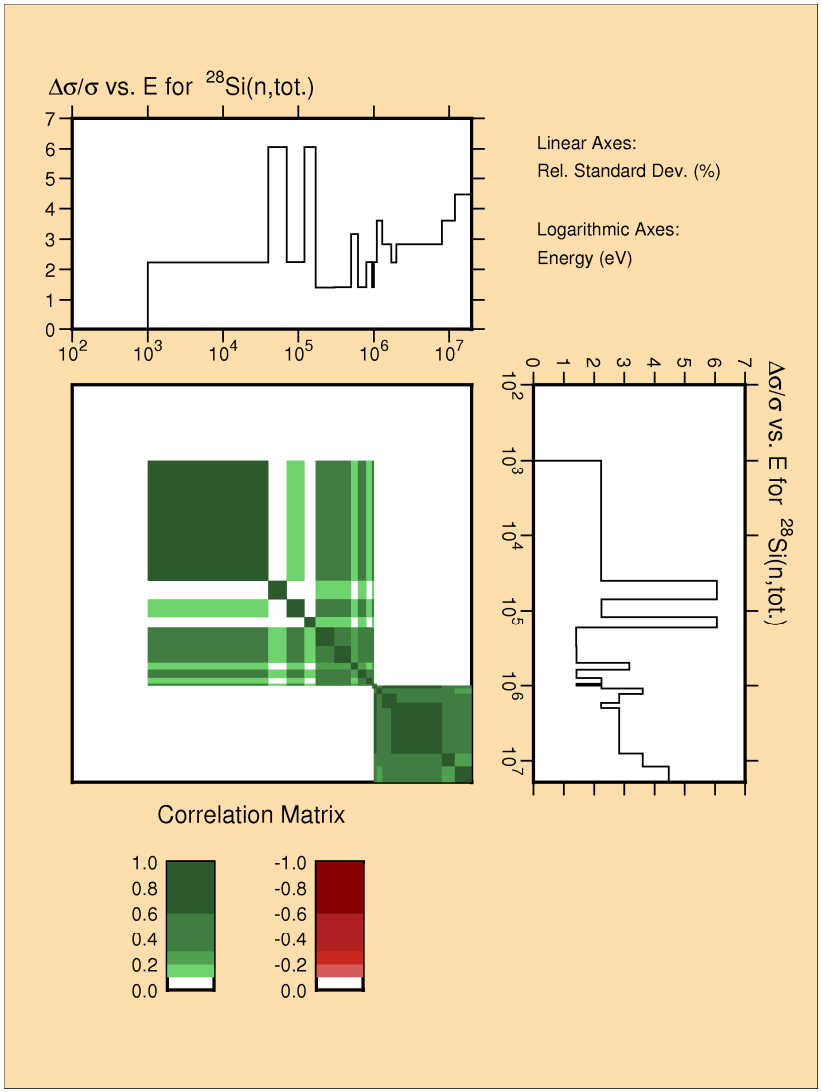
Want about the agreement for ^{nat}Si total cross section?

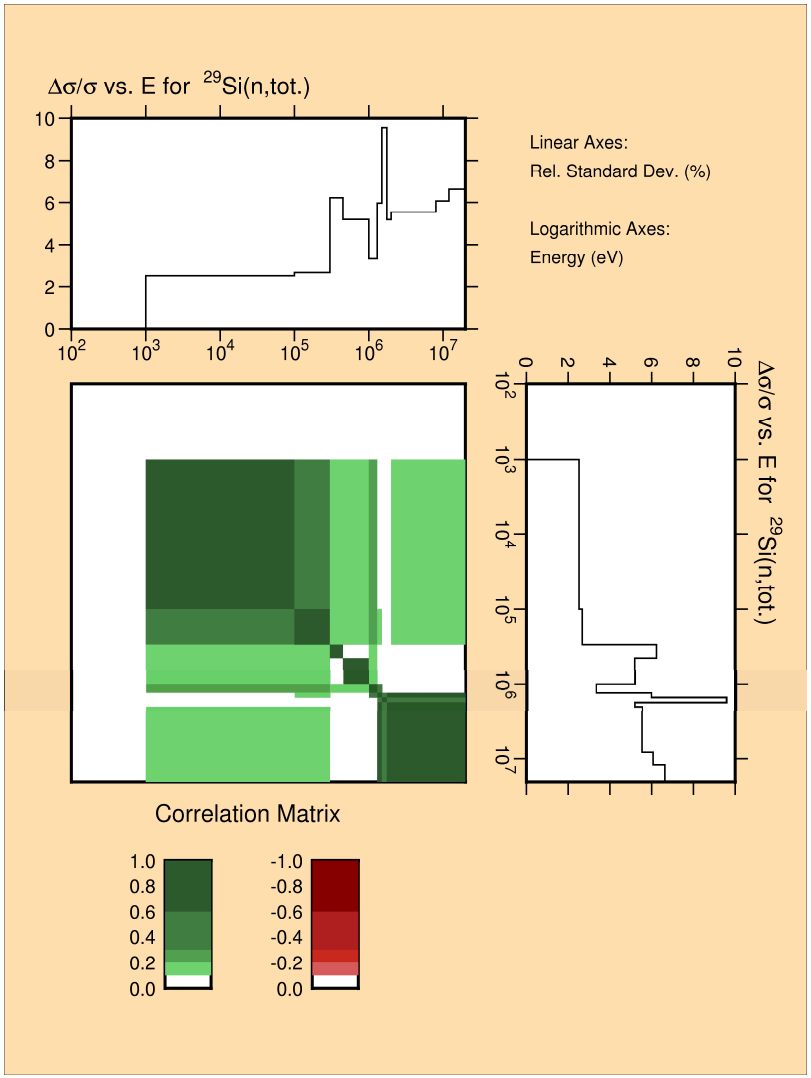


This good agreement is not a surprise since the total cross sections are also in good agreement

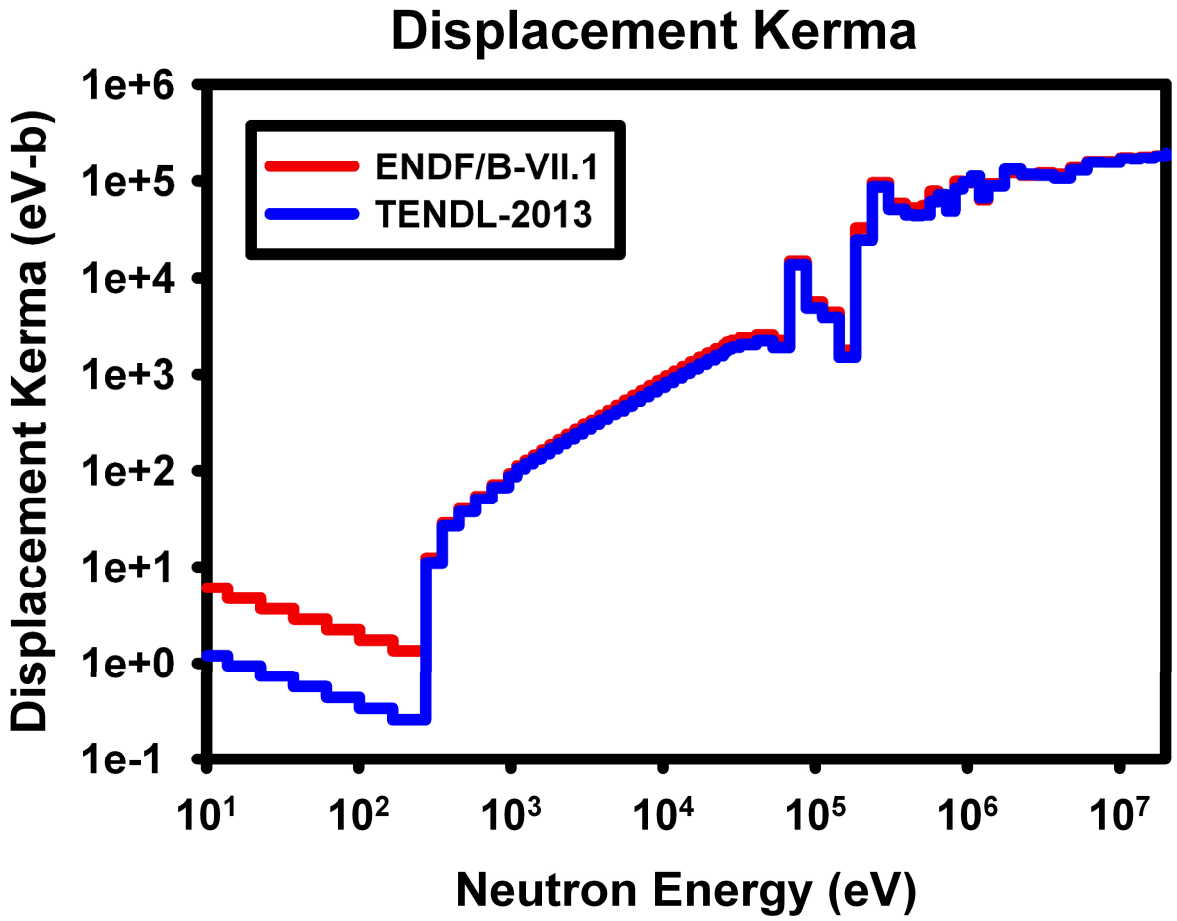


ENDF/B-VI ^{28}Si and ^{29}Si Correlation Matrix

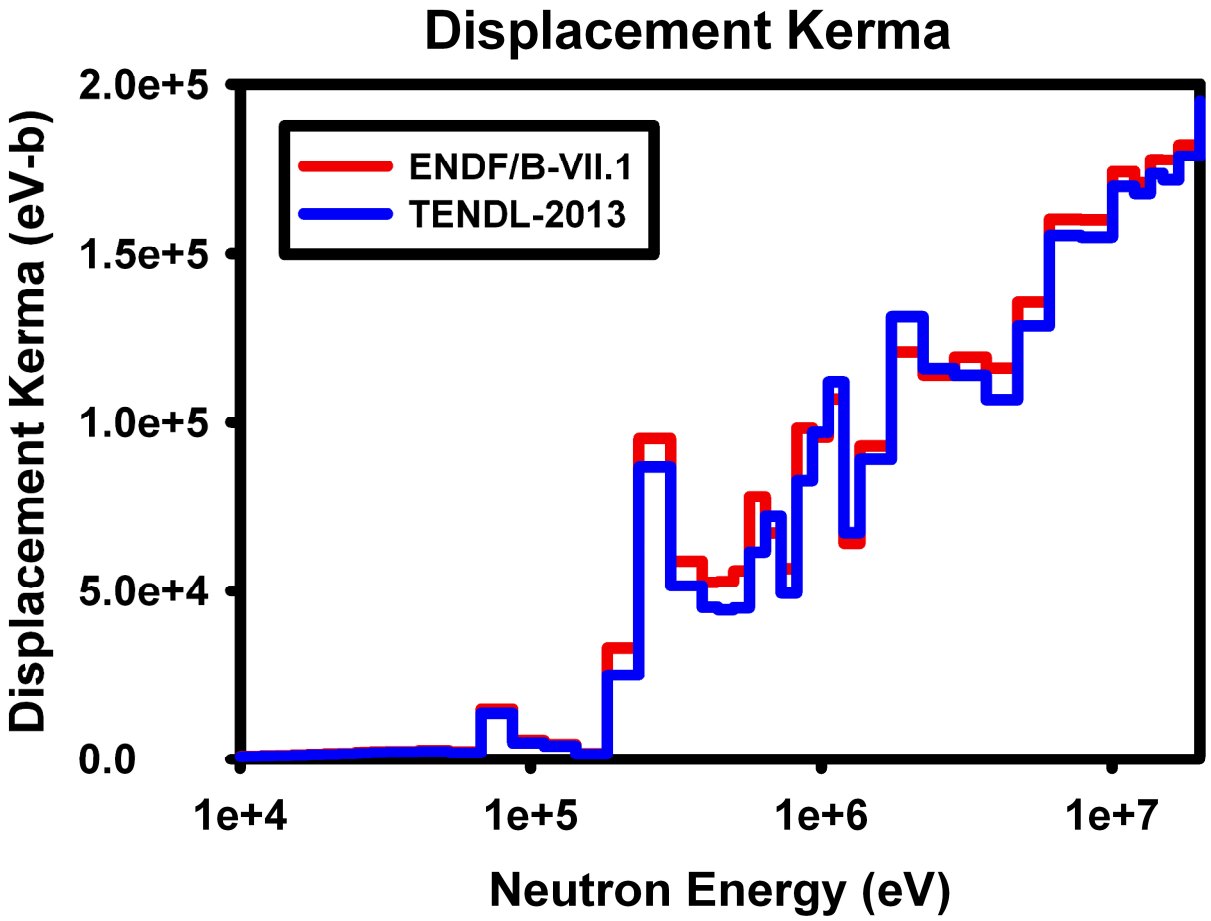




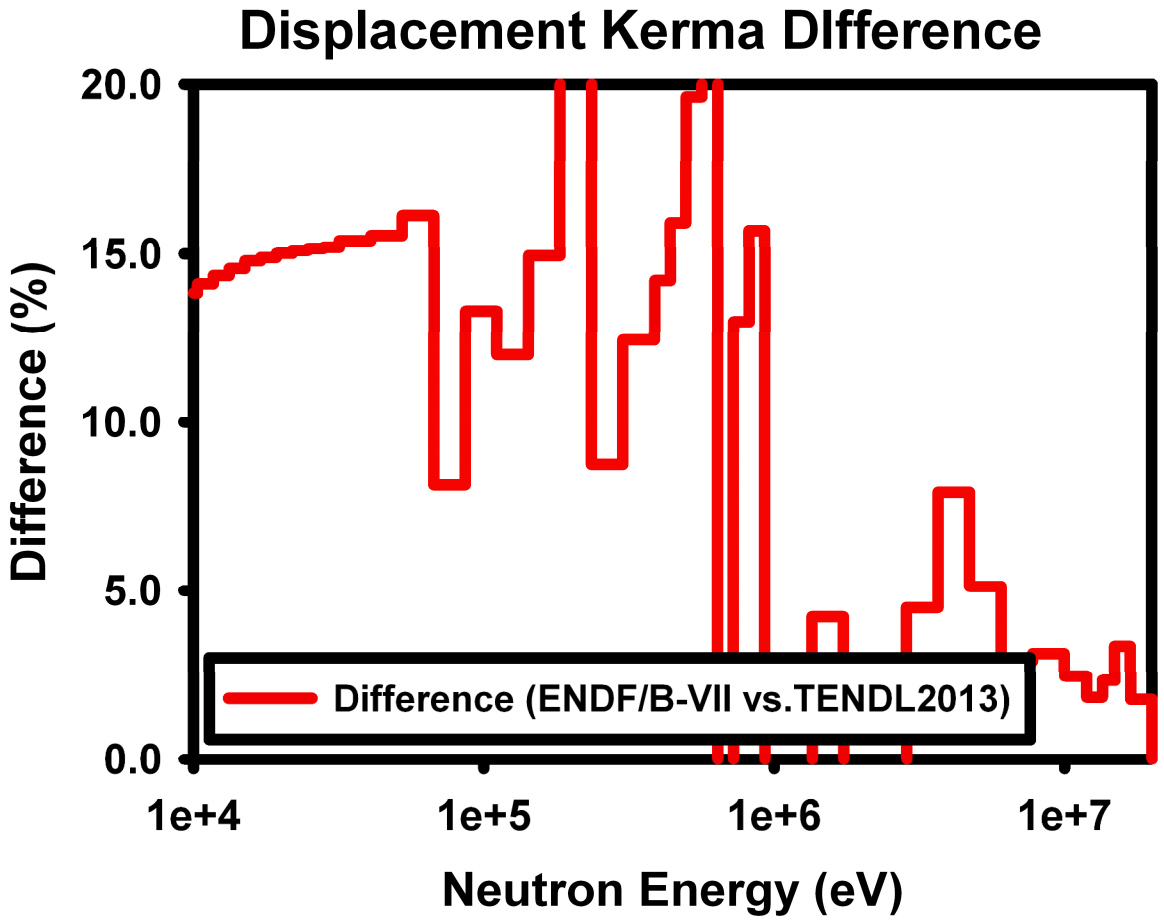
89-group Comparison of Total Displacement Kerma



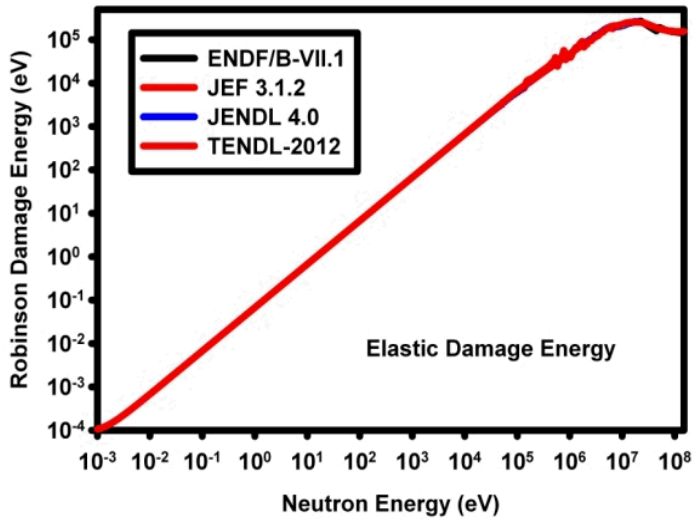
89-group Comparison of Total Displacement Kerma



89-group Comparison of Difference in the Total Displacement Kerma (TENDL-2013 vs. ENDF/B-VII.1



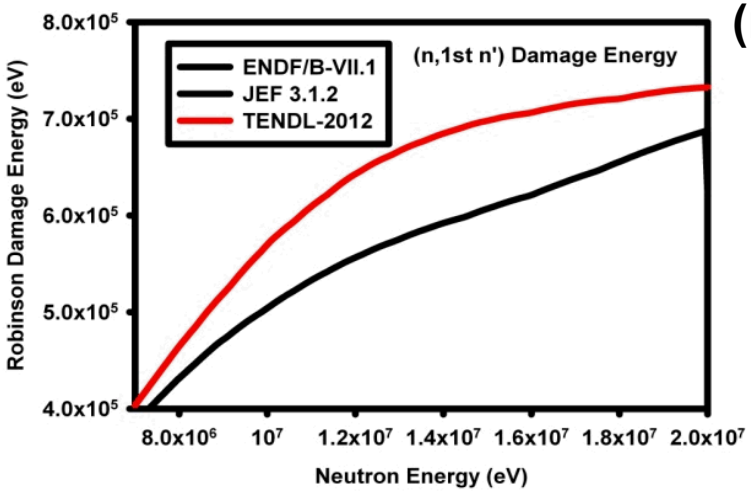
Uncertainty/Variation in Robinson Displacement Energy



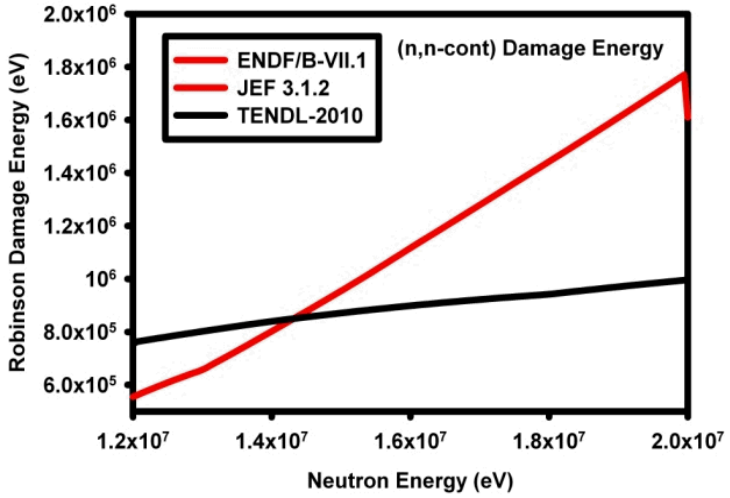
Elastic

Elastic and discrete inelastic damage energies are in good agreement. Continuum inelastic varies and is correlated in energy.

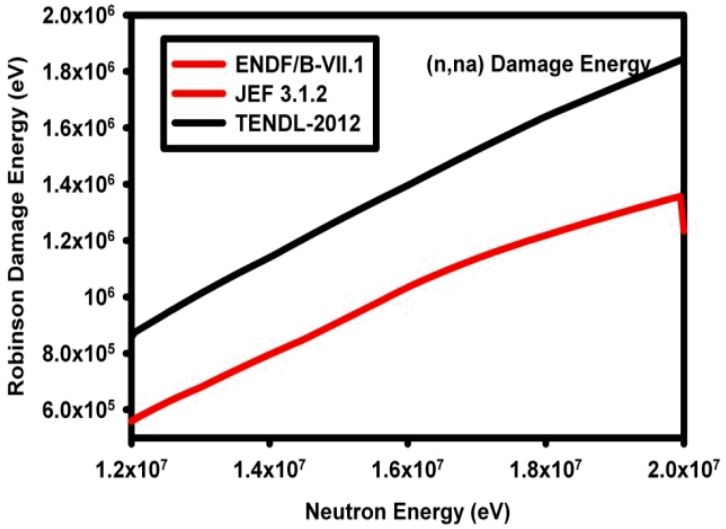
(n,1st n')



(n,n'-continuum)

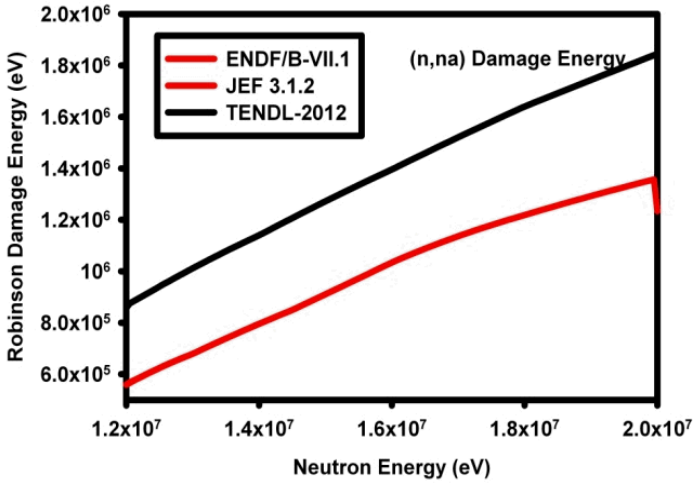


Variation in Reaction-specific Robinson Displacement Energy



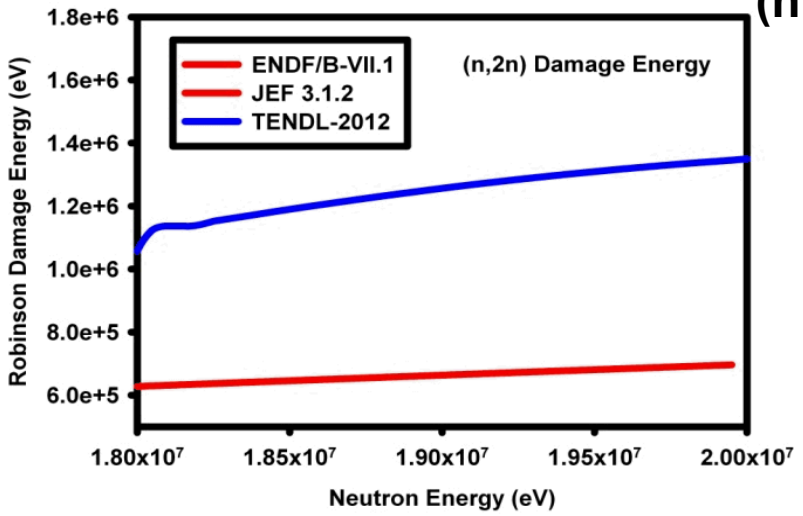
(n,na)

High energy channels show offset in damage energy but strong energy-dependent correlation.

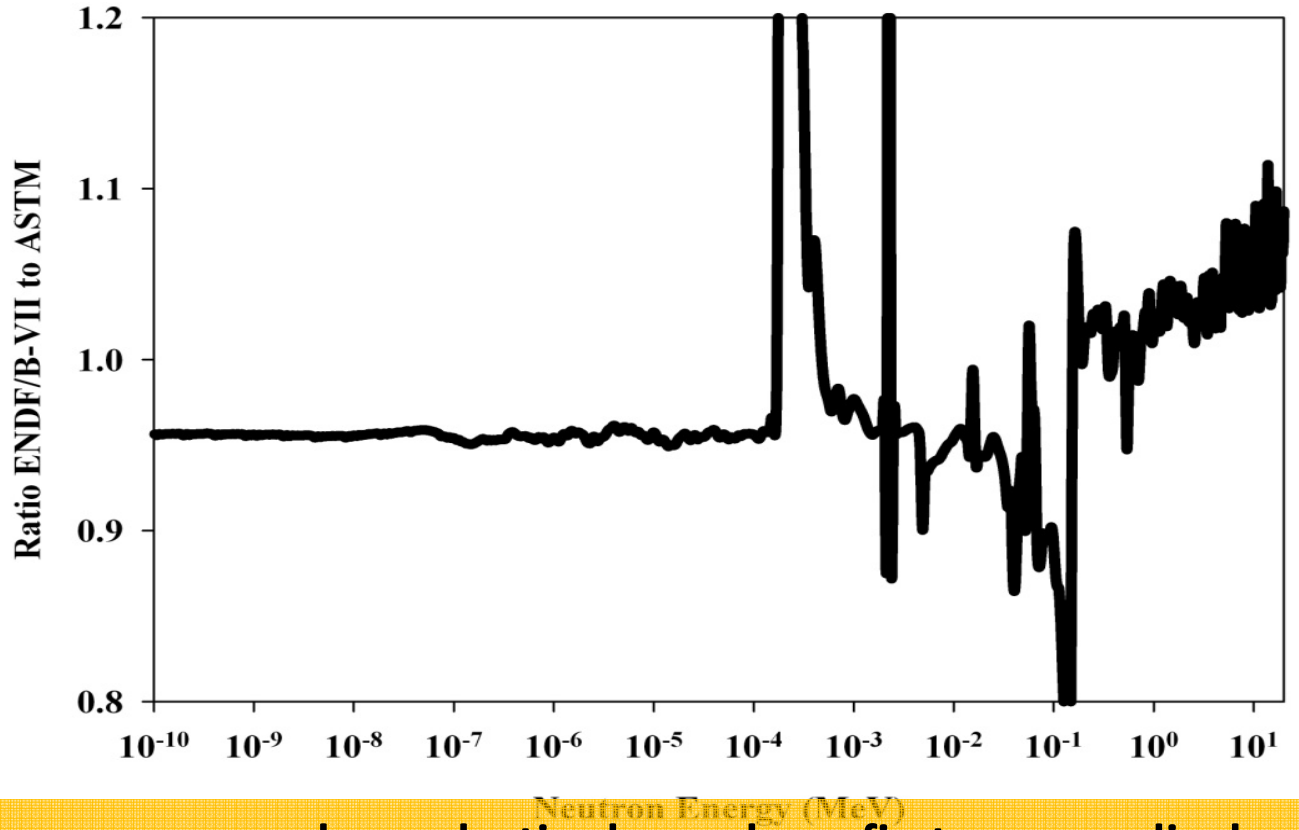


(n,np)

(n,2n)



Ratio of E722-2015 to E722-94 Silicon Displacement kerma



- **Spike near energy where elastic channel can first cause a displacement, i.e. ~ 130 eV.**
- **Spike at 2.25 keV due to ^{30}Si resonance**

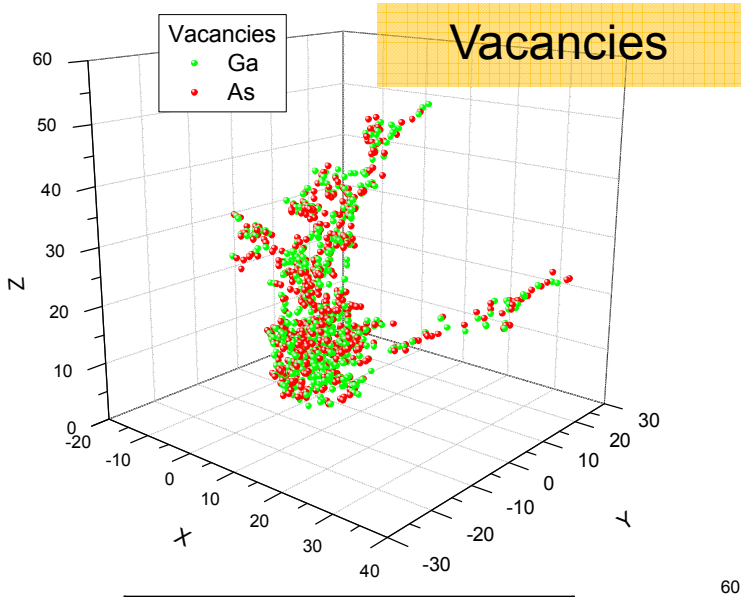
Considerations in the Selection of a Metric

- **Displacement Kerma or 1-MeV(matl.)-Eqv.**
  - **A large portion of the systematic uncertainty will cancel out when one looks at an equivalent damage metric, e.g.**
    - **the effect of the interatomic potential**
    - **Displacement threshold energy**
- **Displacement kerma (calc.) or Equivalent Damage (exptl.)**
  - **Eqv. damage would have a dependence on the type of residual defect, e.g.**
    - **Recombination lifetime in semiconductors**
  - **arc-dpa may be fit to equivalent damage or calculated MD/NRT ratio of primary #FP**

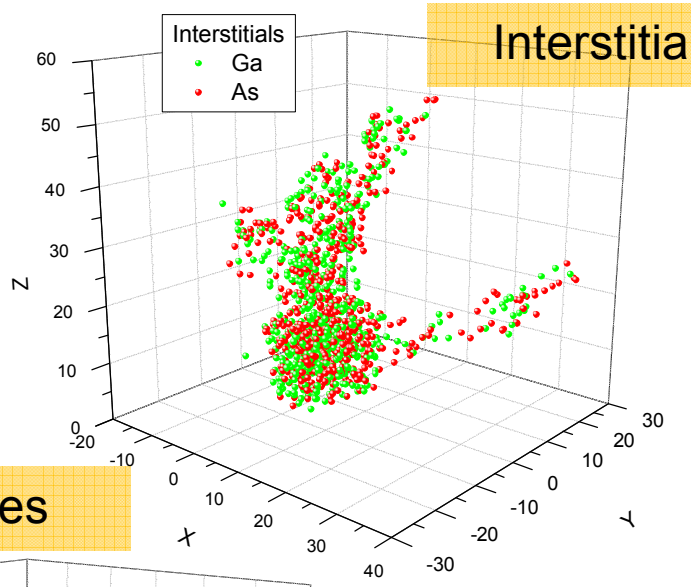
Complication: Polyatomic Lattice

- Polyatomic Materials
  - Consider each recoil atom based on neutron cross section and use Robinson formula with “effective” lattice A and Z
  - Parkin and Coulter for energy partition in polyatomic materials
  - Use MARLOWE for BCA analysis of defect production

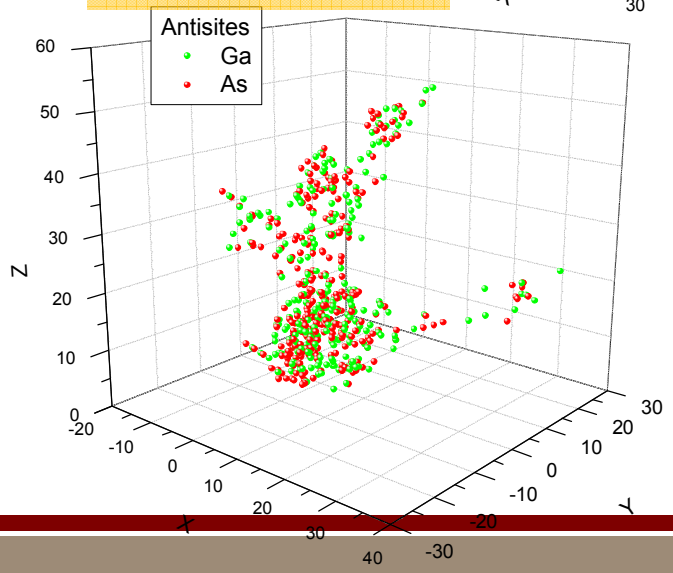
MARLOWE 10 keV As recoil in GaAs



Vacancies



Interstitials



Anti-sites

# of defects in 10 cascades		
	Ga	**As**
Vacancy	**605**	**641**
Interstitial	**624**	**622**
Antisite	**277**	**303**

Spatial coordinates are in units of GaAs lattice constant=0.5653 nm
Cluster diameter ~ 20 to 30 nm.

These plots show defects from 10 recoils summed together

Questions