Phonon contribution to nonionizing energy loss in silicon detectors^{*}

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Abstract: Nonionizing energy loss (NIEL) has been applied to a number of studies concerning displacement damage effects in materials and devices. However, most studies consider only the contribution of displacement damage effects, neglecting the contribution from phonons. In this paper, a NIEL model, which considers the contribution of phonons, has been established using the Monte Carlo code SRIM. The maximum endurable fluence for silicon detectors has been estimated using the equivalent irradiation fluence compared with experimental data for the incident particles. NIEL is proportional to the equivalent irradiation fluence that the detector has received.

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1 Introduction

Silicon detectors have been widely used in nuclear physics experiments due to their perfect position resolution and energy resolution, wide linear range and quicker response time. It is found that a silicon detector cannot withstand too high a radiation fluence because the radiation damage can cause degradation of its electrical properties. Many studies have demonstrated that the degradation of silicon detector properties in a radiation field is linearly correlated to the displacement damage energy [1–3] induced by the nonionizing energy loss (NIEL) [4].

NIEL has been proved to be an effective tool to analyze displacement damage effects in materials and devices in the past few decades [5–7]. For example, it has been applied to solar cells, optical sensors, high energy particle detectors and high temperature superconductors. It has 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 by using the NIEL approach rather than previous techniques. The displacement damage effects produced by different particles over a wide range of energies are approximately proportional to the NIEL induced by the incident particles and the energetic nuclear recoils. It has been pointed out [8] that NIEL can be incorporated into Monte Carlo transport codes to estimate the displacement damage effects. The Monte Carlo code SRIM [9], which 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, can be used to fill blanks in the existing tabulations of NIEL.

Although the NIEL approach has wide applications, the contribution of phonons is not taken into account in the existing literature. Incident particles with energy low enough so as not to induce displacement damage in the lattice atoms will stop in the detectors due to multiple Coulomb scattering. In this case, the energy of the incident particles is totally transformed into phonons, which will participate in the crystal lattice vibration. Thus, the temperature of the sensors will increase and the number of electrons excited from valence band to conduction band will also increase, which may result in an increase in the leakage current and a decrease in the detector's charge collection efficiency or even the failure of the detector. It is important to take phonons into account for the calculation of nonionizing energy loss in materials and devices.

In this paper, the contribution of phonons was taken into account in the calculation of NIEL by using the Monte Carlo code SRIM. The NIEL values of alpha, carbon and bismuth particles were calculated for our own

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specific applications. According to Ref. [10], the NIEL of the incident particles is proportional to the equivalent irradiation fluence that the detector has received, so we can estimate the maximum endurable fluence for silicon detectors by using the equivalent irradiation fluence compared with experiments.

2 NIEL model

NIEL is the energy lost to nonionizing processes (energy per unit length) in units of MeV/cm or MeV cm²/g. In order to calculate NIEL, information is needed about the average recoil energy of the target atoms (*T*), the Lindhard factor (*L*), which partitions the energy into loss ionizing and nonionizing components, and the differential cross section for atomic displacement ($d\sigma/d\Omega$). NIEL can be written as an integral over the average recoil energy of the target atoms [11],

$$\text{NIEL} = \frac{N_{\text{A}}}{A} \int_{T_{\text{min}}}^{T_{\text{max}}} T \cdot L(T) \left(\frac{\mathrm{d}\sigma}{\mathrm{d}T}\right) T_0 \mathrm{d}T, \qquad (1)$$

where $N_{\rm A}=6.02\times10^{23}$ (Avogadro's number), T_0 is the primary particle energy, A is the lattice atoms mass in units of AMU and $T_{\rm max}=4T_0AA_1/(A_1+A)^2$, where A_1 is the recoils atomic mass in units of AMU. We assume that the minimum energy transfer is $T_{\rm min}=2T_{\rm d}$ where $T_{\rm d}$ is the displacement energy. For silicon we use $T_{\rm d}$ (silicon)=21 eV.

Three SRIM data files, INOIZ.TXT, VACANCY. TXT and PHONON. TXT, are necessary to derive the NIEL data. All files give the spatial information in length units of Å. For all data concerning ionization energy loss, vacancy and phonon production, SRIM divides the particle path into 100 length intervals. The total energy loss rate for the incident particles and the recoils is given for each interval. The INOIZ. TXT file contains the information on ionization energy loss rates in units of eV/Å /ions and provides a measure of the particle's energy loss at each interval. The VACANCY.TXT file gives the information on vacancies in units of the number of vacancies/Å /ion, and provides a measure of the number of displacements in each interval. The PHONON.TXT file provides the information on crystal lattice vibrations, with units of number of phonons/Å /ion, and provides a measure of the number of phonons in each interval. We use the files VACANCY. TXT and PHONON. TXT to calculate NIEL, and use all the SRIM files to correlate the particle depth with particle energy.

The vacancy formation rate can be converted into NIEL using the modified Kinchin-Pease relationship between the number of displaced atoms, $N_{\rm d}$, and a given quantity of nonionizing energy $E_{\rm n}$, i.e.,

$$N_{\rm d} = 0.8 \frac{E_{\rm n}}{2T_{\rm d}},\tag{2}$$

where $T_{\rm d}$ is the threshold energy for atomic displacement (usually in the order of a few tens of eVs) and $E_{\rm n} > 2.5T_{\rm d}$.

To calculate NIEL from SRIM, we first need to calculate the energy necessary to produce a vacancy and a phonon. These constants will be designated by M_1 and M_2 respectively. M_1 (the energy needed to produce a vacancy) is given by the following expression [2]:

$$M_1 = \frac{1}{1000} \left(\frac{T_{\rm d}}{0.4} + 2 \right),\tag{3}$$

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 convert eV to keV. M_2 (the energy needed to produce a phonon) is given by the following expression:

$$M_2 = \frac{1}{1000} \cdot \frac{h \cdot c}{\lambda},\tag{4}$$

where the *h* is Planck's constant, *c* is the speed of light, λ is the Raman spectrum wavelength of silicon, and the 1000 is a conversion factor to convert eV to keV. For λ we use λ (silicon)=520 cm. [12]. From Eqs. (3) and (4), the energy necessary to produce a vacancy is 0.0545 keV/vacancy, and that needed for a phonon is 2.38×10^{-10} keV/phonon.

The values for NIEL as a function of depth D are then simply calculated using Eq. (3) and (4) and the expression

$$\operatorname{NIEL}(D) = \{M_1[\operatorname{IONV}(D) + \operatorname{RECV}(D)] + M_2[\operatorname{IONP}(D) + \operatorname{RECP}(D)]\}\frac{10^5}{9}, \quad (5)$$

where IONV(D) and IONP(D) are the number of vacancies and phonons produced respectively by incident particle ionization at depth D, and RECV(D) and RECP(D) are the number of vacancies and phonons produced respectively by incident particle elastic collisions at depth D.

To get NIEL as a function of incident particle energy, we need to get the energy as a function of depth. We can use the SRIM data to calculate the total energy loss as a function of depth by combining the results from the files IONIZ. TXT, VACANCY. TXT and PHONON. TXT. The expression used for this conversion F(D) is

$$F(D) = 10000\{[IONV(D) + RECV(D)] + M_2[IONP(D) + RECP(D)]\} + 10[IONI(D) + RECI(D)], \quad (6)$$

where the factors of 10000 and 10 are the appropriate unit conversion factors, and IONI(D) and RECI(D) are the number of ions and recoil respectively at depth D. The cumulative energy loss $E_{\rm c}(D)$ as a function of position is then calculated using

$$E_{\rm c}(D) = BF(D),\tag{7}$$

where B is the SRIM depth range. The residual energy as a function of penetration depth $E_r(D)$ is then given by

$$E_{\rm r}(D) = E - E_{\rm c}(D), \qquad (8)$$

The relationship between NIEL and incident particle energy is thereby established, so Eqs. (5) and (8) then give the desired results of the NIEL as a function of energy.

3 Results and discussion

Figure 1 shows the results of a SRIM run for 10 MeV protons incident on a double-sided silicon micro-strip detector. The data from the files INOIZ.TXT (black line), VACANCY.TXT (blue line) and PHONON.TXT (red line) are plotted as a function of penetration depth. The displacement threshold energy is set at 21 eV for silicon. The ionization, phonon and vacancy production rate of incident particles (protons) are shown in Fig. 1(a); it can be clearly seen that more than 95 percent of the energy loss can be ascribed to ionizing energy loss, which provides energy to excite or ionize extra-nuclear electrons to generate electron-hole pairs when the particles traverse the detector and collide with lattice atoms. Less than 5 percent of energy loss is nonionizing energy loss which induces lattice atom displacement damage or transforms into phonons to participate in the crystal lattice vibration. It is demonstrated that the main contribution of NIEL is phonons rather than lattice atom displacement damage. Fig. 1(b) shows the results of ionization, phonon and vacancy production rate of the resultant recoil (silicon). It is pointed out that for energetic nuclear recoils, the energy is mainly transformed into thermal energy due to the crystal lattice vibration. That is to say, with multiple Coulomb scattering with the target atoms, the incident particles' energy is transformed into phonons, then the phonons participate in the crystal lattice vibration, which will cause the temperature of the sensors to increase. It has been revealed that the contribution of phonons even exceeds that of ionization for recoils.

The number of vacancies and phonons produced by both the incident particles and the resultant recoils derived from the files VACANCY.TXT and PHONON.TXT must be added together to obtain the total NIEL. In this way, the NIEL as a function of penetration depth is obtained. Fig. 2 shows a plot of the result derived from Eq. (5). It has been revealed that the NIEL reaches its maximum at 700 μ m due to the proton interaction in silicon for both elastic and inelastic scattering.

Figure 3 shows proton energy as a function of penetration depth in silicon, derived from Eq. (8). It can be seen that the incident particle energy decreases with the increase in penetration depth, because of lattice scattering.



Fig. 1. (color online) The ionization, phonon and vacancy production rates of the incident proton (a), and of the recoil silicon (b).



Fig. 2. Proton NIEL as a function of penetration depth, derived from SRIM data.

Figure 4 shows the results for calculated proton NIEL versus proton energy. It shows that the proton NIEL increases with the decreasing of incident energy. When protons traverse into a silicon micro-strip detector, they are affected by atomic Coulomb interactions, and nuclear elastic/inelastic scattering. At low energies, Coulomb interactions induce the production of displaced atoms from their lattice sites. At high energies, nuclear reactions are mostly responsible for displacements.



Fig. 3. Proton energy as a function of penetration depth in silicon.



Fig. 4. Proton NIEL as a function of particle energy.

According to Ref. [13], the incident particle NIEL is proportional to the equivalent irradiation fluence (Φ) that the detector has received. We estimate the maximum endurable fluence for double-sided silicon microstrip detectors by using the equivalent irradiation fluence compared with experiments. Experimentally the maximum proton equivalent irradiation fluence of such a detector is 2×10^{14} cm⁻² [14]. Compared with the experimental data from Ref. [14], the maximum equivalent irradiation fluences for alpha particles, carbon and bismuth ions are roughly estimated as $\Phi_{\alpha} \approx 2 \times 10^{13}$ cm⁻², $\Phi_{\rm C} \approx 5 \times 10^{11}$ cm⁻², $\Phi_{\rm Bi} \approx 2 \times 10^8$ cm⁻², respectively, and the corresponding NIELs are shown in Fig. 5. The

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Fig. 5. NIEL for different particles as a function of incident particle energy.

energies for all incident particles (proton, alpha, carbon and bismuth) are 10 MeV.

4 Conclusion

We have established a NIEL model that considers the contribution of phonons, and have calculated the relationship between NIEL and incident particle energy using the Monte Carlo code SRIM. It has been demonstrated that more than 95 percent of the energy loss is ionizing energy loss, which provides the energy to excite or ionize extra-nuclear electrons to generate electron-hole pairs when the particles enter the detector and collide with lattice atoms. The main contribution of nonionizing energy loss is from phonons rather than from lattice atom displacement damage for incident particles and recoils. The incident particle energy will decrease with increasing penetration depth because of lattice scattering. The proton NIEL is found to increase with decreasing incident energy because of the atomic Coulomb interactions and nuclear elastic/inelastic reactions. The maximum endurable fluence for silicon detectors for protons, alpha particles, carbon and bismuth ions are anticipated to be $\Phi_{\alpha} \approx 2 \times 10^{13} \text{ cm}^{-2}, \Phi_{\rm C} \approx 5 \times 10^{11} \text{ cm}^{-2}, \Phi_{\rm Bi} \approx 2 \times 10^8 \text{ cm}^{-2}$ respectively, calculated using the equivalent irradiation fluence compared with experiment data.

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