Uncertainty in Silicon Displacement Damage Metrics due to the Displacement Threshold Treatment[1]

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Abstract—This paper examines the influence of the displacement threshold energy and the treatment of the threshold on the 1-MeV(Si) response function. This uncertainty contribution is characterized in the form of a covariance matrix.

***Index Terms*—Displacement Kerma, Dosimetry, 1-MeV(Si), uncertainty, covariance matrix**

I. Introduction

The 1-MeV-Equivalent silicon damage function represents the most important metric in assessing neutron damage to semiconductors. The energy-dependence of this metric is captured in ASTM standard E722-14 Standard Practice for Characterizing Neutron Fluence Spectra in Terms of an Equivalent Monoenergetic Neutron Fluence for Radiation-Hardness Testing of Electronics [1]. This response function is also recommended as a direct dosimetry metric in ASTM E1855-15 Standard Test Method for Use of 2N2222A Silicon Bipolar Transistors as Neutron Spectrum Sensors and Displacement Damage Monitors [1] – supporting its use as both a direct characterization of the "quality" of radiation fields and as a sensor used in spectrum adjustments/unfolds to cover an energy region in research reactors not easily covered by non-fission based dosimetry sensors.

This damage metric is important because it captures, through the Messenger-Spratt equation [2], the relationship of the change in the minority carrier lifetime, or the gain degradation in silicon bipolar junction transistors, to the incident neutron fluence and spectrum. This paper examines the importance of the selection of the displacement threshold energy and the threshold model used to characterize the energy-dependent shape of this response near the displacement threshold energy. The guidance found in ASTM E1018-09(2013) Standard Guide for Application of ASTM Evaluated Cross Section Data File requires that dosimetry-quality sensors capture the uncertainty in the response through an energy-dependent covariance matrix. This paper establishes one contribution to this uncertainty by appropriately characterizing the effect on the uncertainty of the treatment of this threshold modeling in the response function.

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II. Damage Metrics

The fundamental metric that one looks at in order to characterize the energy-dependence of the 1-MeV(Si) response is the number of defects introduced by the incident neutrons. Most approaches start with a consideration of the number of Frenkel pairs, or vacancy-interstitial pairs, introduced by the irradiation. This number of initial Frenkel pairs is proportional to the displacement kerma, which is, in turn, related to the non-ionizing energy loss (NIEL).

A displacement model is used to relate the number of displaced atoms, ν_d, to the lattice damage introduced by the recoiling atoms from a neutron interaction. The non-ionizing damage from a recoiling ion is characterized by the ion damage energy, ${}^{ion}T_{dam}$. Several models are used by the community. In order to differentiate these models we adopt the notation of ${}^{type}\nu_d$ to distinguish the various Frenkel pair production models. In order to support a discussion of various damage metrics and, in particular, to provide a clear consistent definition of the damage energy, we elect to break up the displacement model into:

- a threshold function, ${}^{type\text{-}A}\Lambda(E_d, {}^{ion}T_{dam})$;
- a Frenkel pair generation efficiency component, ${}^{type\text{-}B}\zeta_d(E_d, {}^{ion}T_{dam})$; and
- a residual defect efficiency survival term, ${}^{type\text{-}C}\xi({}^{ion}T_{dam})$.

Thus,

$$ {}^{type}\nu_d\left(E_d, {}^{ion}T_{dam}\right) = {}^{type-A}\Lambda(E_d, {}^{ion}T_{dam}) \cdot {}^{type-B}\zeta_d(E_d, {}^{ion}T_{dam}) \cdot {}^{type-C}\xi({}^{ion}T_{dam}) \qquad \text{Eqn. 1} $$

A. Historical Displacement Models

The original Kinchin-Pease model [3-6] relates the number of defects, ${}^{orig\_K\&P}\nu_d(E_d, E_l, T_R)$, to the primary recoil atom energy:

$$ {}^{orig\_K\&P}\nu_d\left(E_d, E_l, T_R\right) = \begin{pmatrix} 0 & 0 \le T_R < E_d \\ 1 & E_d \le T_R < 2 \cdot E_d \\ T_R / (2 \cdot E_d) & 2 \cdot E_d \le T_R < E_l \\ E_l / (2 \cdot E_d) & E_l \le T_R < \infty \end{pmatrix} \qquad \text{Eqn. 2} $$

where E_I is the energy is the energy above which ions lose their energy only through ionization and below which energy loose could be modeled with an elastic hard sphere scattering model; E_d is the displacement threshold energy; and T_R is the recoil atom energy.

When this was coupled with the LSS model for the energy partition function, then there was no longer a need to introduce the E_I energy and the equation could be rewritten as a function of ${}^{ion}T_{dam}$. The commonly seen version of the Kinchin-Pease model uses this LSS energy partition function to define ${}^{K\&P}\nu_d(E_d, {}^{ion}T_{dam})$.

The Kinchin-Pease model is sometimes quoted as using a sharp transition to define ${}^{sp\_K\&P}\nu_d(E_d, {}^{ion}T_{dam})$, the transition being modeled as occurring at E_d. This is the formalism for the damage energy that is built into codes such as NJOY-2012.

The community has examined various forms for the number of Frenkel pairs resulting from different analytic forms of the differential elastic scattering cross section between atoms, represented by a screened Coulomb interaction. The Robinson-Sigmund modification [5], while imposing a consistency condition on the average number of Frenkel pairs produced in a random cascade, calculated an asymptotic solution for $E > 2E_d$ that led to the introduction of a factor of $\beta=(12/\pi^2)/\ln(2)=0.84$ in the Kinchin-Pease expression for the breakpoint energy of the transition region.

B. Norgett-Robinson-Torrens (NRT) Displacement Model

After the original Kinchin-Pease formulation, the radiation damage community did additional theoretical work and computer simulations. A group of experts at an IAEA Specialist's meeting on radiation damage units adopted a modified formulation for the number of displacements. This approach used the Robinson-Sigmund modification of the hard-sphere scattering energy loss model. This model is called the Norgett, Robinson, and Torrens (NRT) Frenkel pair model, or the modified Kinchin-Pease, and is given by:

$$ {}^{NRT}\nu_d\left(E_d, {}^{ion}T_{dam}\right) = \begin{cases} 0 & 0 \le {}^{ion}T_{dam} < E_d \\ 1 & E_d \le {}^{ion}T_{dam} < 2\cdot E_d / \beta \\ \beta \cdot {}^{ion}T_{dam} / (2\cdot E_d) & 2\cdot E_d / \beta \le {}^{ion}T_{dam} < \infty \end{cases} \quad \text{Eqn. 3} $$

where β is an atomic scattering correction and is taken to be 0.8. This adopted value of 0.8 is close to the analytically derived asymptotic value used in the Robinson-Sigmund analysis.

C. Other Displacement Models

Other displacement damage models that assign a different amount of damage energy to the creation of a Frenkel pair can be found in the literature. These models include:

- Synder-Neufeld: ${}^{SN}\varsigma_d\left(E_d, {}^{ion}T_{dam}\right) = \left({}^{ion}T_{dam} + E_d\right) / (2 E_d)$
- Neufeld-Synder: ${}^{SN}\varsigma_d\left(E_d, {}^{ion}T_{dam}\right) = \left({}^{ion}T_{dam} + E_d\right) / (3 E_d)$

Bacon [7, 8] used MD calculations that modeled the many-body effects of the thermal spike phase in the cascade development and found that the results could be fit with an exponential applied to the Frenkel pair generation efficiency term. The Bacon fit the MD results for various metals and observed a trend of decreased Frenkel pair production with increasing recoil ion energy.

Actual device behavior is more complicated than a simple consideration of Frenkel pairs because the defects evolve and all defects are not equal with regard to their effect on the degradation of the minority carrier lifetime. For late-time gain degradation in silicon, the primary contributors are divacancies (V_2) and vacancy-phosphorus (VP) defects, i.e. complex defects that evolve from the primary Frenkel pair damage. Furthermore, defect recombination within clusters could lead to an enhanced recombination of defects for high recoil ion energy. This led to displacement models that incorporated a residual defect efficiency survival term. These models include [9]:

- athermal recombination-corrected dpa (arc-dpa)
- replacement per atom (rpa)

Models for displaced atoms do not cover the total range of ways that "defects" can be introduced into materials through irradiation. All "defects" introduced into materials cannot necessarily be attributed to displaced lattice ions. In silicon, broken bond pairs, not just vacancy-interstitial pairs, can result in electrically active defects in silicon. Defect production from ionization has also been observed in insulating materials such as SiO_2 [10, 11]. This observation complicates attempts to correlate observed defect production metrics with calculated quantities using non-ionizing energy deposition. In silicon semiconductors, trapped charge in the insulating SiO_2 can result in electric field that affect the gain in bipolar semiconductors and further complicates the interpretation.

III. Effect of Metrics

A. Variation of Selected Metric

Figure 1 shows that the difference between the various damage metrics discussed above is negligible except in a narrow neutron energy range between 100 eV and 1 keV. Due to the range of values for the displacement kerma, the logarithmic y-axis in Figure 1 makes the difference between the curves hard to discern. Figure 2 shows an expanded view of this region where the differences are more apparent.

To better highlight this difference, Figure 3 shows the difference between the various quantities, expressed as a percent variation, [displacement kerma – damage energy]/[displacement kerma]*100. Figure 3 shows a significant variation, greater than 50%, between the displacement kerma and the damage energy near 170 eV and a noticeable difference in the general neutron energy region between ~150 eV and ~400 eV. The difference between these metrics in this neutron energy region is due to the fact that elastic scattering is the dominant reaction in this region and conservation of momentum and energy for each elastic interaction results in a maximum energy transfer to a lattice atom given by:

$$E_{recoil} = \frac{4 \cdot A \cdot E_n}{(A+1)^2} \qquad \text{Eqn. 4}$$

where E_n is the energy of the incident neutron and A is the atomic weight of the lattice atom. The case where the lattice recoil energy in silicon from elastic scattering is equal to a displacement threshold energy of 20.5 eV corresponds to an incident neutron energy of ~153 eV. For lower neutron energies the deviations seen in Figure 2 are very small since the displacement kerma is dominated by the contributions from the (n,γ) reaction, which kinematically permits a larger recoil energy for the residual ion, so that the lower integration bound for the displacement threshold energy no longer plays an important role in the damage energy calculation.

IV. Displacement Threshold Energy

A. Experimental

The status of experimental data is succinctly captured in Reference [12]:

> "E_d is poorly known in the material (Silicon). Experimental methods show a widely varying scale of results for E_d in the range of 10 – 30 eV."

The minimum displacement threshold energy in the <111> direction in silicon has been measured as 13 eV [13, 14]. Reference [15] noted an energy difference for creation of divacancies and oxygen-vacancy pairs noting "it is still a convenient concept, however, to refer to an effective threshold (of 21 eV in this case) in this energy range". A good baseline experimental value of 20.5 ± 1 eV comes from the Reference [16] and was derived from capacitance-voltage measurements on gold-silicon Schottky diodes using electron irradiation.

B. Theoretical

Molecular dynamics (MD) calculations by [17] indicate that the silicon displacement threshold energy varies from 10 - 15 eV. Different values could be selected based on different assumptions for the relevant time for observation of a phenomenon, and hence on the time at which the Frenkel pair exists. For an application to electronic lifetime degradation, kinetic Monte Carlo or other defect annealing treatments should be used to transform this early-time displacement metric into a relevant late-time metric.

The application of the E_d in binary collision approximation codes was studied in Reference [18]. They observed:

> "The displacement threshold energy is the energy that a target atom needs to leave its lattice site and form a stable interstitial. Its values given in the literature range from ~9 to 35 eV for silicon ..."

Work in 2008 [12] studied the displacement threshold energy in silicon using density functional theory (DFT) and molecular dynamics simulations. Consistent results were found using both the local density approximation (LDA) and the generalized gradient approximation (GGA). The DFT and Hartree-Fock (HF) methods "provided repulsive potentials which are significantly improved compared to the standard universal ZBL potential" [19]. The average threshold energy, over all lattice directions, for the creation of stable Frenkel pairs was found to be 36 ± 2 eV; in the <100> direction it was 20 ±2 eV; in the <111> direction it was found to be 12.5 ± 1.5 eV. Reference [12] notes that:

> "The common usage of 13 and 15 eV for the value of the parameter (displacement threshold energy) is highly inappropriate, as from our calculations it is clear that the actual value is over a factor of two higher."

C. Recommended

For comparison of 1-MeV(Si) displacement damage, the recommendation, at this time, for the value of E_d is 20.5 eV. This selection is based upon consideration of the best experimental values [16], 20.5 ± 1 eV, and the latest high fidelity DFT-MD modeling [12] value, 24 ±2 eV, and recent comparisons between BCA and MD modeling, which recommend using 20 eV.

V. Effect of the Threshold Treatment

Section *III.A* compared the difference between the displacement kerma, basically the damage energy with a zero eV lower integration bound, and the damage energy when a nominal/recommended displacement threshold energy of 20.5 eV is used and E_d is selected as the lower integration bound for the damage energy integral. As discussed in Section *IV.A* and *IV.B*, there is significant uncertainty in the value for the displacement threshold energy. For silicon, the range found in both experimental investigation and in model-based calculation is between 10 eV and 30 eV.

Figure 4 shows the variation in the damage energy (with E_d as the lower integration bound) that can result from this range of possible values for the displacement threshold energy in silicon. The figure shows the percent difference relative to the nominal/recommended displacement threshold energy of 20.5 eV. The maximum deviation seen in Figure 4 between damage energies with different E_d values [relative to E_d = 20.5 eV] is more than the variation seen in Figure 3 between damage metrics because the deviation, and the denominator of the difference, in Figure 3 is that for the larger displacement kerma, essentially a damage energy with E_d = 0 eV.

The multi-group representation of this variation can be affected by the granularity of the energy bin structure. The above analysis used a fine 640-group structure. When one wants to determine an energy-dependent correlation in a parameter where non-linear error propagation plays an important role, a Monte Carlo sampling process is typically employed. Sample size considerations motivate the use of a coarser energy grid structure, 89-groups in our analysis.

We quantified the change in the damage energy when the displacement threshold energy is varied using a Total Monte Carlo (TMC) approach to capture the nonlinear change in the damage energy. The energy-dependent standard deviation in the magnitude of the response is shown in Figure 5. The energy-dependent correlation matrix is shown in Figure 6.

VI. Conclusion

This paper examined the range of metrics that can be used to characterize the energy-dependence of the 1-MeV(Si) response as manifest by the observed degradation in the minority carrier lifetime. The sensitivity to the selection of the

damage energy metric was examined and the "NRT damage energy" was selected as the most appropriate damage metric. Using this metric, the uncertainty in the displacement threshold energy was examined from both an experimental and theoretical perspective, and the effect of this uncertainty was propagated into the response function and characterized by a covariance matrix.

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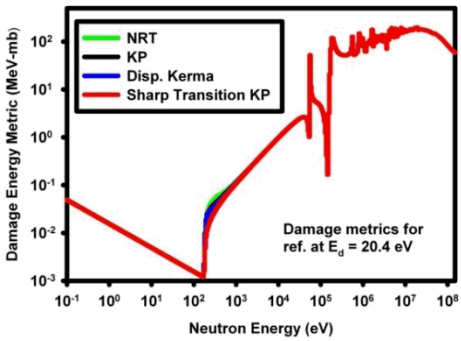

Figure 1. Comparison of Variation of the Damage Energy Metric

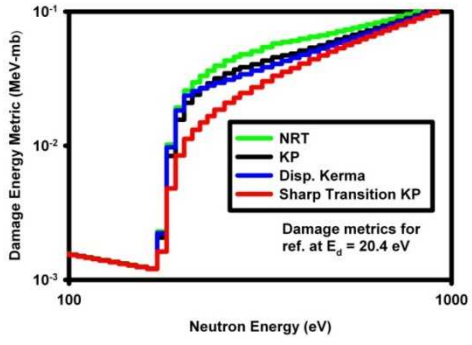

Figure 2. Expanded View of the Comparison of Variation of the Damage Energy Metric

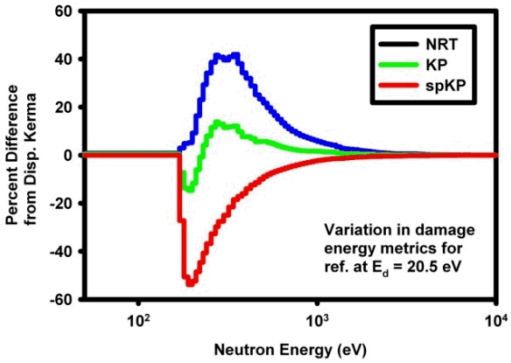

Figure 3. Percent Difference between Displacement Kerma and Damage Energy

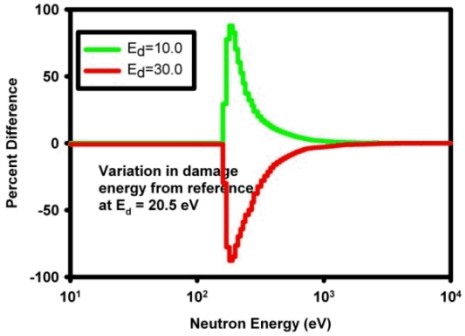

Figure 4. 640-Group Representation of the Percent Variation in the Damage Energy Induced by the Choice of the Displacement Threshold Energy

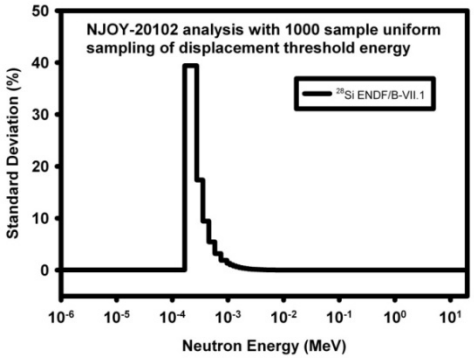

Figure 5. 89-Group Representation of Standard Deviation of the Damage Energy when the Displacement Threshold Energy is Varied

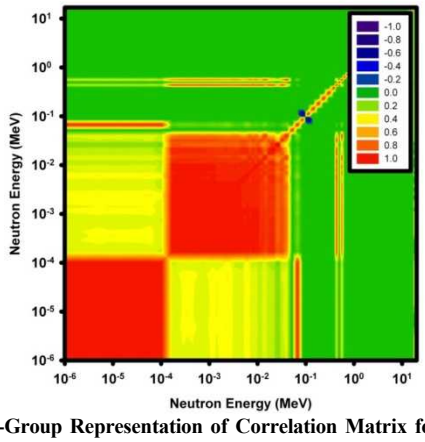

Figure 6. 89-Group Representation of Correlation Matrix for the Damage Energy when the Displacement Threshold Energy is Varied with Uniform Sampling