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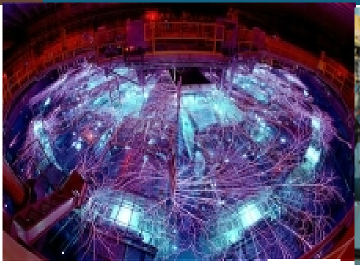
Uncertainty Considerations that Impact the Use of Dosimetry Metrics in Modern Semiconductors



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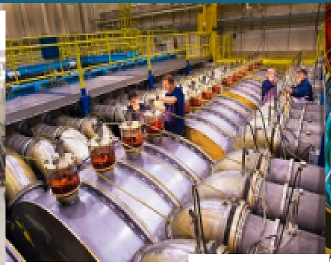

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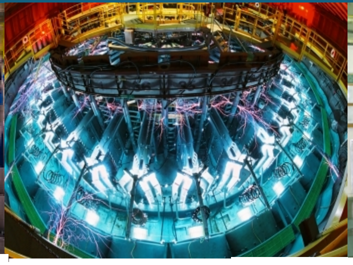

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PRESENTED BY

Patrick Griffin, Laboratory Fellow, Org. 1000

R&A#: xxxx

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Name/Org: Patrick Griffin/SNL Date: 07/12/2022
Guidance (if applicable) ____________________

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Flow of Presentation:

- Dosimetry Metrics – Terminology
- Focus on Calculated Metrics vs. Observed Behavior
- Electronic Materials of Interest
  - Main semiconductor materials: Si, GaAs, GaN, SiGe, SiC
  - Other materials:
    - Semiconductors: [$HfSe_2$]; Dielectrics: [SIO_2, HfO_2, $Hd_{0.5}Zr_{0.5}O_2$]; Dopants: [B, P, Sb, In]; Metals: [Au, Cu, W]; Capacitors [Ta, gel];
- Examples of Nuclear Data Needs (with motivation for uncertainties) for Semiconductors

Why is the understanding of energy-dependent uncertainties in semiconductor damage metrics important? Consider the use of semiconductors in space and for instrumentation in power reactors.

Formulation of Calculated Damage Metrics

- **<u>Calculated</u> metrics**
  - Total cross section
  - Kerma
    - Total kerma
    - Displacement kerma
    - Ionizing kerma
  - NRT damage energy
  - dpa
  - Recoil atom distributions
    - For: Single event effects
    - Convert to: LET distributions

$$ {}^{facility}D_{type} = {}^{type}\mathbb{C} \bullet {}^{facility}\Phi \bullet \int_0^\infty \phi^{facility}(E) \bullet \Re_{type}(E) \bullet dE $$

$$ \Re_{type}(E) = \sum_{i,j_i} \sigma_{i,j_i}(E) \int_0^\infty dT_{R,j_i} \int_{-1}^1 d\mu \cdot f\left(E,\mu,T_{R,j_i}\right) \cdot {}^{type-A}\Lambda\left(E_d, {}^{ion}_{type-B/D} T_{R,j_i}\right) \bullet $$

$$ {}^{type-B}\zeta\left(E_d, T_{R,j_i}, {}^{type-D}T_{dam}\right) \bullet {}^{type-C}\xi\left(T_{R,j_i}\right) $$

- Recoil spectrum
- Damage partition
- Threshold treatment
- Recoil ion efficiency

$$ {}^{O_{i,x}}\Theta(T_{R,i,x}, E) = \sum_{i,j_i} \delta\left[j_i, O_{i,x}\right] \cdot \phi(E) \cdot \sigma_{i,j_i}(E) \cdot \int_{-1}^1 d\mu \cdot f\left(E,\mu,T_{R,j_i}\right) $$

$$ \mathscr{L}(E) = \sum_{i,j_i} {}^{GaAs}S\left[T_{R,j_i} \Rightarrow LET\left({}^{A^{j_i}}_{Z^{j_i}}P\right)\right] \bullet {}^{O_{i,j_i}}\Theta(T_{R,j_i}) $$

Nuclear Data is used to determine the response functions for radiation damage to semiconductors.

Applied Damage Metrics for Semiconductors

Damage Metrics	Comments / Description / Application
Total Dose	Used to measure the response of calorimeters. Approximated by the calculated total kerma assuming charged particle equilibrium.
Displacement Dose	Approximated by the calculated displacement kerma in complex materials.
NIEL	Proportional to displacement dose; defined for all incident particles; at high incident energies, includes the effect from nuclear interactions. Corrected for nuclear reactions and CP transport.
1-MeV(GaAs)-Equivalent 1-MeV(GaAs) Fluence	Derived from 1-MeV(matl) damage energy by dividing the damage energy by the reference 1-MeV damage energy, 95/70 MeV-mb for Si/GaAs. Corrected for recombination.
Ionizing Dose	Used to measure transient response of some detectors, e.g., photoconductive detectors (PCDs). Approximated by the calculated ionizing kerma.
Frenkel Pair Density	Proportional to the NRT damage energy. Computed using $2^*E_d/\beta$, where β is an atomic scattering correction term, to account for the energy per Frenkel pair. Recombination corrected.
Track Density	Used as a fluence monitor. Proportional to the total cross section. Treashold tratment,.
Minority Carrier Recombination Lifetime	An experimental metric derived from carrier removal rates in bulk materials, lifetime changes in optoelectronics, or gain degradation in BJTs and HBTs.
Material embrittlement	Used to correlate with material dpa. Proportional to the NRT damage energy

Semiconductors – Nuclear-data related Sources of Uncertainty

- Cross Sections
  - **Cross reaction correlations** – can be addressed using TENDL random libraries
- Recoil Spectra
  - Limited availability in ENDF/B-VIII.0; found in TENDL-2021
  - **No uncertainty** even supported in ENDF-6 format
  - Sparse **experimental validation data** (none for semiconductor materials)
- Stopping Power
  - Lack of **experimental data** for GaAs or GaN, so calculations used
- Damage Partition Function
  - Treatment of alpha particle damage – **limitations in Robinson formalism** violated
  - Treatment of polyatomic lattice materials – limitation in Robinson formalism for dissimilar A/Z for lattice/recoil atoms, requires use of BCA/MD. CP studies.

A common theme is the lack of experimental data and limitations of nuclear data library formats.

Uncertainty Considerations in Semiconductors Metrics

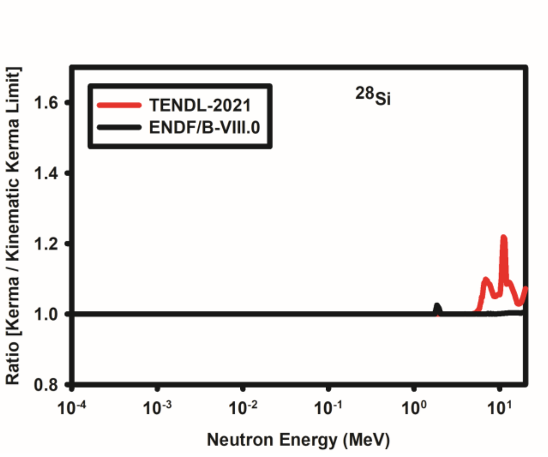
- Uncertainty components (std. dev. & correlation) reside in:
  - Nuclear data evaluations (data and model) – [previous slide]
  - Unaccounted for model-defect used to generate the data representations.
    - Systematic correlations due to optical model representation that go beyond what is captured by parameter variation.
  - Models used to generate damage metrics, e.g.:
    - Damage partition function
    - Threshold treatment in Frenkel pair generation
  - Propagation of uncertainty into damage metrics, e.g.:
    - Cross reaction-channel correlations
    - Stopping power correlation over energy and between different recoil atoms
  - Relationship between a calc. damage metric and an observed damage mode:
    - e.g., use of primary Frenkel pair creation for transistor gain degradation.

There are many uncertainty aspects to consider, e.g., how the data is used.

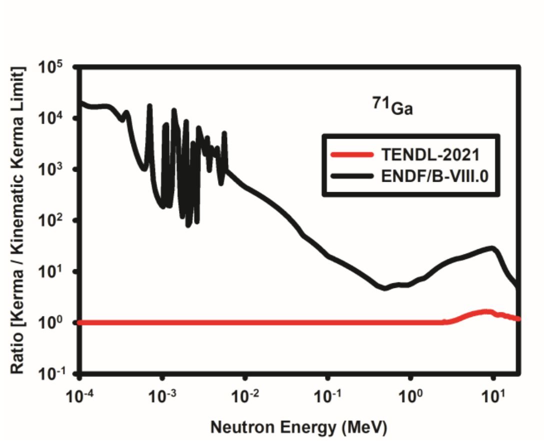
Radiation Damage in Semiconductors - kerma

- First quality metric: **Energy Balance** (kerma / kinematic kerma limit)
  - Easily assessed with codes, such as NJOY-2016 (MT301/MT443)
  - Serious issues in ENDF/B-VI and prior versions.

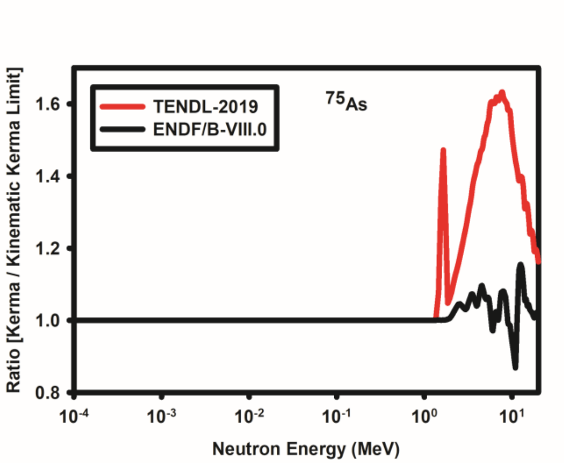
✓ Status is now **adequate**. Modern cross section evaluations are, generally, checked for this.



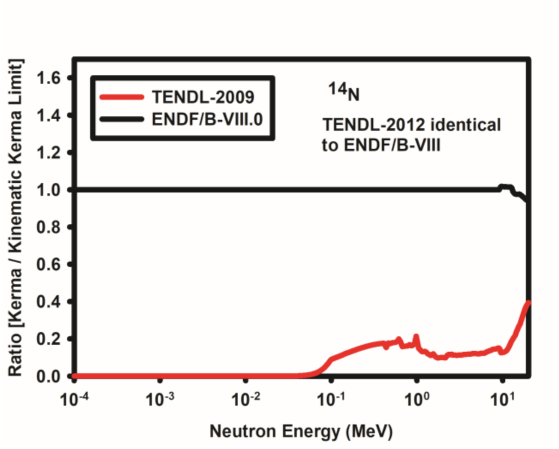
^{28}Si energy balance



^{71}Ga energy balance



^{75}As energy balance



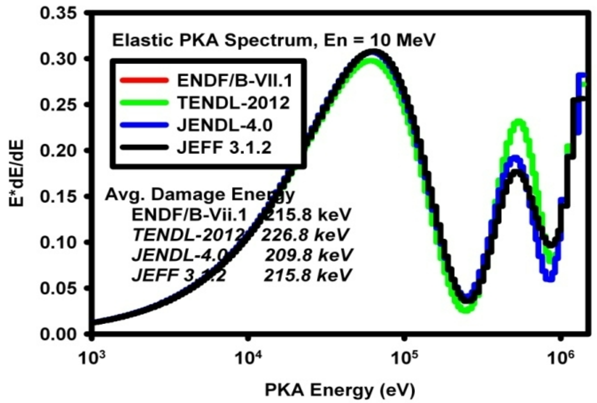
^{14}N energy balance

The energy balance in nuclear data remains a concern. Nuclear data and model-dependent aspects. An acceptable evaluation can usually be found.

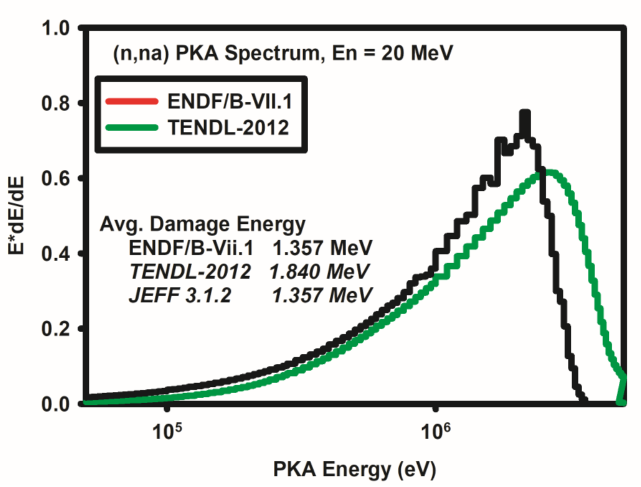
Radiation Damage in Semiconductors - kerma

- Second quality metric: **Recoil Energy Distribution**
  - Comparisons are best metric:
    - Little experimental data, use model-based variation between different evaluations / codes
  - Serious issues in ENDF/B-VI and prior versions.

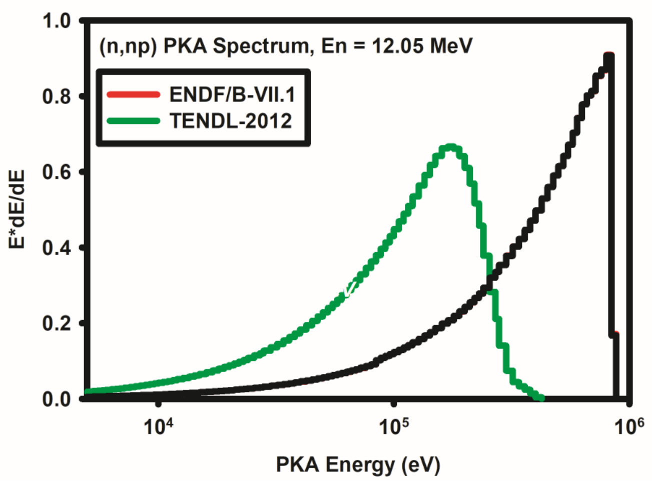
REJECTED Status is **marginal**.



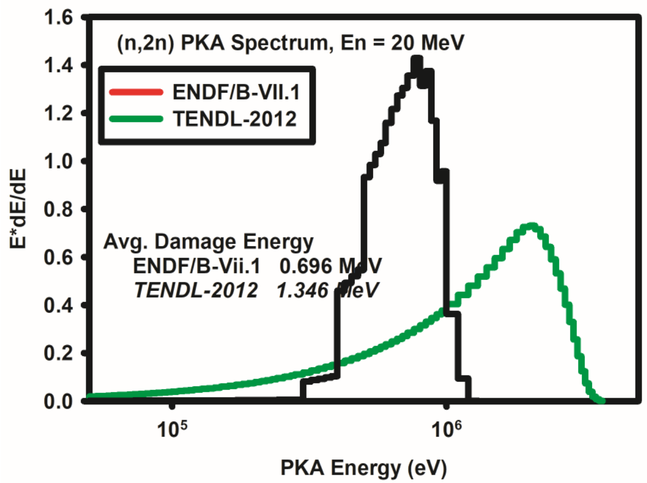
^{28}Si recoil: elastic



^{28}Si recoil (n,nα) E_t= 10.3 MeV



^{28}Si recoil (n,np) E_t= 12 MeV

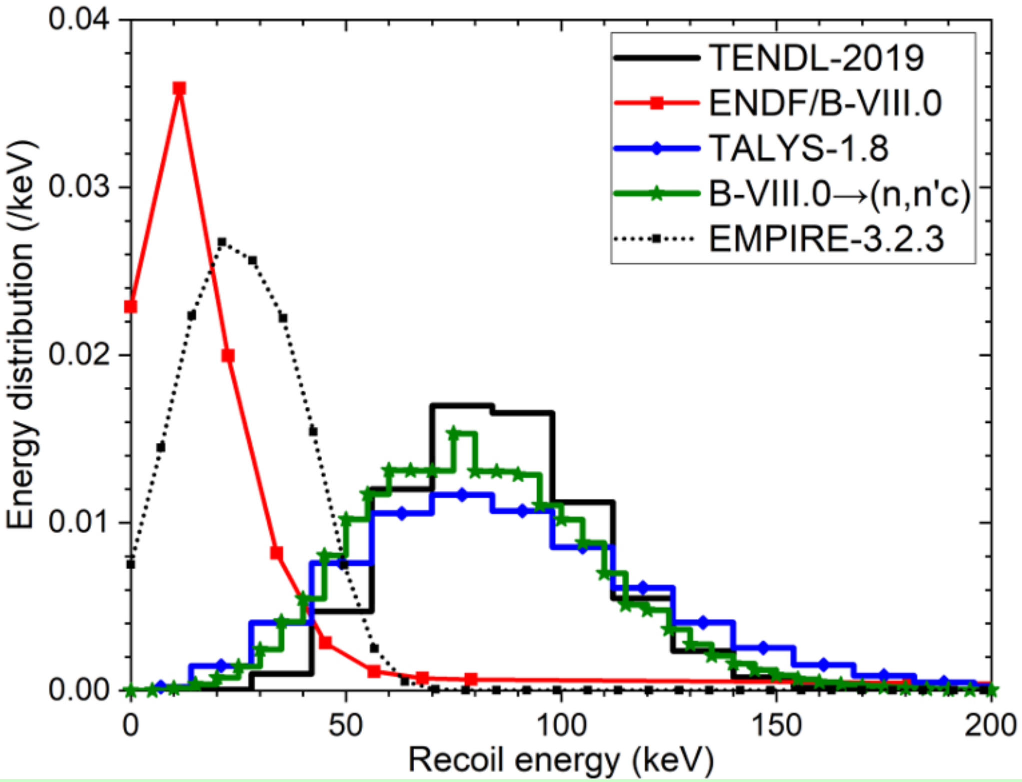


^{28}Si recoil (n,2n) E_t= 17.8 MeV

Significant variations observed when kinematics do not constrain spectrum – and when close to the reaction threshold energy.

It is even worse when data verification is not performed.

- ENDF-6 MF6 does not support capturing the uncertainty in recoil spectrum.
- Some literature reports big differences – often code bug, user error or data format issue.
  - Data verification steps too often fail to carefully look at the MF6 data – many errors occur – often related to the CM/Lab coordinate system.
- Direct experimental data for heavy recoil particles is very limited. Rather, it is inferred from kinematics.
  - Comparison of MF6 and reaction kinematics is a good verification step – and should be required (Chen recommendation).



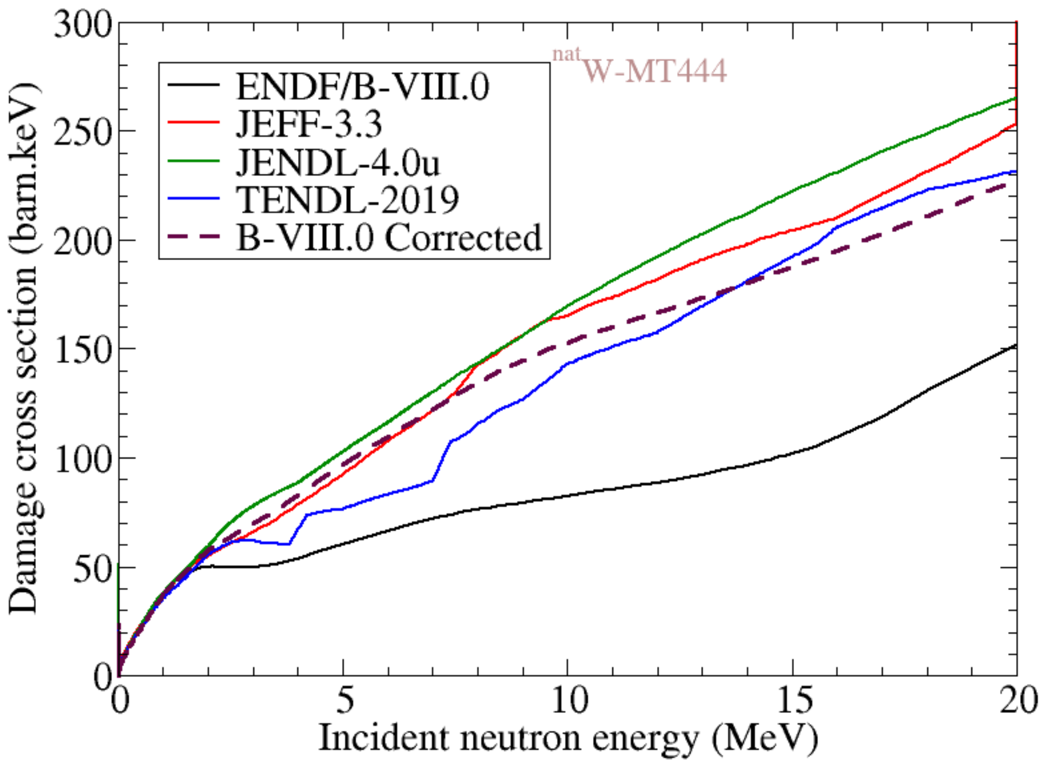
Recoil Spectra of $^{184}W(n,2n)^{183}W$ at 14-MeV Incident Energy

S. Chen, D. Bernard, J. Nucl. Matl., Vol 562, April 2022.

There is a major need to look more closely at recoil atom spectra and the associated uncertainty.

Implications for Displacement Kerma Due to Recoil Spectra Uncertainty:

- Even when data is corrected to catch formatting issue, there are large differences between nuclear data evaluations.
  - Consider the displacement kerma (damage cross section) in tungsten.
  - Presumed format errors caused a 3X error
  - Evaluation differences were still resulted in ~25% variation in the damage metric.
    - These are all recent evaluations!
    - Low energy elastic damage is in good agreement because the recoil is derived purely from conservation of momentum and energy.



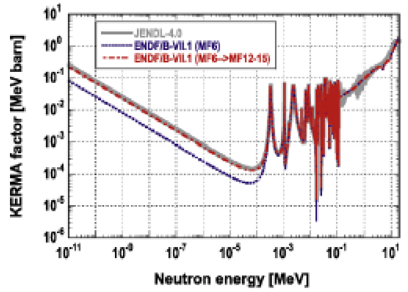
Total Damage Cross Section of ^{nat}W

S. Chen, D. Bernard, J. Nucl. Matl., Vol 562, April 2022.

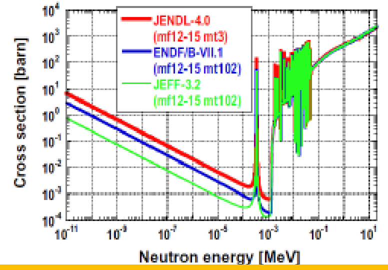
There is a major need to look more closely at recoil atom spectra and the associated uncertainty.

Radiation Damage in Si Semiconductors - kerma

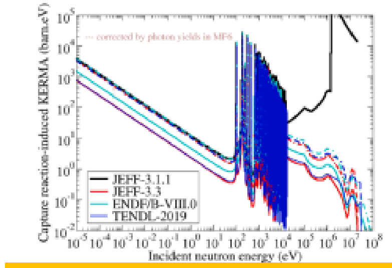
- Consideration: Photon Spectra for neutron capture
- Quality metric: consistent treatment
  - Photon spectrum matters – not just energy:1 photon vs. 2 photons with same energy
  - Consider NJOY-2016 treatment of thermal capture
    - MF6 vs. MF12 representation (e.g., Konno and Chen)
      - Difference seen in TENDL evaluations that have both formats
    - Discrete vs. continuum representation [NJOY treatment issue]
  - Kimura et al., 9th ISRD found ASTM thermal displacement kerma Si kerma 2X too large based on reactor experimental damage.
  - Use of PGAA spectra vs. modeled with limited nuclear structure
  - Fidelity of thermal neutron capture vs. high energy neutron capture
  - Status is poor.



Konno, FED, 109, 2016.



Chen, JNM, 562, 2022.



Chen, JNM, 562, 2022.

Serious limitations seen even in (n,g) reaction treatment.

Semiconductors – further complexities

- Responses (calc.) mapped to experimental damage metrics (obs.)
  - Ionizing dose (calc.) – trapped charge in oxide (obs.)
    - Issue 1: charge recombination due to local density of ionization
    - Issue 2: presence of high-Z materials: vias and high-κ dielectrics
    - Issue 3: small feature size and lack of electron equilibrium
  - Damage energy (calc.) – change in minority carrier lifetime (obs.)
    - Issue 1: recoil-energy depended correction, arc-dpa
    - Issue 2: sensitivity to charge state of residual defect, e.g. $V\text{-}V^{o}$ vs. $V\text{-}V^{-}$
    - Issue 3: annealing of defects – interplay between temperature/time and current injection on defect populations, e.g. Si DLTS observations.

Our easily calculated damage metrics do not always capture some of the important physics in the device response. Application-dependent!

Statistical Issues: there is a significant cascade-to-cascade variation in FPs

pdf for Si Ions

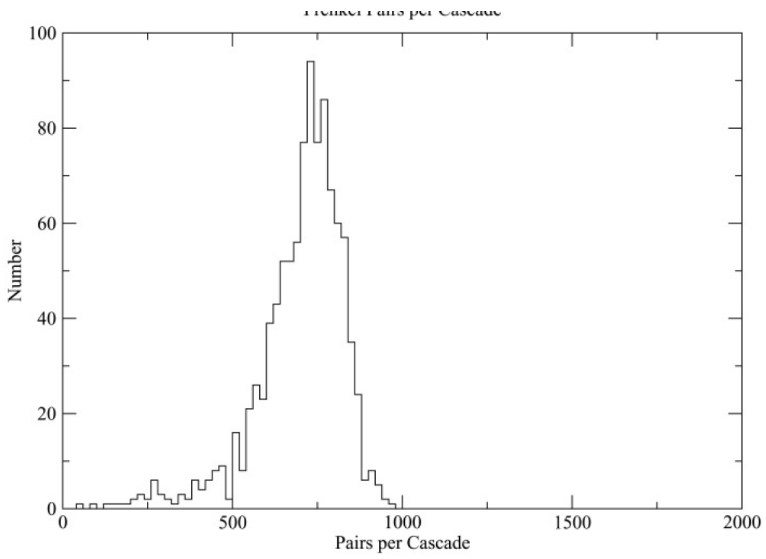
pdf for 1-MeV neutrons in Si.

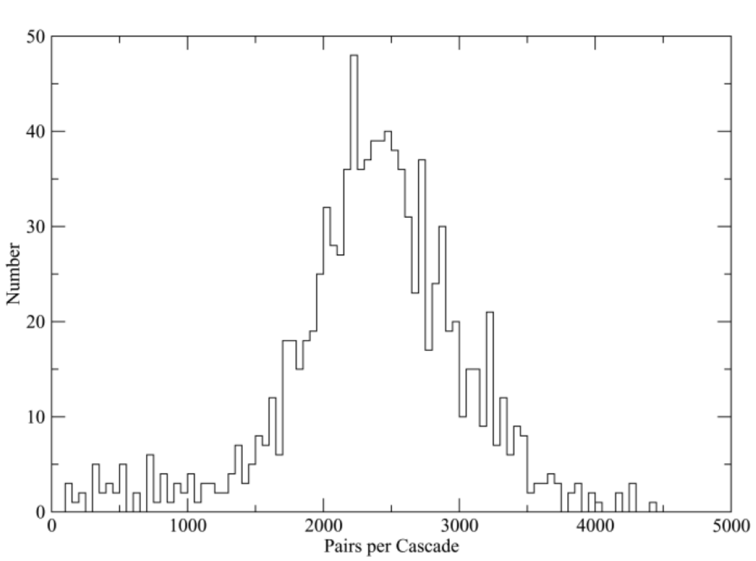
100 keV
$\langle FP \rangle$ = 680; FWHM = 129

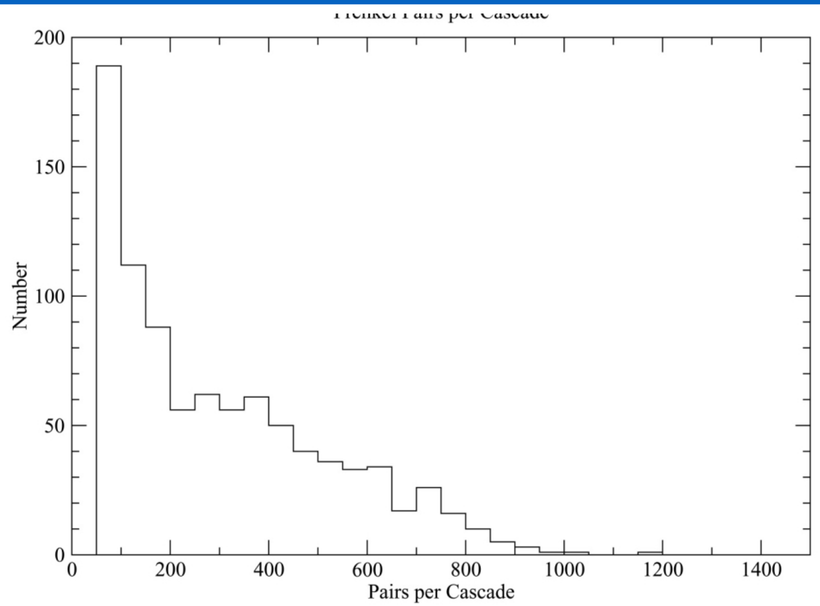
1 MeV
$\langle FP \rangle$ = 2320; FWHM = 656

$\langle FP \rangle$ = 244; FWHM = 216

$\langle E_{recoil} \rangle$ = 38 keV; FWHM = 31 keV

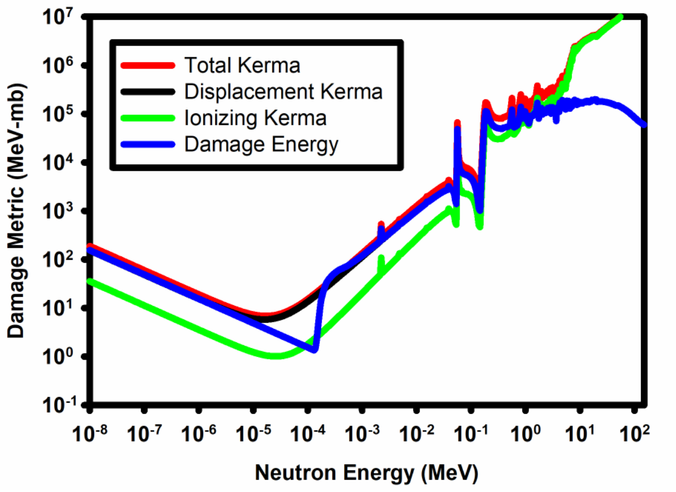




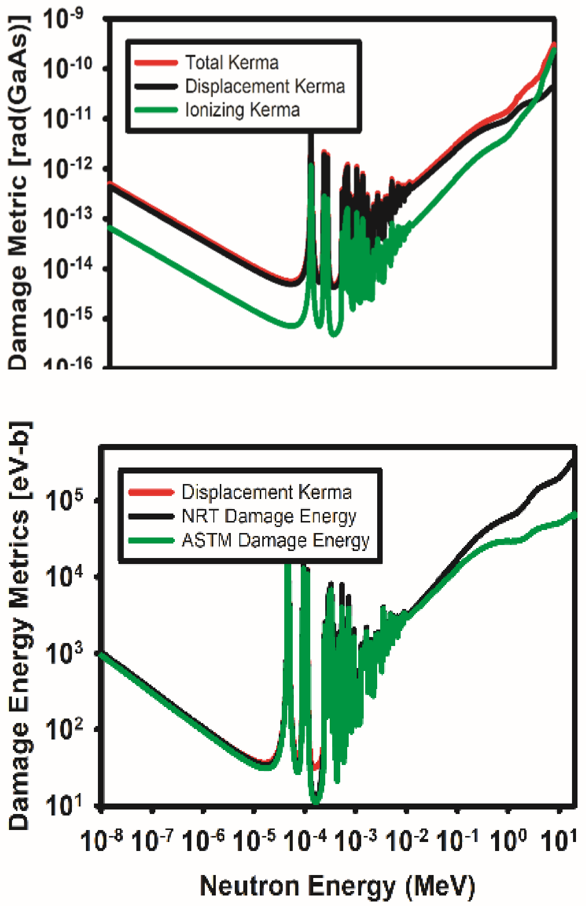


The distribution is critical! At the neutron level, it is not even a normal distribution. The variation in the pdf can be as large as the mean value.

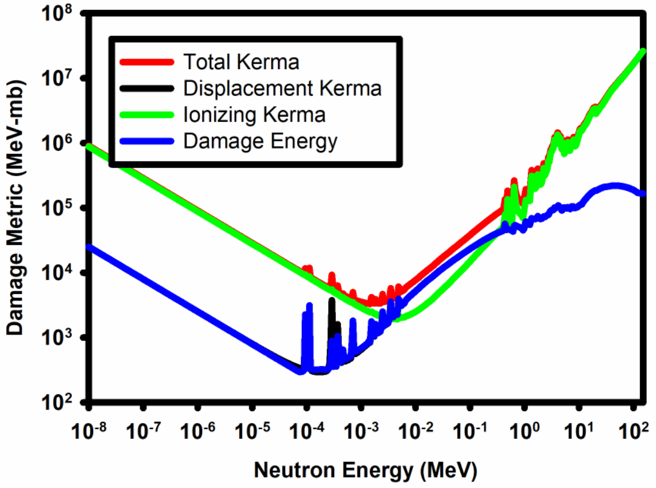
Semiconductor Response Functions



Silicon



GaAs



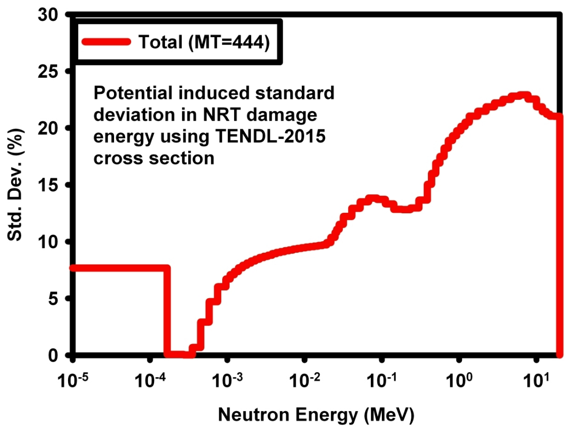
GaN

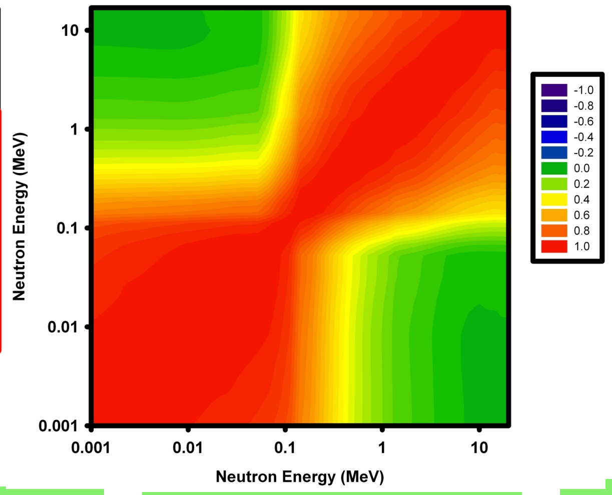
We can generate energy-dependent response functions for most semiconductor materials. The issue is the ability of these calculated responses to capture the observed behavior!

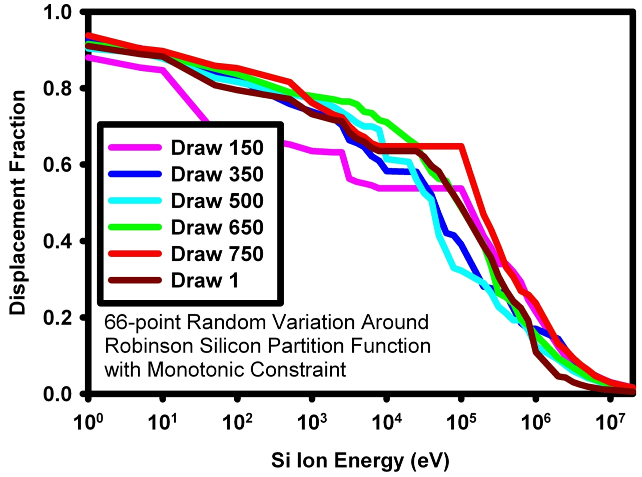
There is a strong energy-dependent correlation in the damage partition function

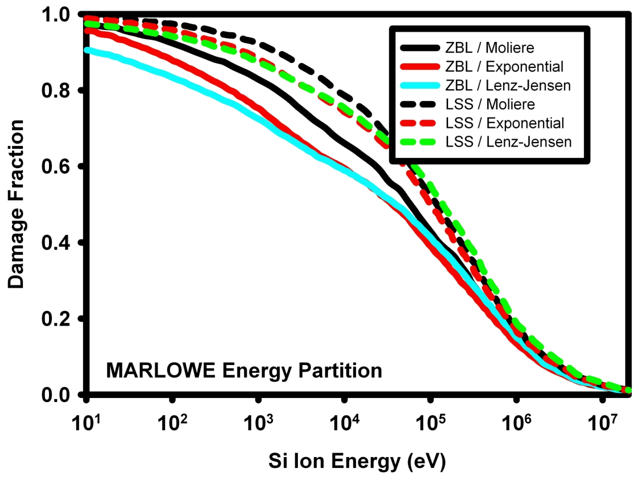
Neutron-based

Si ion-based









Std. dev. in Si damage partition function

Correlation Matrix

Statistical draw of damage partition function

Effect of potential on damage function

Neutron-based uncertainty based upon TENDL-2015 random ENDF files for recoil spectra.
Si ion-based uncertainty based on MARLOW-based BCA calculations.

A strong energy-dependent correlation can result in a 2X change in integral uncertainties!

Summary – the Most Significant Sources of Uncertainty for the Radiation Response in Semiconductors

- Matching a **computed** response function to an **observed** radiation effect of interest
- Correlations between reaction channels
- Uncertainty in the recoil spectrum
- Verification of the recoil spectra in nuclear data evaluations
- Uncertainty in the treatment of the damage partition function for polyatomic materials
- Equivalence of damage metrics due to contributions of light and heavy recoil atoms, e.g., proton damage vs. neutron damage.
- Characterization of stochastic variation in applications

There is a big need for fundamental advances here – both in the characterization of the underlying nuclear data and in modeling the damage metric!

Questions?