SAND2018-9258C

SAND2018-xxxx C

Impact of Nuclear Data Uncertainty in the Modeling of Recoil Atom Energy Distributions in Silicon

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Abstract

Recoil ion distributions in silicon and the resulting distribution of the linear energy transfer (LET) are important metrics in microdosimetric studies and in the investigation of single event effects. A rigorous methodology is presented for quantifying the uncertainty in these metrics due to the underlying uncertainty terms, including that due to the nuclear data. The methodology uses a Total Monte Carlo approach so that the nonlinear uncertainty propagation is rigorously treated. The uncertainty is captured in the form of a recoil energy or LET-dependent covariance matrix.

LET Dosimetry Metric

- Most radiation damage metrics are scalars values and can be represented as:

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

where the neutron response function has the form:

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

and the energy-dependent uncertainties from the response and the neutron spectrum can be separated.

- LET is, however, a distribution and is equal to the product of the recoil ion spectrum and the corresponding maximum (over lower energies) ion electronic stopping power, which can be represented by a convolution over the neutron spectrum and the recoil atom production cross section:

$$LET(let) = S(T_R \rightarrow let) \bullet \Theta(T_R) =$$

$$\mathbb{C} \bullet S(T_R \rightarrow let) \bullet \sum_{i,j_i} \int_0^\infty dE \bullet \phi(E) \bullet \sigma_{i,j_i}(E) \bullet \int_{-1}^{1} d\mu \bullet f\left[E,\mu,T_{R,j_i}\right] \bullet T_{R,j_i}$$

- The Si recoil atom stopping power in a lattice, contribution to neutron kerma, and uncertainty are:

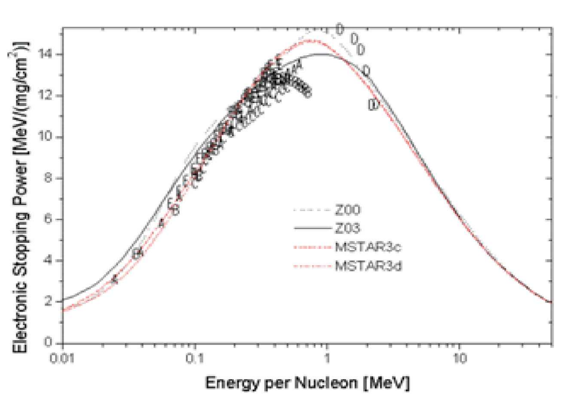

Fig. 1. Si stopping power in silicon lattice

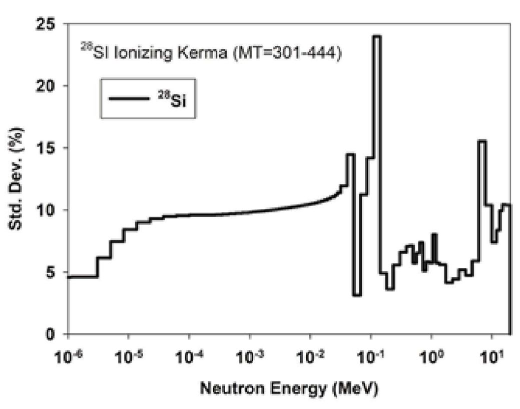

Fig. 2. Neutron energy-dependent ionizing kerma

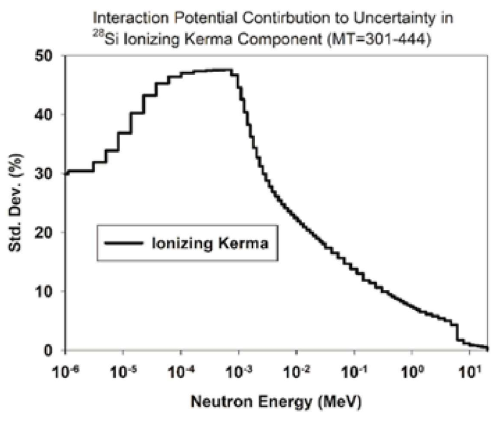

Fig. 3. Uncertainty in neutron ionizing kerma

Uncertainty Treatment

- Total Monte Carlo (TMC) treatment used to capture the contribution from uncertainty in the nuclear data
  - Used 300-sample TENDL-2015 random cross sections
- Least squares uncertainty in neutron spectrum captures spectrum uncertainty
- Analytic fit to experimental stopping power captures uncertainty and ion energy-dependent correlation
- Brute force Monte Carlo (BFMC) used to propagate uncertainty

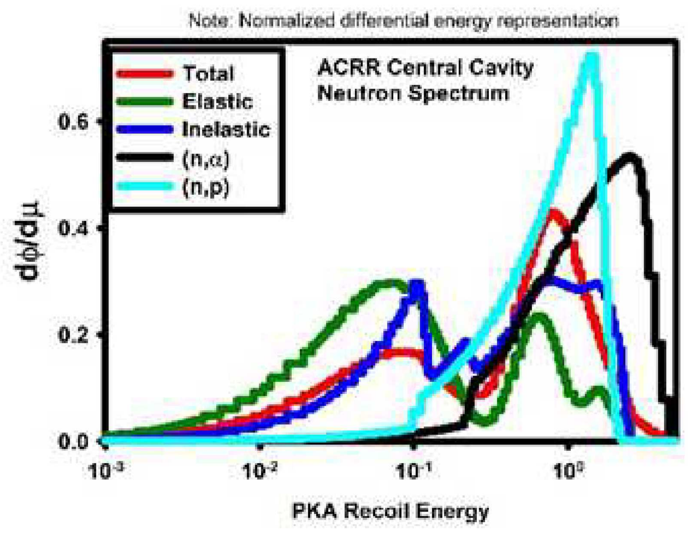

Fig. 4. Recoil spectra for various reaction channels in the ACRR reference pool-type reactor spectrum

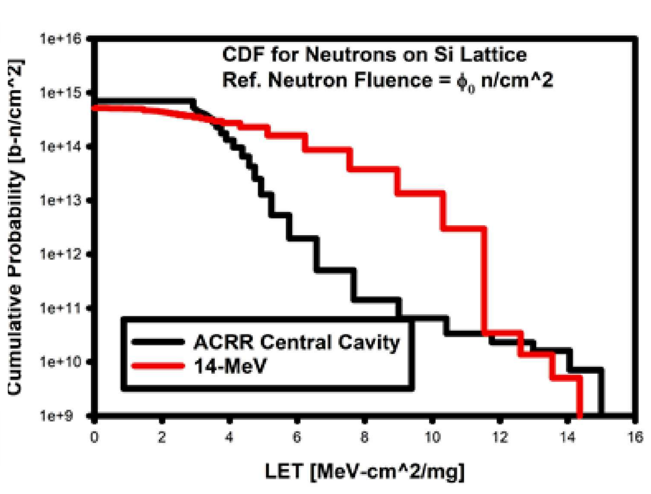

Fig. 5. LET distribution for two representative neutron spectra

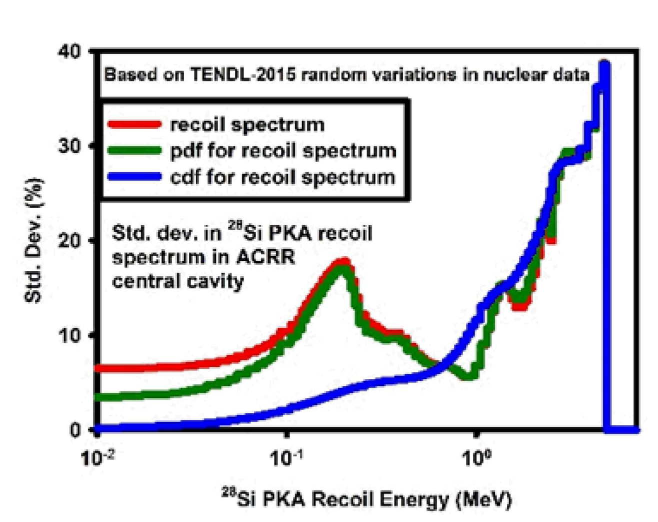

Fig. 6. Energy-dependent standard deviation for dosimetry metrics

Correlation Matrix for Uncertainty Metrics

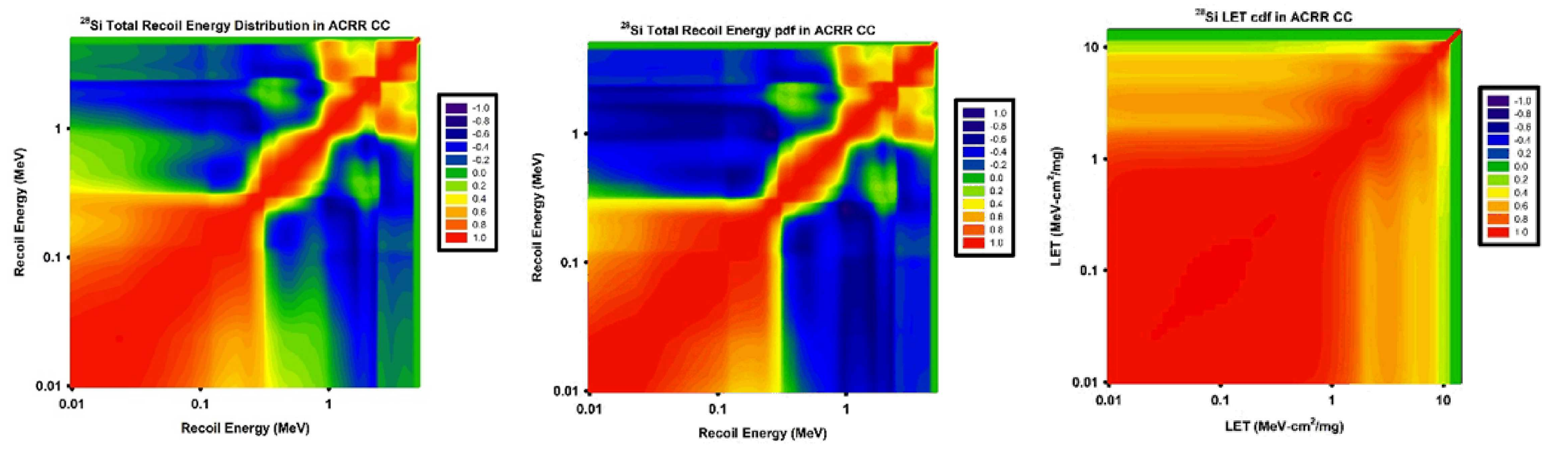

Fig. 7 a/b/c. Correlation matrix for the various ^{28}Si uncertainty metrics in the ACRR central cavity spectrum. a) nuclear data uncertainty in primary recoil atom energy; b) normalized pdf for nuclear data uncertainty in recoil energy; c) cdf for LET distribution

Conclusion

This work has quantified the uncertainty in the recoil atom energy distribution and in various electronic deposition damage metrics due to the underlying nuclear cross section data and the damage partition function. The nuclear data uncertainty characterization is the result of a rigorous TMC approach that preserves the aspects of the nonlinear uncertainty propagation through the calculations. It is presented in the form of a covariance matrix so that it can be further propagated in support of various applications.

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