Nonionizing Energy Loss (NIEL) for Heavy Ions

S.R. Messenger[1], E.A. Burke[2], G.P. Summers[3,4], M.A. Xapsos[4], R.J. Walters[4], E.M. Jackson[1], and B.D. Weaver[4]

[1]SFA, Inc., Largo, MD 20774

[2]Consultant, Woburn, MA 01801

[3]Physics Department, University of Maryland Baltimore County, Baltimore, MD 21250

[4]Code 6825, Naval Research Laboratory, Washington, DC 20375

Abstract

The concept of nonionizing energy loss (NIEL) has been found useful for characterizing displacement damage effects in materials and devices. Published tabulations, however, are limited with respect to target materials, particle types and energies. In this paper we show how the NIEL database can be significantly expanded to include heavy ions in the coulombic limit by using the Monte Carlo code SRIM. The methodology used to extract NIEL from SRIM is described. This greatly adds to the number of materials and incident particles for which the NIEL concept can be applied. To show that values so derived are consistent with previous calculations, we compare alpha particle NIEL for GaAs derived from SRIM with a direct analytical calculation. The SRIM code is limited in that only coulombic interactions are considered. General rules of thumb are also described which permit prediction of NIEL for any target material over a large energy range. Tabulated values of NIEL for alpha particles incident on Si, GaAs and InP are presented.

I. INTRODUCTION

Nonionizing energy loss (NIEL) [1-3] has been applied to a number of problems concerning displacement damage effects in materials and devices over the past decade. Examples have included solar cells, high temperature superconductors, optical sensors, and high energy (>GeV) particle detectors. The utility of the concept rests upon the fact that, to a good approximation, displacement damage effects produced by many different particles over a wide range of energies are proportional to the nonionizing energy losses of the primary particle and the energetic nuclear recoils it produces. For example, in the case of high temperature superconductors, it was found that the reduction in the critical temperature was proportional to NIEL when the latter varied by over 8 orders of magnitude [4,5]. It has also been demonstrated that the number of ground experiments required to characterize the response of devices such as solar cells to complex radiation environments can be significantly reduced [6,7] by using the NIEL approach rather than previous techniques. It has been pointed out [3] that NIEL, which is analogous to ionization energy loss or stopping power [6], can be easily incorporated into existing Monte Carlo transport codes to estimate displacement damage effects. This considerably simplifies the task of forecasting the response of devices irradiated at one particle energy to that at another energy, or a spectrum of energies.

Although the NIEL approach has wide applications, published tabulations are limited with respect to the target materials, particle types and energies. This is due in part to the fact that calculations over a wide energy range are not straightforward. They can involve coulombic, nuclear elastic and spallation (nuclear inelastic) interactions. Summers *et al.* [1] have tabulated electron (and ^{60}Co γ's) and proton NIEL values for Si, GaAs, and InP as a function of energy. Van Ginneken [3] has published NIEL curves for electrons, protons, pions, muons, photons, and neutrons in silicon as a function of energy. In this paper we show how existing programs and data can be used to markedly extend the number of particles and materials to which the NIEL concept can be applied. Our purpose here is to give other users the ability to calculate NIEL values for their own specific applications.

We have found that the Monte Carlo code SRIM (formerly TRIM) [8] can be used to fill gaps in the existing tabulations of NIEL. This code describes ionization and displacement damage interactions for all positive ions over a wide range of energies and for a large number of elements and compounds including multi-element compounds such as high temperature superconductors. It is limited to coulombic and non-relativistic interactions, but for heavy ions, the useful energy range can extend beyond 100 MeV. We have found that our previous calculations for protons and alpha particles overlap SRIM results over a broad energy region. The results compare on an absolute basis, i.e. no fitting parameters are needed.

In this paper we first briefly review the concepts of NIEL and displacement damage dose. We then present several applications of NIEL, some of which have not been published to date or have received only limited distribution. This is followed by sections giving a detailed description of the methodology used to derive NIEL from SRIM, and methods of obtaining approximate estimates of NIEL for protons, alpha particles and electrons. The essential points are summarized in the last section. Two appendices are included, the first one describing a step-by-step procedure in the SRIM-NIEL calculation, and the second one giving tabulated NIEL values for alpha particles incident in Si, GaAs and InP in the coulombic limit.

II. NONIONIZING ENERGY LOSS (NIEL)

NIEL is the rate at which energy is lost to nonionizing events (energy per unit length) [1,2]. It is a direct analog of the linear energy transfer (LET) or stopping power for ionization events [6]. The units of NIEL are typically MeV/cm or MeV cm^2/g. The calculation of NIEL requires information regarding the differential cross section for atomic displacements ($d\sigma/d\Omega$), the average recoil energy of the target atoms (T), and a term which partitions the energy into ionizing and nonionizing events, called the Lindhard partition factor (L). NIEL can be written as an integral over solid angle [1,2], i.e.

$$\mathrm{NIEL}(E) = \frac{N}{A}\int_{\theta_{min}}^{\pi}\left(\frac{d\sigma(\theta,E)}{d\Omega}\right)T(\theta,E)L[T(\theta,E)]d\Omega \quad (1)$$

where the N is Avogadro's number, A is the atomic mass, and θ_{min} is the scattering angle for which the recoil energy equals the threshold for atomic displacement.

At present, NIEL can be calculated analytically for electrons, protons, and alpha particles over a large range of particle energies. This is due to the availability of analytical forms for the differential cross sections for atomic displacement. For protons and alpha particles having non-relativistic energy, the simple Rutherford differential cross section can be used for elastic events. For energies where relativistic effects become important, optical model calculations can be used to account for nuclear elastic events for many positive ions. For higher energies (>100 MeV for protons), nuclear inelastic contributions can be obtained using empirical data. Fortunately, for electrons, coulombic events are dominant over the entire energy range of interest. The Mott expression for the differential cross section is used in the electron NIEL calculation [9]. Various approximations are used for the Lindhard factor. References 1 and 2 contain much of the details of the NIEL calculation.

The results of NIEL calculations were tabulated for electrons and protons in Si, GaAs, and InP in the proceedings of the 1993 NSREC [1]. Included herein (see Appendix II) are tabulations for alpha particle NIEL for these same elements for energies up to 50 MeV. Only the Rutherford interaction is included in this calculation. The calculations for the compounds GaAs and InP were obtained from combining the individual NIEL contributions from the constituent atoms using the Bragg rule (i.e. via weight fractions). The thresholds for atomic displacements in Si, Ga, As, In, and P were 21, 10, 10, 6.7, and 8.7 eV, respectively [1,10,11].

III. EXAMPLES OF NIEL APPLICATIONS

The effects of irradiation on the electrical parameters of many materials have been found to display a simple relationship with NIEL. As an example, the particle-induced degradation of the transition temperature of high temperature superconductors has been shown to be linearly proportional to NIEL [4,5]. Figure 1 shows the results for several different superconductor materials, where a large range of particles and energies has been plotted. It can be seen in Fig. 1 that the change in the transition temperature is linearly dependent on NIEL for over 8 orders of magnitude. The heavy ions shown in Fig. 1 range in atomic number from 2(He) to 54(Xe).

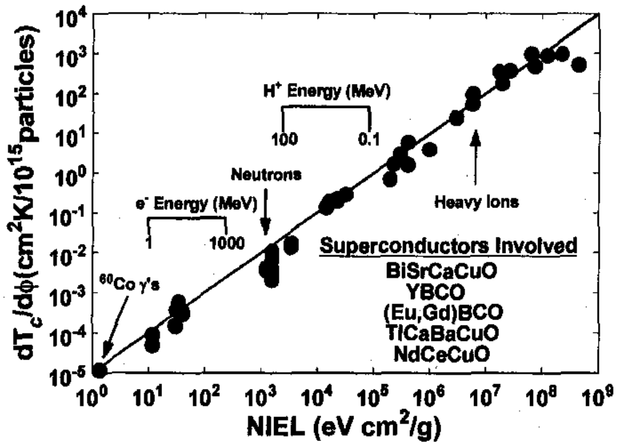

Figure 1. Radiation-induced change in the transition temperature as a function of NIEL [4,5]. A linear dependence exists for over 8 orders of magnitude. The heavy ions shown range in atomic number from 2(He) to 54(Xe)

More recently the particle-induced degradation of many device parameters has been analyzed in terms of another concept, i.e., displacement damage dose, D_d [6,7]. D_d, which is the product of NIEL and the particle fluence, is exactly analogous to ionizing dose where the latter is the product of the LET and the particle fluence. The concept of D_d can greatly simplify the prediction of displacement damage effects in complex particle environments because only a few ground measurements are required to generate the expected effect of an entire spectrum of energetic particles. As an example we consider the case of GaAs/Ge solar cells. Figures 2a and 2b shows the results for the normalized maximum power degradation of GaAs/Ge solar cells, as reported by Anspaugh [12,13]. Anspaugh reported the radiation response of GaAs/Ge solar cells for 8 proton and 4 electron energies. Figure 2a shows the results, normalized to pre-irradiation values, plotted as a function of particle fluence. Replotting this data as a function of D_d in Fig. 2b yields a single, characteristic curve. The curve shown in Fig. 2b could obviously have been obtained by measurements made at only one particle energy.

The applicability of the D_d approach has now been demonstrated in the analysis of actual space radiation data. Figure 3 shows the maximum power degradation of GaAs/Ge solar cells measured as a function of time on the PASP Plus space experiment, flown on the APEX satellite. [14,15]. In this experiment, solar cell data were taken for a total of 373 days in a proton-dominated orbit. The maximum power degradation data shown by the solid circles in Fig. 3, as measured by the space experiment, was for albedo-free and temperature-corrected conditions for cells covered by 6 mil

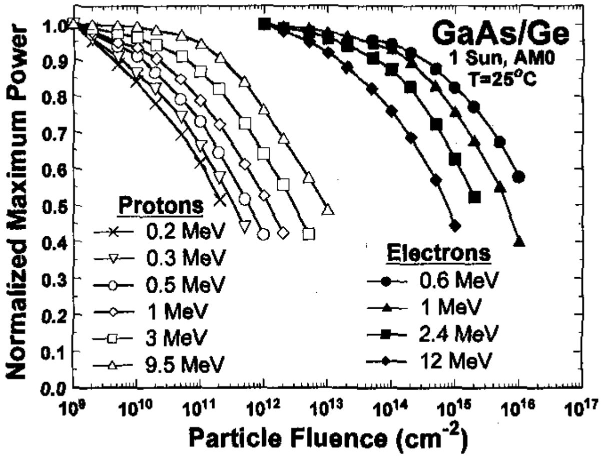

Figure 2a. Normalized maximum power degradation of GaAs/Ge solar cells as a function of proton and electron fluence [12,13]. The normalization was with respect to pre-irradiation values.

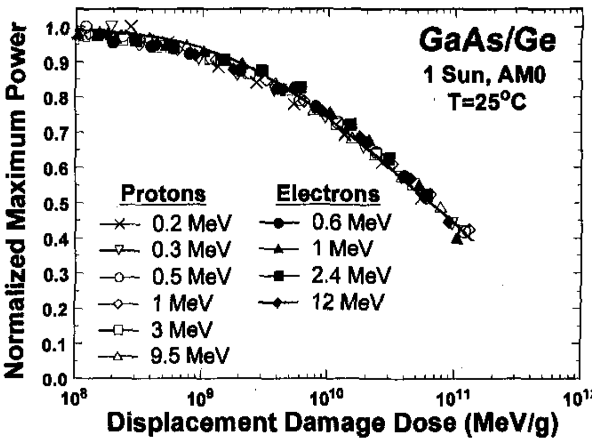

Figure 2b. Normalized maximum power degradation of GaAs/Ge solar cells as a function of displacement damage dose. The effects of the many different particles and energies shown in Fig.2a can be reduced to a single, characteristic curve.

CMG coverglasses. Because of the cell location the backshielding was effectively infinite. In the calculations, the values for D_d were determined for each day of the mission using the appropriate slowed-down proton spectrum that traversed the coverglass [16,17]. The incident spectrum was taken from the standard AP-8 proton environment and IGRF magnetic field models using the given ephemeral data for the APEX orbit (2552x363 km, 70° inclination, 8/3/94 to 8/11/95). The line in Fig. 3 shows the results of the calculation as generated by a computer code called SAVANT [15], presently being developed in a joint effort by NRL and co-workers at NASA Glenn Research Center. It can be seen that the calculation correctly predicts the actual degradation to a typical accuracy of better than 1%, including the undulations caused by precession of the orbit.

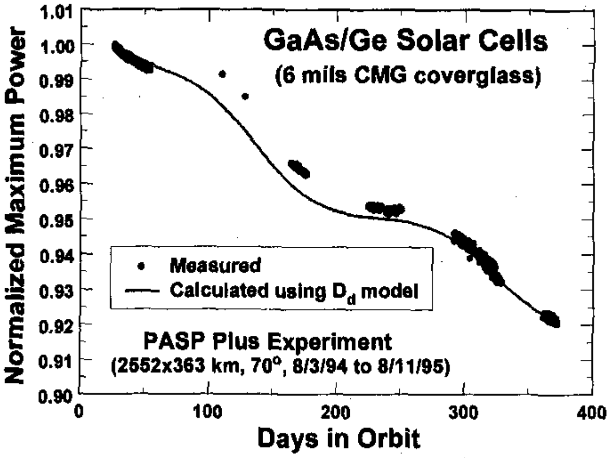

Figure 3. Measured and calculated normalized maximum power degradation of GaAs/Ge solar cells onboard the PASP Plus space experiment [14]. The displacement damage dose model is seen to predict the actual degradation with an accuracy of better than 1% over the entire mission. The solid line was calculated using the computer code SAVANT [15], being developed jointly by NRL and NASA Glenn Research Center.

IV. SRIM-NIEL CALCULATION

In this section we outline how NIEL can be determined using the widely used computer code SRIM [8]. A more detailed description can be found in Appendix I. SRIM [8] is a Monte Carlo code used for calculations of ion penetration in a wide range of solids. Examples include semiconductors, metals, inorganic insulators, polymers and high temperature superconductors.

Two data files from SRIM known as IONIZ.TXT and VACANCY.TXT contain the information necessary to derive the NIEL data. In the case of both ionization energy loss and vacancy production SRIM divides the particle path into 100 distance intervals. The total energy loss rate is given at each interval for both the incident particle and the resultant recoils. The file IONIZ.TXT provides ionization energy loss rates in units of eV/Å/ion, while the file VACANCY.TXT provides vacancy formation information in units of the number of vacancies/Å/ion. Both files give the spatial information in units of Å. Figure 4 shows such SRIM output, with the results presented in units of keV and μm. The IONIZ.TXT file provides a measure of particle energy at each interval while VACANCY.TXT provides a measure of the number of displacements. The SRIM file VACANCY.TXT is used in the calculation of NIEL, while both SRIM files are used in the correlation of particle depth with particle energy.

The vacancy formation rate can be converted into NIEL using the modified Kinchin-Pease relationship between the number of atomic displacements, N_d, and a given quantity of nonionizing energy, E_n [18], i.e.,

$$N_d = 0.8\frac{E_n}{2T_d} \qquad (2)$$

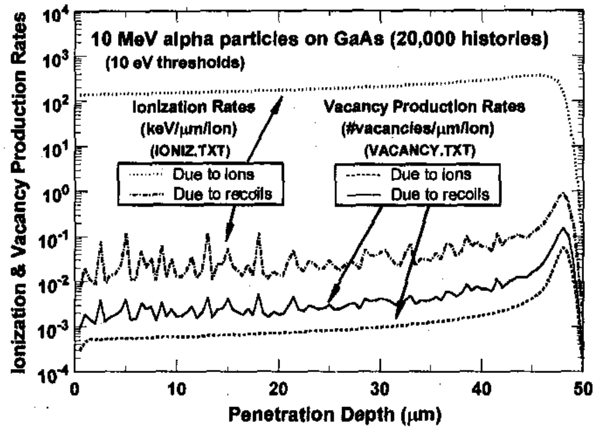

Figure 4. Results of a SRIM run for 20,000 10 MeV alpha particles incident on GaAs. The data from the files IONIZ.TXT and VACANCY.TXT are plotted as a function of penetration depth. The units on the ordinate are keV/μm/ion and # vacancies/μm/ion for the ionization and vacancy data, respectively. The displacement threshold energies were set at 10 eV for both Ga and As.

where T_d is the threshold energy for atomic displacement (usually on the order of a few tens of eV's). Equation (2) applies for $E_n > 2.5T_d$. The number of vacancies produced by both the incident particle and the resultant recoils must be added together to obtain the total NIEL. In this way the NIEL as a function of penetration depth is obtained. Figure 5 shows a plot of the results.

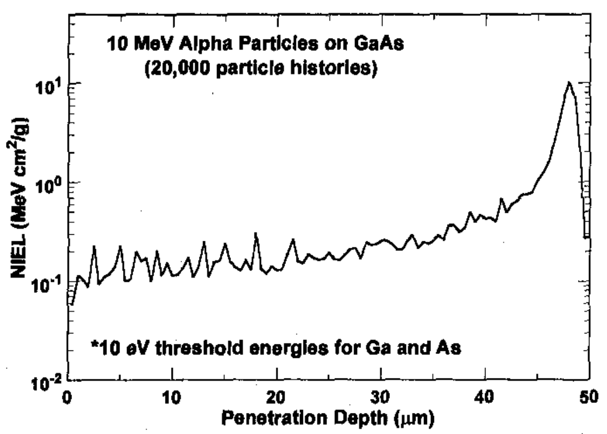

Figure 5. NIEL as a function of ion penetration depth derived from SRIM data. Only the SRIM file VACANCY.TXT is required for this result.

In order to obtain the NIEL as a function of particle energy from the results shown in Fig. 5, we must first determine the incident particle energy as a function of depth. This can be accomplished by combining the results from the files IONIZ.TXT and VACANCY.TXT to determine the total energy lost in each of the 100 path intervals. The result is shown in Fig. 6.

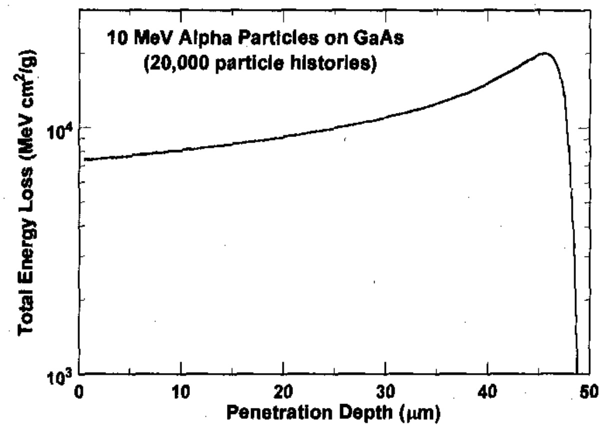

Figure 6. SRIM results for the total energy loss as a function of penetration depth for 10 MeV alpha particles incident on GaAs.

Figure 6 resembles the result for ionization loss except at the end of the track where displacement interactions become dominant. By subtracting the total cumulative energy losses along the particle track it is possible to establish the particle energy as a function of depth. The result of this operation is shown in Fig. 7. The connection between NIEL and particle energy is thereby established. The final result is given in Fig. 8, which compares the results of the SRIM calculation with a first principles analytical calculation of the alpha particle NIEL as a function of energy.

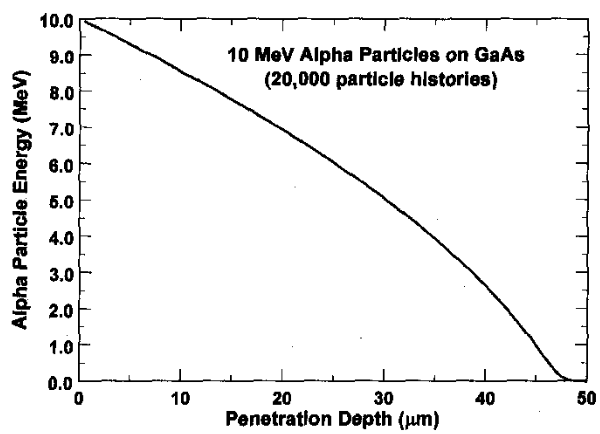

Figure 7. Alpha particle energy as a function of depth in GaAs derived from the data shown in Fig. 6.

Figure 8 also shows the results obtained using SRIM but with an incident alpha particle energy of only 1 MeV. Notice that the SRIM-derived NIEL values coincide absolutely with the analytic curve for a certain energy range, and then deviate from it. For 10 MeV alpha particles, the analytic and SRIM-derived NIEL values start to deviate at about 100 keV. Using 1 MeV alpha particles, the deviation energy is extended a little lower, to about 20 keV. The divergence is due in part to straggling. That is, the analytic calculation gives the NIEL corresponding to a specific particle energy, whereas in the SRIM results, the particles are slowed down from a higher energy. Therefore at a given depth the particles will have a range of energies.

The Monte Carlo origin of the results shown in Fig. 8 is evident at the higher particle energies for each incident alpha particle where there are fewer interactions per unit pathlength. As the particle slows down, the statistics improve and the fluctuations become less apparent. The high energy fluctuations can be improved using a larger number of particle histories. However, due to the statistics involved, a factor of 100 more particle histories only gives a factor of 10 better resolution.

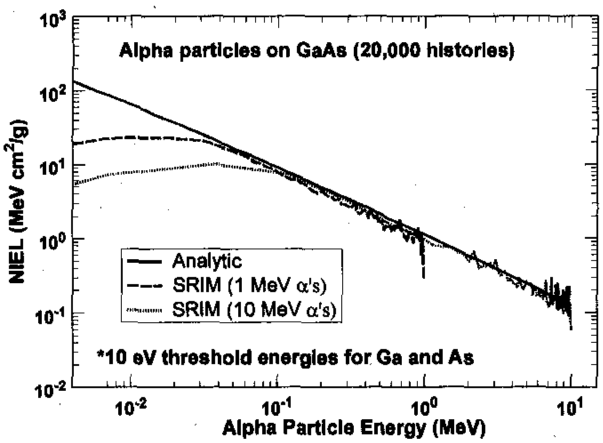

Figure 8. NIEL as a function of particle energy derived from the data shown in Figs. 5 and 7. Also shown is the SRIM result for incident 1 MeV alpha particles to show that the choice of incident particle energy can be important.

V. NIEL AT HIGH ENERGIES FOR LIGHT PARTICLES

For electrons, protons and alpha particles the NIEL is relatively insensitive to the nature of the target. This is especially true of protons as shown in Fig. 9 where analytical NIEL values for electrons, protons, and alpha particles incident on various elements (C, Si, Y, and In) and the compound GaAs are plotted as a function of particle energy. Many of these calculations have been described in earlier publications [1,2]. The values of the displacement threshold energies were taken from References 10 and 11. The values for Y and In are those for elements when they are in an compounds and are intended to illustrate how NIEL varies with atomic number. This arises because NIEL must be calculated for each element separately in a compound and combined using the Bragg rule. For the alpha particle and electron NIEL calculations, only the coulombic contributions are included. The proton NIEL values also include an optical model calculation for the nuclear elastic contribution. Nuclear inelastic contributions are not included in any of the calculations shown in Fig. 9.

Figure 9 allows the effect of Z to be shown on the results. In the alpha particle case, the lower Z elements have larger NIEL values at a given energy. A slight Z dependence can also be observed in the proton NIEL, especially at lower proton energies. Also in the proton NIEL case, the Z dependence of the optical model calculations can be observed. Nuclear elastic contributions were only significant for the lower Z elements for energies higher than about 10 MeV. The electron NIEL values display no clear Z dependence, but show ambiguities at the lower energies. This is due in large measure to the value of the displacement threshold energy used in the calculation.

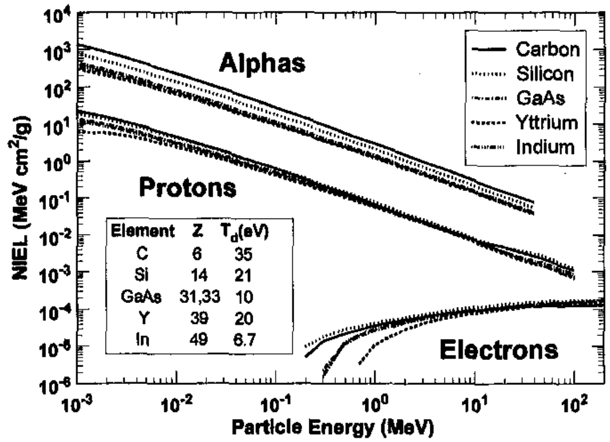

Figure 9. Analytical calculations of NIEL for electrons, protons, and alpha particles for several different target materials.

For a given element, the effect of displacement threshold energy is an important consideration in the calculation of the electron NIEL, especially at energies near threshold. Figure 10 shows this effect for electrons in silicon where the calculations were performed using atomic displacement threshold energies of 5, 12.9, 21, and 30 eV, respectively. The low energy portion of the curve is shifted to the right as the displacement threshold is increased. As the energy range where the shift occurs can be of considerable interest (especially at 1 MeV for solar cell irradiations), the determination of the threshold energy for atomic displacement is a key factor in the NIEL calculation for electrons. The values of 5 and 30 eV are used here for the purpose of illustrating the impact of threshold energy. The value of 12.9 eV has often been cited as a suitable value for Si but 21 eV has proven to yield better agreement with experiments when a broad spectrum of electrons are involved. The threshold energy also affects the energy at which the NIEL falls to zero for incident protons and alpha particles (not shown in Fig. 9), but there is negligible effect at higher energies which usually is usually the region of interest.

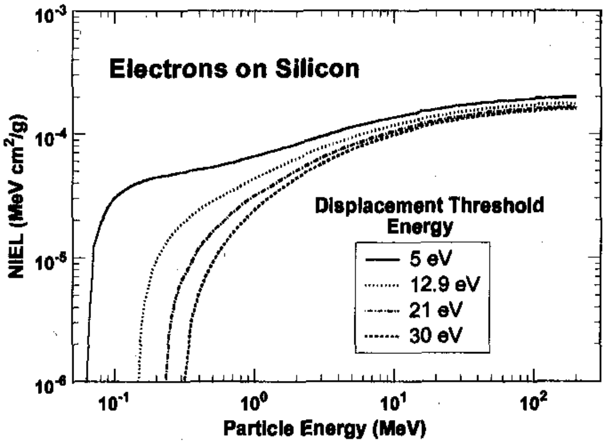

Figure 10. The effect on the NIEL for electrons in silicon of varying the threshold energy for atomic displacement from 5 to 30 eV.

VI. SUMMARY

We have reviewed a number of successful applications of NIEL and the related concept of displacement damage dose. Several examples have been given which demonstrate how the effects of irradiation on the electrical parameters of different materials display a direct dependence on NIEL. Exploiting this dependence allows accurate prediction of device performance in a complex radiation environment from analytical calculations based on a minimum of ground-based test data. The chief impediment to further applications has been the lack of tabulations for a variety of materials and particle types over a wide range of energies. The NIEL calculations are not straightforward since they involve coulombic, nuclear elastic and spallation reactions. Consequently, available data tabulations have been limited in scope and have been confined to electrons and light ions.

A procedure has been outlined to show how NIEL for heavy ions can be extracted from the SRIM code. This not only adds to the number of particles for which data is available but vastly increases the types of target materials for which NIEL can be determined. The chief limitation of the SRIM code is that nuclear elastic and spallation interactions are not included. Although the results are therefore confined to the energy region where coulombic interaction dominate, the methodology enables the transformation of data obtained with heavy ions into an equivalent fluence of monoenergetic particles, e.g. 10 MeV protons or 1 MeV equivalent electrons.

Finally we have shown that proton and alpha particle NIEL is relatively insensitive to the atomic number of the target atom up to the energy range where nuclear elastic interactions become important. However, the electron NIEL is quite sensitive to the value of the threshold energy for displacements that is employed.

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APPENDIX I

ALGORITHM FOR DERIVING NIEL FROM SRIM

The input parameters are the incident particle energy (E, in keV), the threshold energy for atomic displacement (T_d, in eV), the target density (ρ, in g/cm^3), and the input depth range of the SRIM run (B, in μm). One also needs the data from the 2 SRIM files called IONIZ.TXT and VACANCY.TXT. The text at the beginning and end of these files will need to be stripped for use in any algorithm. For IONIZ.TXT, there will be 3 columns of data. They represent the ion depth (D, in Å), the ionization energy loss (eV/Å/ion) due to both ions (IONI) and recoils (RECI). For VACANCY.TXT, there will also be 3 columns of data. They represent the ion depth (D, in Å), the vacancy production rate (# vacancies/Å/ion) due to both ions (IONV) and recoils (RECV).

To calculate NIEL from SRIM, we first need to calculate the energy necessary to produce a vacancy. This constant will be designated the variable M and is given by the expression [17] (in units of keV/vacancy)

$$M = \frac{1}{1000}\left(\frac{T_d}{0.4}+2\right) \qquad \text{(A1)}$$

where the 2 is added to allow for the binding energy loss that SRIM assigns to each vacancy, and the 1000 is a conversion factor to get eV's to keV's. The values for NIEL as a function of depth D are then simply calculated using Eq. (A1) and the expression (in units of MeV cm^2/g)

$$\mathrm{NIEL(D)} = \mathrm{M[IONV(D)+RECV(D)]}\frac{10^5}{\rho} \qquad \text{(A2)}$$

To get NIEL as a function of incident particle energy, we need to get the depth (i.e. range) as a function of energy. We can use the SRIM data to calculate the total energy lost per micron due to both ionization and vacancy production as a function of depth. The expression used for this conversion ((F(D), in units of keV/μm) is

$$\begin{aligned}\mathrm{F(D)} = {} & \mathrm{10000M[(IONV(D)+RECV(D)]} + \\ & \mathrm{10[(IONI(D)+RECI(D)]}\end{aligned} \qquad \text{(A3)}$$

where the factors of 10000 and 10 are the appropriate unit conversion factors. The cumulative energy loss $E_c(D)$ (in keV) as a function of position is then calculated using

$$E_c(D) = BF(D) \qquad \text{(A4)}$$

where B is the SRIM depth range (in μm). The incident particle energy as a function of penetration depth E(D) is then given by

$$E(D) = E - E_c(D) \qquad \text{(A5)}$$

Equations A2 and A5 then give the desired result of the NIEL as a function of energy.

APPENDIX II

NIEL FOR ALPHA PARTICLES IN Si, GaAs, AND InP*

Alpha Particle Energy (MeV)	Si (MeV cm^2/g)	GaAs (MeV cm^2/g)	InP (MeV cm^2/g)
7.940E-05	1.660E+03	8.732E+02	1.392E+03
1.260E-04	2.005E+03	1.106E+03	1.439E+03
2.000E-04	1.867E+03	1.048E+03	1.261E+03
3.160E-04	1.556E+03	8.820E+02	1.018E+03
5.010E-04	1.219E+03	6.954E+02	7.821E+02
7.940E-04	9.172E+02	5.263E+02	5.817E+02
1.259E-03	6.713E+02	3.871E+02	4.223E+02
1.995E-03	4.813E+02	2.788E+02	3.012E+02
3.162E-03	3.395E+02	1.977E+02	2.118E+02
5.012E-03	2.363E+02	1.383E+02	1.473E+02
7.943E-03	1.627E+02	9.586E+01	1.015E+02
1.259E-02	1.109E+02	6.583E+01	6.932E+01
1.995E-02	7.497E+01	4.487E+01	4.703E+01
3.162E-02	5.025E+01	3.039E+01	3.171E+01
5.012E-02	3.342E+01	2.045E+01	2.126E+01
7.943E-02	2.206E+01	1.370E+01	1.418E+01
1.259E-01	1.448E+01	9.129E+00	9.411E+00
1.995E-01	9.466E+00	6.053E+00	6.222E+00
3.162E-01	6.157E+00	3.996E+00	4.098E+00
5.012E-01	3.986E+00	2.625E+00	2.689E+00
7.943E-01	2.568E+00	1.715E+00	1.757E+00
1.259E+00	1.647E+00	1.116E+00	1.144E+00
1.995E+00	1.053E+00	7.240E-01	7.425E-01
3.162E+00	6.704E-01	4.683E-01	4.800E-01
5.012E+00	4.260E-01	3.020E-01	3.093E-01
7.943E+00	2.702E-01	1.942E-01	1.990E-01
1.259E+01	1.713E-01	1.245E-01	1.277E-01
1.995E+01	1.085E-01	7.969E-02	8.193E-02
3.162E+01	6.883E-02	5.093E-02	5.252E-02
5.012E+01	4.373E-02	3.256E-02	3.367E-02

*The displacement threshold energies were 21 eV for Si, 10 eV for Ga and As, 6.7 eV for In, and 8.7 eV for P [10,11]. The energies listed were calculated as powers of 10 to better accommodate many orders of magnitude, i.e. the energy range is $10^{-4.1}$, $10^{-3.9}$, ..., $10^{1.7}$. This knowledge may make interpolation easier. A cubic spline interpolation technique is suggested.