UNCERTAINTY OF SILICON 1-MeV DAMAGE FUNCTION*

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ABSTRACT

A covariance matrix for the silicon 1-MeV neutron displacement damage function is developed. This uncertainty data will support the electronic radiation hardness-testing community and will permit silicon displacement damage sensors to be used in least squares spectrum adjustment codes.

1. Introduction

The electronics radiation hardness-testing community uses the ASTM E722-93 Standard Practice[1] to define the energy dependence of the nonionizing neutron damage to silicon semiconductors. This neutron displacement damage response function is defined to be equal to the silicon displacement kerma as calculated from the ORNL Si cross-section evaluation.[2] Experimental work has shown that observed damage ratios at various test facilities agree with the defined response function to within 5%.[3] This paper provides an energy-dependent description of the uncertainty in the silicon damage function and provides a complete covariance matrix. This information can be used to provide a much more complete precision and bias section for ASTM E722.

This paper uses two methods to examine the uncertainty in the silicon 1-MeV displacement kerma. The first approach, which will be referred to as "observed" in this paper, is to examine the energy-dependent variation resulting from the existing cross section evaluations. The second approach is to correctly combine and weight the existing ENDF/B-V covariance data for the silicon cross section components, so that they represent the covariance for the displacement kerma.

2. Observed Silicon Displacement Variation

2.1. Silicon Cross Sections

A survey of existing cross sections has found twenty-one different silicon evaluations.

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Six of these were identified as being recent and relatively independent. They include evaluations from the ENDF/B-VI, JENDL-3[4], JEF 2.2[5], BROND 2 (revision 1)[6], and CENDL libraries as well as the private ORNL evaluation, and are used in this analysis. Because all of these evaluations do not use the same subset of reaction channels, a set of five generic reaction channels were identified and all reaction components were mapped into these five reactions. The reactions include the elastic, inelastic, (n,p), (n,α), and (n,γ) reactions. The (n,2n), (n,3n), and (n,nd) channels were combined with the inelastic channel. The (n,d), (n,np), and (n,2p) reactions were combined with the (n,p) channel. The (n,nα), (n,t), and (n,^{3}He) channels were combined with the (n,α) channel. This grouping was necessitated by the availability of covariance data and only applied to the uncertainty estimates. The displacement kerma from each reaction channel was modeled with the exact evaluated cross sections and recoil energy distribution models. This grouping should not affect the application of the resulting covariance matrix for radiation hardness testing purposes.

Cross sections and displacement kerma for each evaluation and from each reaction channel were studied and compared. A statistical analysis of these cross section files, with the reactions grouped into the five main channels, was performed and the results were used to generate the observed energy-dependent uncertainties for the silicon displacement kerma.

The elastic cross section is the largest component at all energies. The order of importance of the displacement components, for an irradiation with a normal reactor spectra, is elastic, inelastic, (n,p), (n,α), and (n,γ). Figure 1 shows the relative energy-dependent importance of the various cross section contributions in the ORNL evaluation. The displacement kerma is affected by both the cross section and the recoil energy of the reaction products. Above about 5 MeV, the inelastic displacement damage begins to dominate the displacement kerma. Figure 2 shows the relative energy-dependent importance of the various reaction channels to the displacement damage. Reactions which result in a proton or alpha particle in the outgoing channel are combined in Figure 2 based on the similarity of the emitted particles. The analysis treated each of these channels separately.

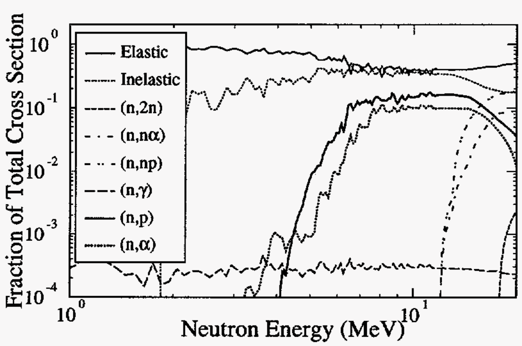

Figure 1. Silicon Cross Section Components

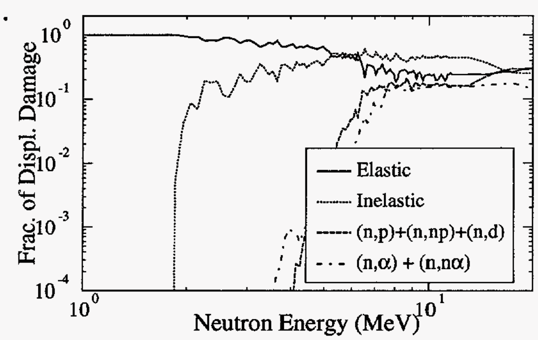

Figure 2. Silicon Displacement Kerma Components

2.2. Displacement Methodology

The displacement kerma is obtained by multiplying the cross section by the recoil energy that goes into creating displacements and summing over reaction channels. Equation 1 shows the formula used to compute the displacement kerma

$$D(E) = \sum_r \sigma_r(E) \int_0^\infty dE' \int_{-1}^{1} d\mu f(E,\mu) g(E \rightarrow E') P(E_R[E,E',\mu]) \quad (1)$$

where:

$\sigma_r(E)$ = cross section for reaction r at energy E

$f(E,\mu)$ = angular distribution (function of energy, E, and angle, μ)

$g(E \rightarrow E')$ = secondary energy distribution

$E_R[E,E',\mu]$ = Primary knock-on atom (PKA) recoil energy

$P(E_R)$ = Robinson partition function[7]

The NJOY91 code[8] (version 118) was used to compute the displacement kerma for all results reported in this paper. When neutron spectra were folded in with cross sections, a fine-group 640-bin SAND-II multigroup energy grid[9] was used.

3. Silicon Damage Covariance

3.1. Displacement Covariance

Covariance matrices for the silicon cross-section components [elastic, inelastic, (n,p), (n,α), and (n,γ)] for the ENDF/B-V silicon evaluation exist as part of the COVERV covariance data library.[10] Figure 3 shows the energy-dependent uncertainty (the square root of the diagonal elements of the covariance matrix, expressed as a percentage) for several reaction channels. The covariance matrices were weighted by the displacement effectiveness (the ratio of the reaction displacement kerma to the reaction cross section) and combined to form a displacement covariance matrix. A covariance matrix may be hard to interpret due to the varying normalization of each row and column. For clarity the covariance matrix is usually depicted by giving the energy-dependent uncertainty and the relative correlation matrix. Figure 4 shows the calculated standard deviation for the silicon displacement kerma. Figure 5 shows the calculated relative correlation matrix for the silicon displacement kerma.

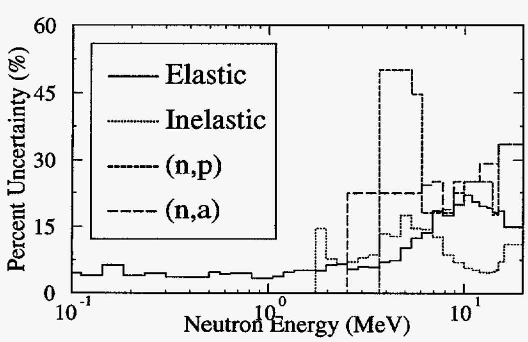

Figure 3. Uncertainty of Si Cross Section Components

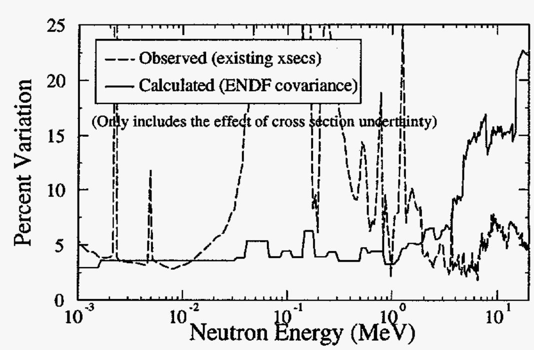

Figure 4. Uncertainty of Si Displacement Kerma

Figure 4 also shows the standard deviation for the "observed" silicon displacement kerma. At high energies the "observed" variation among the six silicon evaluations is seen to be much less than that indicated by the COVERV uncertainty estimates. Significant contributions to the displacement kerma at these energies come from the inelastic and (n,p) reactions. Due to the reliance on nuclear models, normalized by a limited set of measurements at energies below 9 MeV and at 14 MeV, the high energy "observed" data is probably highly correlated. Since the methodology used to estimate the "observed" variation did not treat this correlation, the "observed" uncertainty is underestimated.

Large differences are seen for the energy-dependent "observed" displacement kerma in the resonance region of Figure 4. The variation in the threshold region below 100 keV is not important for most integral displacement damage measurements, however the difference near 0.2 MeV is the major contributor to the observed variation.

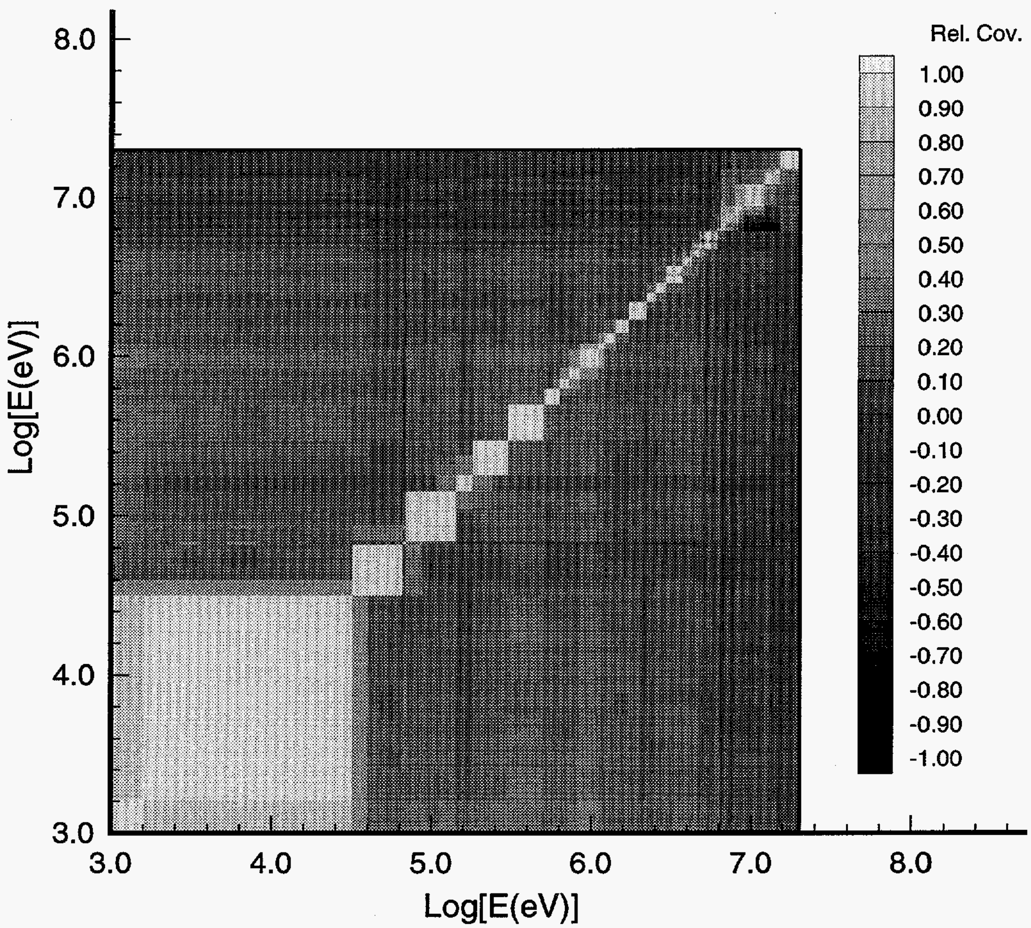

Figure 5. 1-MeV(Si) Relative Correlation Matrix

3.2. Variation in Silicon Elastic Cross Section

Analysis of the contributions to the "observed" variations seen in Figure 4 shows that the difference in displacement kerma is directly attributable to differences in the "observed" silicon elastic cross section. The major difference in the elastic displacement kerma comes from contributions near the 0.2 MeV resonance from the various evaluations. This discrepancy between the JEF and BROND cross section as compared to the ENDF, JENDL and CENDL cross sections needs to be resolved.

Initial speculations were that some of the variation in the elastic channel displacement kerma may have been due to the energy-dependent angular distributions and recoil modeling of the elastic angular distribution. This modeling varies considerably between evaluations. In fact, as shown in Figure 6, the difference is directly attributable to differences in the magnitude of the elastic cross section. The experimental data and code predictions for the elastic cross section in this region need to be re-examined and the sensitive nuclear data parameters identified.

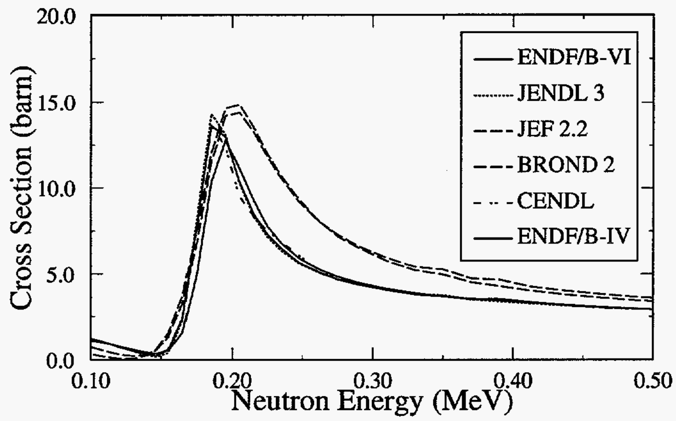

Figure 6. Silicon Elastic Cross Section

3.3. Propagation of Covariance

Neutron spectra, spanning the range from fast-burst reactor cavity spectra to pool-type reactor spectra, have been folded with the silicon damage covariance matrix to provide uncertainties in the calculated displacement kerma. Two estimates of the energy-dependent uncertainty in the silicon displacement kerma have been made. The first estimate represents the observed point-by-point uncertainty between the cross-section evaluations. The second estimate represents the uncertainty derived from the component-weighted sums of the ENDF/B-VI cross-section uncertainty values.

Four estimates of the spectrum-averaged displacement kerma have been made. The first estimate, σ_{calc}, represents the correct propagation of the displacement kerma with the reactor spectra using the calculated covariance matrix. The second estimate, $\sigma_{FC\text{-}calc}$, folds the group-averaged calculated damage uncertainty values with the reactor spectrum. This estimate does not treat the actual correlations between the various energy groups and between reaction channels. This estimate corresponds to the assumption of a fully correlated covariance matrix[11] and a mathematical analysis shows that it must always be greater than the case where the correlation is properly treated. The third estimate, σ_{obs}, represents a statistical analysis of the variation in the spectrum-averaged displacement kerma from the various cross section evaluations. This estimate, since the statistics are performed after the spectrum integration, includes all of the energy- and reaction-dependent correlation. The fourth estimate, $\sigma_{E\text{-}obs}$, folds the energy-dependent observed variation in the various displacement components with the reactor spectrum. This estimate, like the second, does not properly treat the energy- and reaction-dependent correlations and produces a larger uncertainty estimate consistent with the assumption of fully correlated errors. Table 1 shows the resulting silicon damage uncertainty for the SPR3CC fast-neutron spectrum produced in the central cavity of the Sandia National Laboratories (SNL) SPR-III fast burst reactor.

A comparison of the spectrum average of the silicon damage standard deviation with the fully propagated damage uncertainty for the calculated and the "observed" models demonstrates the importance of the off-diagonal elements of the covariance matrix. The true uncertainty is about half what would be obtained if the energy-dependent uncertainties are folded with the spectrum without a proper treatment of the energy- and reaction-dependent correlations.

Table 1. Uncertainty Analysis of Spectrum-Averaged Si Displacement Kerma in SPR-III Spectrum

Reaction	Reactor Spectrum: SPR3CC				
	Contribution	σ_{calc}	$\sigma_{FC\text{-}calc}$	σ_{obs}	$\sigma_{E\text{-}obs}$
Total	100.0%	2.27%	4.51%	5.55%	9.24%
Elastic	90.5%	2.55%	5.06%	6.32%	10.28%
Inelastic	8.8%	5.47%	11.32%	4.89%	12.81%
(n,p)	0.4%	17.09%	24.54%	20.97%	26.9%
(n,α)	0.2%	18.43%	23.31%	25.18%	29.3%
(n,γ)	<0.002%	83.2%	85.6%	183.7%	189.6%

This range of uncertainty in the silicon kerma is representative of typical research reactor spectra. Table 2 shows the correctly propagated uncertainty for other reactor environments available at the SNL facilities. A complete description of the reactor environments can be found in References 12 and 13.

Table 2. Silicon Damage Uncertainty For Various Reactor Environments

Spectrum Designator	Spectrum Description	Si Damage Uncertainty	
		σ_{calc}	$\sigma_{FC\text{-}calc}$
SPR3CC	SPR-III central cavity at fuel centerline.	2.27%	4.51%
SCR4	SPR-III 17-inch leakage	2.27%	4.52%
SPR_80A3	SPR-III 80-inch leakage	2.28%	4.50%
POLYCA48	2.54-cm Cd-poly liner in SPR-III cavity	2.24%	4.56%
PB23	Leakage from Pb box located 12-inches from SPR center.	2.34%	4.45%
ACF9	ACRR, a pool-type reactor, central cavity	2.29%	4.52%
WB7	Water bucket in ACRR cavity	2.28%	4.55%
TPB13	Pb-B bucket in ACRR cavity	2.31%	4.51%

Table 2 shows that the uncertainty in the spectrum-averaged response of silicon displacement damage sensors due to the knowledge of the cross section is about 2.3% for most reactor environments. This is comparable to the uncertainty in many dosimeters used routinely for spectrum determinations. This small an uncertainty in displacement kerma is not unexpected when one considered that 99% of the damage in reactor spectra comes from the elastic and inelastic reaction channels, which are well characterized.

This analysis has addressed only the uncertainty of the silicon displacement-damage response function. The behavior of a given silicon device may also be influenced by ionization effects, neutron rate effects, and annealing of initial defects. All of these effects must be considered in assigning an overall uncertainty to a reading from a silicon displacement sensor.

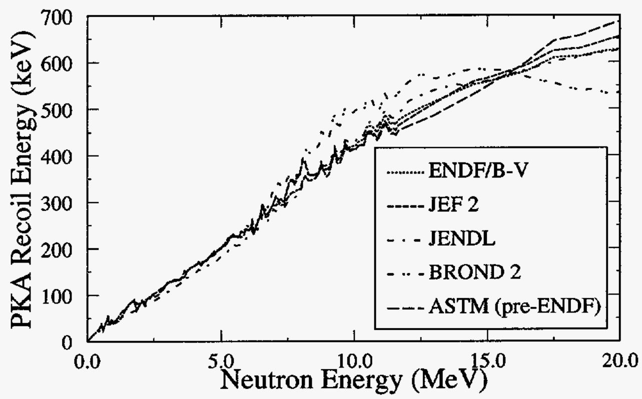

Figure 7. Variation in Observed Silicon PKA Spectrum

4. Future Work

This analysis of the contributions to the silicon displacement uncertainty has highlighted the importance of the contributions from the elastic cross section. Refinement in the elastic cross-section representation from 0.2 to 0. 4 MeV is important to any significant decrease in the calculated silicon damage uncertainty.

This analysis has accounted for the effect of cross section uncertainty on the uncertainty in the silicon displacement kerma. The uncertainty in the modeling of the recoil of the residual nuclei after an interaction has not been treated. Figure 7 shows that the various silicon cross sections show some variation in the predicted recoil spectrum for the primary knock-on atoms (PKA). This variation is only weakly coupled into the displacement kerma through the displacement partition function. Future work should quantify this contribution to the uncertainty of the silicon damage function.

5. Significance of Results

Energy-dependent damage covariance matrix is made available to the radiation testing community. The covariance matrix has been incorporated into the SNLRML[14] cross section compendium and will be distributed through the Oak Ridge National Laboratory Radiation Shielding Information Center as part of version 2 of the PSR-345 and DLC-178 code packages. This covariance will enable silicon displacement monitors to be used as sensors in spectrum adjustment codes.[15] The importance of cross-reaction and energy-dependent correlations is illustrated by comparison of two energy-dependent uncertainty estimators and four spectrum-averaged uncertainty estimators. Future work is needed to quantify the uncertainty component due to the modeling of the PKA recoil energy.

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