NIEL Calculations for High-Energy Heavy Ions

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Abstract—Calculations of NIEL are reported for heavy ions prominent in the space environment for energies ranging from 200 MeV per nucleon to 2 GeV per nucleon.

Index Terms—Displacement damage, fragmentation, heavy ion, NIEL.

I. INTRODUCTION

METHODS have been described for calculating nonionizing energy loss (NIEL) due to Coulombic interactions for many ions and targets at energies ranging from threshold to the GeV range [1]–[3]. For protons and helium ions at energies above 100 MeV per nucleon, nuclear nonelastic mechanisms also contribute substantially to NIEL. Results that include these interactions have been reported [1], [4], [5]. There still exists a large gap in our knowledge of NIEL for relativistic heavy ions, as shown in Fig. 1, which delineates what NIEL values are known as a function of incident ion atomic number, Z, and incident ion energy for a given target material such as silicon. The large area in the figure corresponding to relativistic heavy ions is addressed in this work.

At energies in excess of about 100 MeV per nucleon heavy ions can undergo fragmentation interactions where the incident ion and target are reduced to isotopes with lower charge and mass. Due to the large number of reaction products that emerge from these high-energy heavy ion reactions, at first glance calculating NIEL appears to be rather prohibitive. Consequently the effects of nuclear fragmentation interactions on NIEL have not been reported for heavy ions with atomic number greater than that of helium. Since heavy ions are present in the space environment (for example see [6] for a detailed description), the contribution they make to displacement damage in detectors, microelectronics and solar arrays remains an open question. This question is becoming more significant as missions to the Moon and Mars are being proposed in NASA's new space initiative. On the other hand ionization effects of these fragmentation interactions have been extensively studied because of their potentially damaging biological and material effects [7], [8].

In this paper we first examine the contribution to NIEL from heavy ion fragmentation reactions. This includes fragmentation
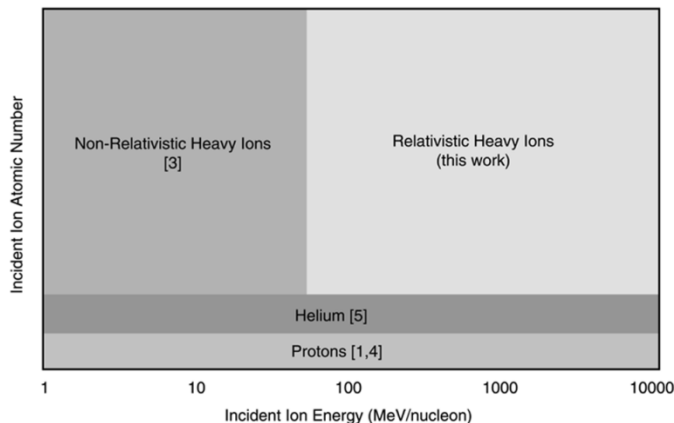
Fig. 1. Delineation of known NIEL values and those values addressed in this work.

of both the incident (primary) ion and the target. These results are obtained using experimental data on fragmentation cross sections [9], [10] combined with the relativistic expression for NIEL [1], [2]. Adding these results to the relativistic Coulomb contribution of the primary ion leads to estimates of NIEL for high-energy heavy ions in the space environment.

II. FRAGMENTATION INTERACTIONS

A. Primary Ion and Target Fragmentation

The current picture of the fragmentation process is one where a very fast-moving ion collides with a target nucleus. Both are reduced to smaller nuclei and a number of other particles, primarily nucleons. The primary fragments, i.e., those coming from the incident ion continue to move without appreciable change of direction or velocity except for a relatively small energy exchange with the target [10]. The target fragments emerge in an excited state and with a significantly lower kinetic energy than the primary fragments. Although ionization studies have typically only considered the contribution of the primary fragments, here we consider the effect of the target fragments as well.

Since fragmentation of the incident ion has been studied the most, it will be considered first. The production of each primary fragment has a partial cross section associated with it, which is a measure of the probability of its production. There are generally a large number of primary fragments that emerge. For example, an incident ion such as argon that has 40 nucleons can result in as many as 36 isotopes in the fragmentation process. The partial cross section associated with the production of a particular fragment species can be calculated by first determining the partial cross section for an incident proton. An example of a basic equation for this is [9]

$$\sigma_p = \sigma_0 f(A) f(E) e^{-P\Delta A} \exp\left(-R|Z - SA + TA^2|^\nu\right) \Omega \eta \xi. \tag{1}$$

Here σ_0 is a normalizing factor, while $f(A)$ and $f(E)$ apply to heavy targets with $Z > 30$. The factor $\exp(-P\Delta A)$ accounts for the reduction of cross sections as the difference of product and target mass increases. The second exponential yields the distribution of cross sections for the production of different isotopes of an element with atomic number Z. The parameter Ω is related to nuclear structure as described in [11]. The quantity η depends on the pairing of protons in the nucleus (e.g., even-even and even-odd). Finally, ξ accounts for enhancement of light evaporation products as described in [12]. Tabulated values of these parameters are provided for a range of projectile-target combinations [[9], and references therein].

The cross sections of nucleus-nucleus $(N_1 - N_2)$ interactions can now be calculated by scaling the proton partial cross sections. The scaling relation is

$$\sigma(N_1 - N_2) = \sigma_p \cdot S_c \cdot \varepsilon_n \varepsilon_L \varepsilon_1 \varepsilon_\Delta. \quad (2)$$

N_1 is the ion which is fragmented in a collision with the target N_2. The factors ε_n, ε_L, ε_1, and ε_Δ are corrections for neutron deficient products, light products, nucleon stripping, and reactions with large change in mass ΔA, respectively. Tabulations are available for the appropriate factors in (2) as a function of the projectile and the target as well as the energy [9]. The above equations permit the calculation of partial cross sections for most ion-target combinations of interest.

The partial cross sections determine the probability of a particular isotope being produced in a fragmentation interaction. In addition to that information the average energy of the fragment is needed in order to determine NIEL. A very standard assumption used in analysis of ionization data is that the nucleons in the fragment have the same velocity and momentum as the original projectile [7], [8], [13]. This is the so-called straight-ahead approximation. In the examples shown here this assumption is applied.

In addition to the high-energy fragments of the incident ion, the contribution of target fragments to NIEL is also considered. When the incident particle is a proton or helium ion the target fragments generated contribute to NIEL and the process is commonly referred to as spallation. Analysis of this proton and alpha particle nuclear inelastic contribution to NIEL for a variety of target materials [4], [5] shows that it scales approximately as the reaction cross section. This provides motivation for estimating the inelastic NIEL for heavier ions by scaling the alpha particle inelastic NIEL by the known ratio of reaction cross sections. It turns out that this estimate of the inelastic NIEL is sufficient for our purposes because it is much smaller than the Coulombic contribution for many incident heavy ions and relativistic energies of interest.

III. RESULTS

Tables I and II illustrate the contribution of the incident ion fragmentation process to NIEL relative to the Coulomb contribution. Table I shows results for carbon ions incident on a carbon target at energies ranging from 250 to 2100 MeV per nucleon. Table II shows results for 600 MeV per nucleon carbon, oxygen, argon and iron incident on carbon targets. The middle column

TABLE I
CALCULATED NIEL FOR HIGH ENERGY CARBON IONS ON CARBON TARGETS

Energy/Nucleon (MeV/n)	Primary Ion NIEL (MeV•cm²/g)	Primary Fragment NIEL (MeV•cm²/g)
250	9.39×10^{-3}	1.58×10^{-6}
600	4.83×10^{-3}	1.55×10^{-6}
1050	3.29×10^{-3}	1.56×10^{-6}
2100	2.06×10^{-3}	1.70×10^{-6}

TABLE II
CALCULATED NIEL FOR 600 MEV PER NUCLEON IONS ON CARBON TARGETS

Incident Ion	Primary Ion NIEL (MeV•cm²/g)	Primary Fragment NIEL (MeV•cm²/g)
^{12}C	4.83×10^{-3}	1.55×10^{-6}
^{16}O	9.54×10^{-3}	3.42×10^{-6}
^{40}Ar	6.63×10^{-2}	1.00×10^{-5}
^{56}Fe	1.55×10^{-1}	1.46×10^{-5}

in both tables is the Coulomb contribution to NIEL for the incident ion calculated using the relativistic form for Rutherford scattering [1], [2]. The NIEL associated with the primary fragments is also calculated using this model. For an incident carbon ion, there are 11 isotopic fragments ranging from ^{11}C to ^{6}Li and ^{6}He. The column on the right is the contribution to NIEL from the fragmentation of the incident ion. These results were obtained by weighting the values of NIEL for each fragment by the corresponding partial cross section to obtain the average NIEL of the primary fragments. It is seen that the contribution of the primary fragments to the total NIEL is very small. This is a direct consequence of the large difference between fragmentation cross sections and the relativistic Coulomb cross sections for the incident ion. The total sum of the partial fragmentation cross sections ranged from 240 to 260 mb. In contrast, the primary carbon ions had Coulomb interaction cross sections that ranged from 187 to 983 b. Examination of cross sections for a number of different ions show a similar effect and this is expected to be characteristic of all relativistic heavy ion interactions of interest.

The contribution of primary ion fragmentation to NIEL has been shown to be negligible. However, this is not necessarily true for target fragmentation. When the incident particle is a proton or helium ion, for example, it is known that the nuclear nonelastic contribution to NIEL is important at high energies. In the following, we will show the general trends observed as a function of incident ion atomic number and energy with and without our estimate of the contribution of target fragmentation.

Fig. 2 shows results for NIEL due to Coulombic interactions only, i.e., it excludes target fragmentation. Results for heavy ions with Z-values ranging from 1 to 26 are shown for a silicon target. In the space environment the flux of ions with Z greater than 26 (iron) falls off rapidly with increasing Z. It is seen that for the energies considered, there is a monotonic increase in
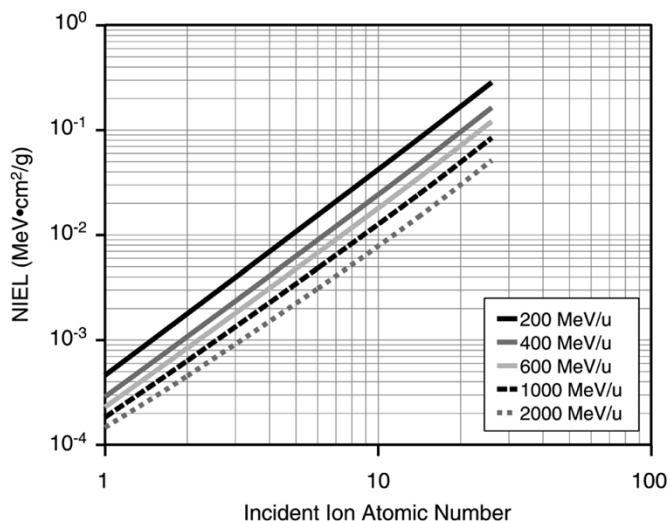
Fig. 2. Heavy ion NIEL in silicon at high energies, excluding target fragmentation.
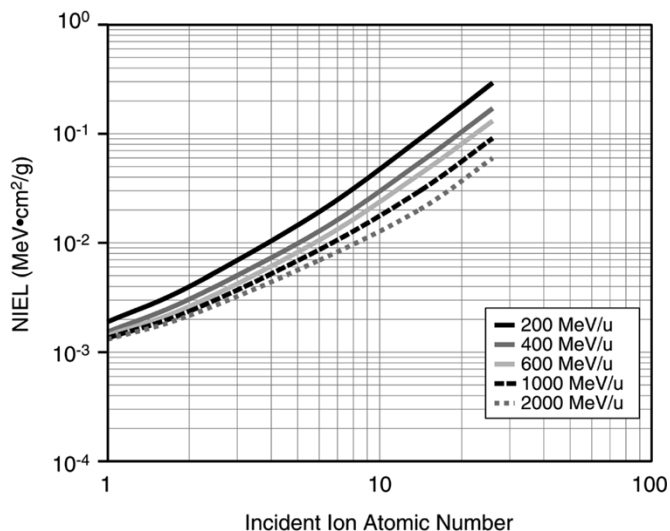

Fig. 3. Heavy ion NIEL in silicon at high energies, including target fragmentation.

NIEL with incident ion atomic number that is proportional to Z^2 to first order, as expected.

Fig. 3 shows results analogous to those in Fig. 2 except that the effect of target fragmentation is included. Results for this nuclear nonelastic contribution were obtained with the MCNPX code for protons and alpha particles [4], [5], while results for heavier ions were scaled according to the reaction cross sections given in the work of Tripathi [14], [15], as discussed above. Fig. 3, thus, fills in what has previously been a large gap in our knowledge of NIEL, shown in Fig. 1 by the relativistic heavy ion region. When target fragmentation is included for the energies considered in this work, the effects are most pronounced for protons and alpha particles. With increasing incident ion atomic number, the target fragmentation becomes less significant because the Coulomb cross section rises much more rapidly with Z than does the reaction cross section. A rule of thumb is that for the materials and energies considered here, target fragmentation should be accounted for when incident ion Z-values are less than about 10.
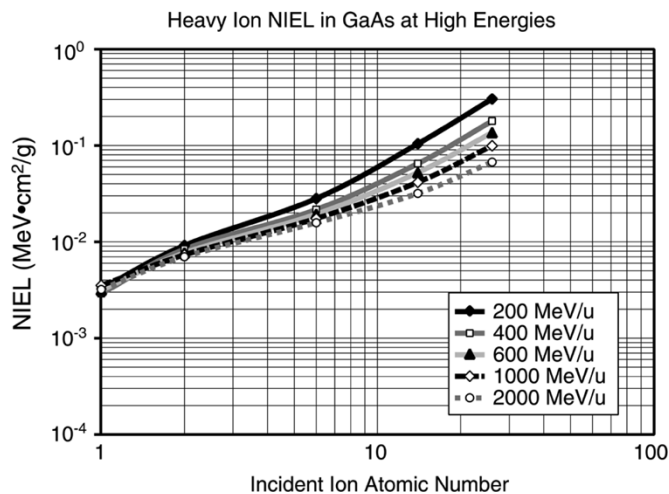

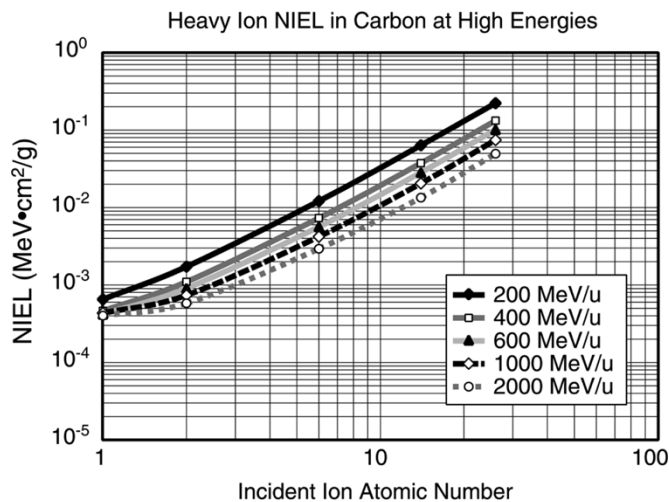Fig. 4. Heavy ion NIEL in GaAs at high energies.

Fig. 5. Heavy ion NIEL in carbon at high energies.

Figs. 4 and 5 show the full NIEL results for GaAs and C targets, respectively, including target fragmentation. These targets have significantly different atomic numbers than Si so that a range of target Z-values is covered. The results for carbon can also be combined with the results for silicon to obtain NIEL values for SiC, a material sometimes discussed for possible use in severe environments.

The description of heavy ion NIEL for a broad range of energies useful for space applications is now reasonably complete. Linear energy transfer (LET) values, commonly used for studies of ionization effects, are known over a similar broad range of energies. Since NIEL is the displacement damage analog of LET [16], it is interesting to compare the two. This is done in Figs. 6 and 7 for carbon and iron ions incident on silicon. This allows for quantitative comparisons to be made about the mechanisms of the ion's energy loss due to displacements and ionization.

It is interesting to review some of the features of these new NIEL results in the context of previous results. Table III provides a bird's eye view of NIEL in silicon as a function of incident ion energy. The ions considered are H, He, C, Si, and Fe. NIEL is characterized with respect to the ion's threshold energy (E_{th}), the peak value of NIEL, the ion energy corresponding to
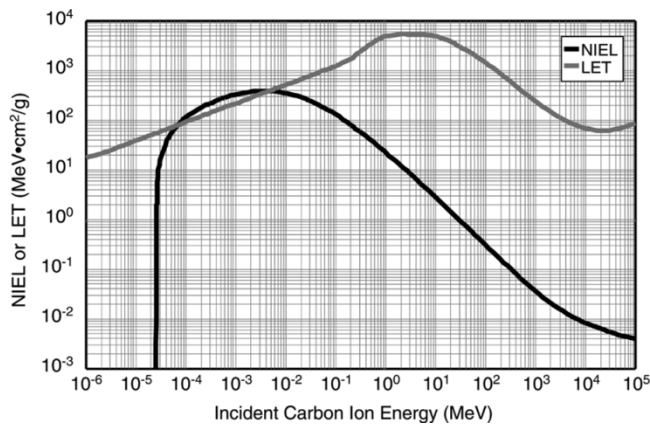
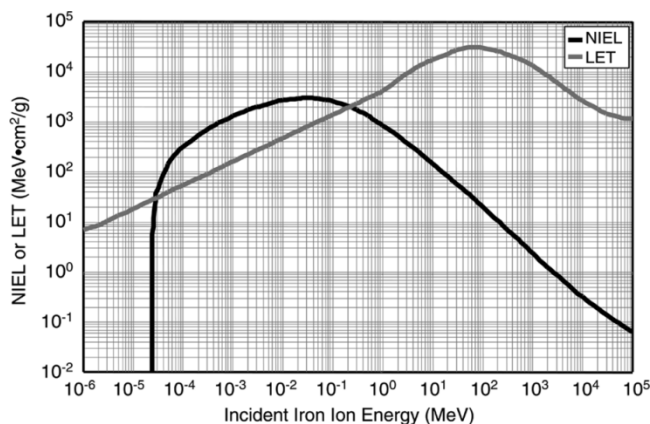Fig. 6.   Comparison of NIEL and LET values for carbon ions incident on silicon.

Fig. 7.   Comparison of NIEL and LET values for iron ions incident on silicon.

TABLE III
FEATURES OF NIEL IN SILICON

Ion	E_{th} (eV)	Peak NIEL (MeV•cm²/g)	E_{pk} (MeV)	$NIEL_{HE}$ (MeV•cm²/g)	E_{eq} (MeV)
H	158	5.032	0.001	0.00116	70
He	48	54.38	0.001	0.00171	900
C	25	385.4	0.003	0.00381	1.5×10^4
Si	21	1362	0.010	0.00511	2.0×10^5
Fe	24	3000	0.030	0.00662	1.0×10^6

the peak NIEL (E_{pk}), the plateau value of the nonelastic NIEL at high energies $(NIEL_{HE})$, and the estimated ion energy at which the Coulombic and nonelastic contributions to NIEL are equal (E_{eq}).

The ion's threshold energy for creating a displacement is based on the expression for the maximum energy transfer to a silicon atom by the ion, and the assumption that the threshold for atomic displacement is 21 eV. The minimum E_{th} occurs when the ion is the same mass as the target.

As the incident ion energies increase, a maximum NIEL value is observed as is shown in the third column. Note that the peak NIEL for iron is about 600 times that of protons. The peak value always occurs in the region governed by the screened Coulomb

potential [3] as is evident by examining the relatively low energies (E_{pk}) at the peak. The new results in this paper begin at energies of 200 MeV per nucleon and are well into the relativistic range. No significant Coulomb screening effect is present at these energies.

The plateau value of the nonelastic NIEL at high energy is shown in the second column from the right. The values for H and He are obtained with the MCNPX code [4], [5]. Those for the heavier ions are estimated using reaction cross section values [14], [15] to scale the MCNPX results to the high energy region. Finally, the last column gives an estimate of the ion energy where the Coulombic NIEL is approximately equal to the nonelastic NIEL. The reason E_{eq} increases so rapidly with ion atomic number is that the Coulombic contribution increases rapidly with Z, as can be seen from the peak NIEL values. With increasing energy, the Coulombic contribution for heavy ions such as Fe takes much longer to come down to values comparable to the nuclear nonelastic values.

Thus, it appears that for ions with Z-values heavier than about 10, the contribution of target fragmentation is a small correction to the total NIEL value for most energies of interest.

IV. CONCLUSION

Estimates of NIEL for high-energy heavy ions have been obtained. The relativistic Coulomb interaction of the incident ion with the target is the most important contribution. A correction for target fragmentation should also be added, which is most significant for high-energy, low-Z ions. The effect of fragmentation of the incident ion can be ignored. The practical consequences of this is that we can now make estimates of NIEL values for all the ions present in cosmic rays that have significance for radiation effects applications.

An important implication of the above conclusion is that NIEL spectra can now be constructed which include all cosmic ray species of interest. These would play a role similar to the LET spectra originally devised by Heinrich [17] for studying ionization phenomena. For some applications, this may considerably simplify the assessment of displacement damage produced in the space environment.

General methods for calculating NIEL for arbitrary ions, ion energies and materials have now been developed [[3]–[5], this work]. These will be available in a Windows compatible code to be distributed by the NASA Space Environments and Effects (SEE) Program.

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