Alpha Particle Nonionizing Energy Loss (NIEL)

Insoo Jun, Michael A. Xapsos, and Edward A. Burke

***Abstract*-- A method previously developed for proton nonionizing energy loss (NIEL) calculations was extended to alpha particles. The alpha particle NIELs for representative device materials are presented from the damage threshold energy to 1 GeV/n. The method used the Ziegler, Biersack, Littmark (ZBL) screened potential for Coulomb interactions and the MCNPX "thin target approximation" for nuclear interactions. The alpha NIEL obtained in this study was compared to the proton NIEL from the previous study. It is seen that for silicon, the NIEL for alphas is about 16 times the NIEL for protons at 1.0 MeV/n where the Coulombic interaction dominates. The ratio drops at higher energies because of the nuclear contributions. Furthermore, a simple radiation transport analysis indicates that in a representative space environment, the contribution of alphas to the damage dose can be comparable to the proton contribution, and that shielding has a marked influence on the relative contributions.**

I. INTRODUCTION

NONIONIZING ENERGY LOSS (NIEL) was computed for representative device materials and reported in [1], [2] for proton energies that ranged from the damage threshold to 1 GeV. The Ziegler, Biersack, Littmark (ZBL) screened Coulomb potential at lower energies and the relativistic kinematics at higher energies were used to compute the Coulomb contribution to NIEL. Nuclear elastic and inelastic interactions were fully accounted for by utilizing a high energy charged particle transport code MCNPX [3] and appropriate physics models implemented in the code. The results were consistent with those from previous studies, and will enable extension of NIEL calculations to many materials. The method developed has applications in the ion implantation and space radiation effects fields. The method has been used to simulate proton damage effects on bandgap engineered HgCdTe detectors [4] and on light output variations in gallium nitride (GaN) light emitting diodes [5]. Especially, the study by Khanna et al. [5] showed that the proton damage constant on a GaN light emitting diode (CREE Model C430-DH85) follows the "total" NIEL curve in the energy range of 2 to 115 MeV, demonstrating the importance of including the nuclear interactions for the proper NIEL and damage correlation.

Alpha particles are the second most abundant constituent in solar particle events and galactic cosmic rays. There is also a small amount of alpha particles in the Earth's inner radiation belt [6]. Although the relative abundance of alpha particles in the space environment is small compared to that of protons (e.g., see Fig. 1), damage effects of alpha particles may be significant because work with bipolar transistors has shown they are about 16 times more damaging than protons at a given energy [8]. While NIEL for protons, electrons, neutrons, etc. have been studied extensively and published in many places [e.g., see [9] and reference therein], the availability of published alpha particle NIEL is limited [8], [10]. Furthermore, only the Coulomb contribution was included in the computations at that time. Alpha particle NIEL that includes contributions from all relevant physical interactions (Coulomb and nuclear elastic/non-elastic) has not been available. It is essential for NASA to evaluate potential damage effects that can be caused by heavy ions in interplanetary space, particularly for manned or robotic missions targeting the Moon or Mars where heavy ion environments is expected to dominate. In this paper we address this problem for alpha particles for various materials relevant for device applications. Incident alpha particle energies covered are from 100 eV to 4 GeV (= 1 GeV/n).

II. ATOMIC COULOMB INTERACTIONS

The analytical model reported earlier by Messenger et al. [2] was used in this study, where the ZBL screened Coulomb potential was employed. The effect of using the screened potential becomes appreciable at lower energies, where a reduction of the Coulomb potential because of the electrostatic screening of the nuclear charges by the space charge of the innermost electron shells becomes important. The classical Rutherford potential does not account for this screening effect properly, resulting in overestimation of NIEL at lower energies. This is clearly illustrated in Fig. 2, where the alpha particle NIEL computed by two different Coulomb potential formulas are shown for silicon. We did

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not include the relativistic effect here because its contribution to the total NIEL is small in the energy range considered in this paper.

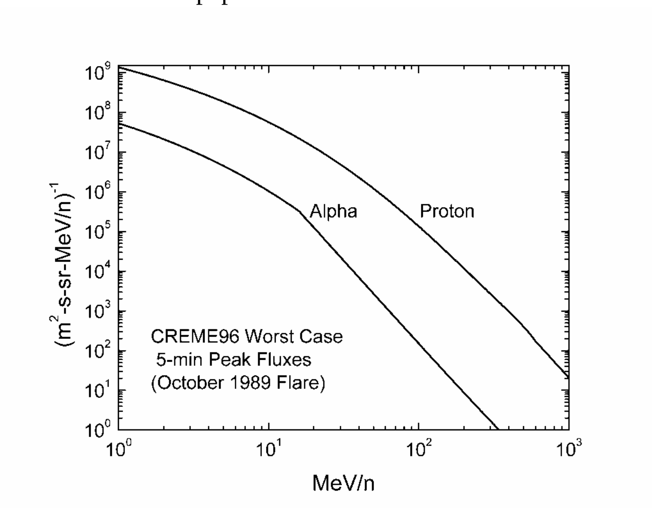

Fig. 1. Worst case 5-min averaged proton and alpha particle differential spectra during the October, 1989 solar energetic particle event from CREME96 [7]. The proton flux is greater than 25 times the alpha flux at 1 MeV/n, the ratio is 54 at 10 MeV/n, and the ratio is ~900 at 100 MeV/n.

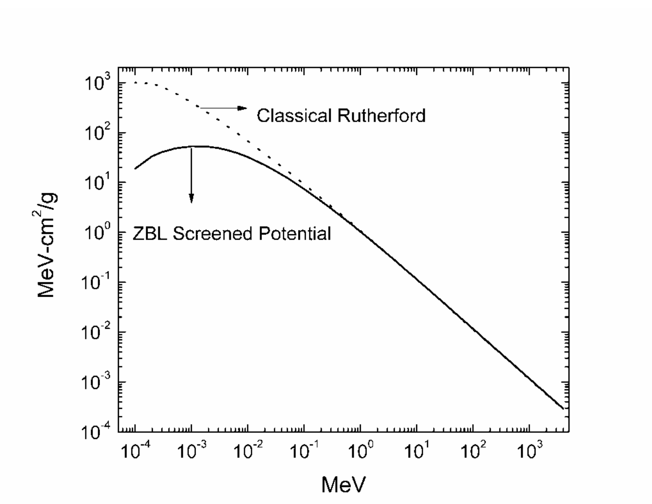

Fig. 2. Alpha particle NIEL for silicon due to the Coulomb scattering, computed using two different formalisms.

III. NUCLEAR INTERACTIONS

In order to develop appropriate results for the high energy ions encountered in space, it is essential to properly account for the nuclear elastic and inelastic interactions. The basic MCNPX "thin target approximation" method developed for computing proton and neutron NIEL from the nuclear interactions [1], [11] was applied in this paper for incident alpha particles. The basic formulation is explained in detail in [1] and [11]. During the MCNPX simulations, we ensured that the target thickness was thin enough that multiple nuclear interactions would not occur in the target, but at the same time thick enough that we would have reasonable statistics within practical Monte Carlo run time. The criterion used for choosing the target thickness as a function of incident ion energy is worth mentioning here and described in the following. To start, for a given incident energy, 10% of the continuous slowing down approximation (CSDR) range was used as a target thickness and the thickness was varied to see how it affects the final result. It became evident that once the target thickness becomes thin enough, reducing the thickness further does not affect the final results very much. For example, for a 100 MeV/n alpha particle incident on silicon case (CSDA range is 9.787 g/cm^2), the nuclear NIEL changed from 2.87×10^{-3} MeV-cm^2/g with a 0.01 cm target thickness to 2.79×10^{-3} MeV-cm^2/g with a 0.005 cm target thickness, and these results were within the computational uncertainty, ~5%. After repeating this process at several incident energies for Si, we simplified the process for determining the target thickness. The energy range was divided into three broad regions: $E < 10$ MeV/n, $10 \le E < 100$ MeV/n, and $E \ge 100$ MeV/n. At each energy region, the target thicknesses were set to 0.0001 cm, 0.001 cm, and 0.01 cm, respectively. In most cases, it was verified visually using SRIM [12] that the incident alphas completely penetrate the target without going through the large angle deflections. Fig. 3 shows the results for silicon, which details the separate contributions of nuclear elastic and non-elastic interactions. As can be seen, the non-elastic interactions have a marked effect on the alpha particle NIEL above about 100 MeV.

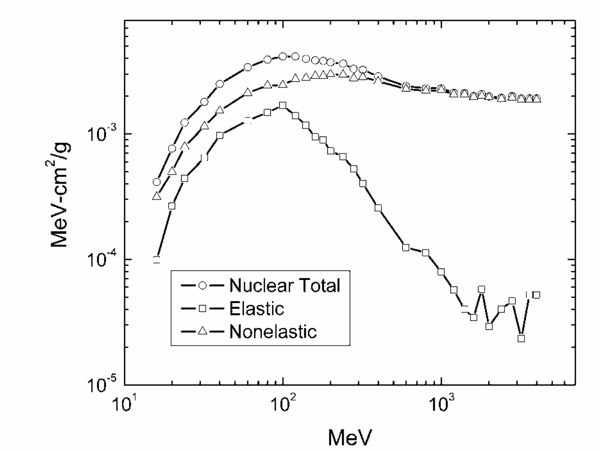

Fig. 3. Alpha particle NIEL for silicon due to the nuclear interactions. The fluctuation of the elastic NIEL at higher energies (> 1 GeV) is due to insufficient number of particles simulated during the MCNPX calculations. However, its contribution is negligible, as shown, and thus no further effort was done to refine the elastic NIEL at these high energies.

Complete description of the relevant nuclear physic is described in [1] for the proton incident case. Most of the physics described therein is still applicable to the alpha particle incident case, except for high-energy intra-nuclear-cascade (INC) model. We used the ISABEL [13], [14] INC model implemented in MCNPX. The ISABEL code was derived from the VEGAS INC code [15]. It allows hydrogen, helium, anti-protons as projectiles and has the capability of treating nucleus-nucleus interactions as well as particle-nucleus interactions (although this capability has not been yet fully tested in the version of MCNPX used in this study: MCNPX version 2.5.e). It allows for interactions between particles both of which are excited above the Fermi sea. The nuclear density is represented by up to 16 density steps, rather than the three of the Bertini INC.

IV. RESULTS

Fig. 4 shows the comparison of the alpha particle NIEL for silicon obtained in this study with that of Messenger et al. [10]. All known damage studies such as shown in [10] have previously been done at alpha energies where the Coulomb interaction dominates. The effects of using the ZBL screened Coulomb potential at lower energies and of including nuclear contributions at higher energies are evident. Table 1 contains the alpha particle NIELs for 10 materials selected for this study: carbon, aluminum, silicon, phosphorous, gallium, copper, germanium, arsenic, selenium, and indium. The table also includes the displacement damage threshold energy ($\equiv E_{th}$) for each material used in the Coulomb NIEL calculations.

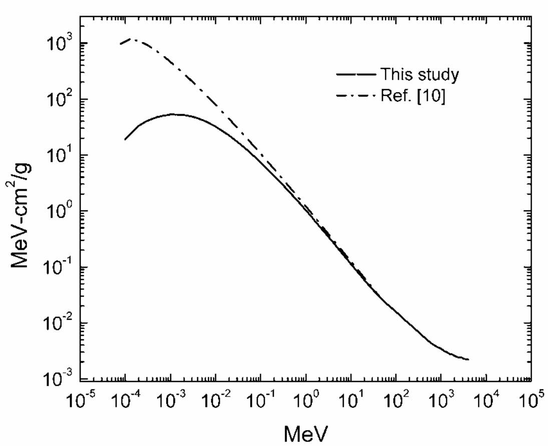

Fig. 4. Alpha particle NIEL for Si from this study and from Messenger et al. [10].

Fig. 5 is a comparison of the new NIEL results for alpha particles in silicon to previous results for protons calculated with the same methods. It is seen that the NIEL for alphas is about 16 times the NIEL for protons at 1.0 MeV/n where the Coulombic interaction dominates. The ratio drops at higher energies because of the nuclear contributions. A significant unknown in the space arena is what the relative damage contribution of protons and alpha particles is for a spectrum such as that shown in Fig. 1. A reasonable method of assessing this is to make use of displacement damage dose. Displacement damage dose was first proposed by Dale, et al. [16] and has been used extensively in areas such as photovoltaics [17]. It is completely analogous to the ionization dose and represents the damage energy per unit target mass. A simple radiation transport analysis was performed where the proton and alpha particles having the energy spectrum in Fig. 1 are impinging on the sphere of bare silicon (i.e., no shielding) of the 0.5 cm radius and the damage dose was computed over the silicon volume. The results showed the contribution of alphas to the damage dose averaged over the silicon region is 15 times smaller than the proton contribution, while the integrated total number of alpha particles is ~40 times less than that of protons. Note that MCNPX transports protons and alpha particles only down to 1 MeV/n. If we consider the lower (<1 MeV/n) energy particles' contribution to the damage dose, we expect that the alpha contribution will be comparable to the proton contribution, mainly because of the great difference in NIEL at the lower energies. It is expected, therefore, that shielding will have a marked influence on the relative contributions. In order to investigate the effect of shielding on the relative contributions to the damage dose, we performed another transport analysis, but at this time with a 1 cm spherical shell aluminum shield added to the silicon sphere. The results showed that the proton contribution to the damage dose is now >250 times larger than the alpha contribution. It has to be noted, however, that the radiation transport analysis discussed here did not account for the effects of possible secondary particles, such as neutrons or pions. Inclusion of secondary particles in the latter transport calculation shows that neutrons are the most important secondary particle to consider. In the absolute sense, the secondary neutrons increased the damage dose in the silicon region by 12% for the alpha particle incident case and by 240% for the proton incident case. The proton damage dose in this case became ~540 times larger than the alpha damage dose in the alpha and proton environments used in this study.

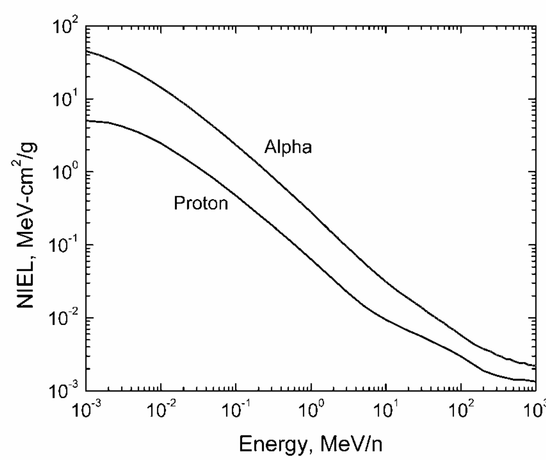

Fig.5. Proton and alpha particle NIEL for silicon from 1 keV/n to 1 GeV/n

TABLE I

NUMERICAL NONIONIZING ENERGY LOSS (NIEL) FOR THE 10 MATERIALS STUDIED IN THIS PAPER. THE VALUES SHOWN INCLUDE THE CONTRIBUTIONS FROM COULOMBIC INTERACTIONS AS WELL AS NUCLEAR ELASTIC AND NON-ELASTIC INTERACTIONS.

	Carbon	Aluminum	Silicon	Phosphorous	Gallium	Germanium	Arsenic	Indium	Copper	Selenium
E_{th} (eV)	35	20	21	9	10	20	10	7	25	20
Energy	MeV-cm^2/g									
10 eV/n				1.06×10^{1}						
20	3.66×10^{1}	1.45×10^{1}	1.30×10^{1}	2.26×10^{1}	3.51×10^{0}		2.61×10^{0}	1.25×10^{0}		
50	8.87×10^{1}	3.63×10^{1}	3.33×10^{1}	3.77×10^{1}	9.68×10^{0}	5.28×10^{0}	8.32×10^{0}	4.42×10^{0}	5.84×10^{0}	4.27×10^{0}
75	1.03×10^{2}	4.40×10^{1}	4.10×10^{1}	4.32×10^{1}	1.23×10^{1}	8.30×10^{0}	1.07×10^{1}	5.80×10^{0}	9.71×10^{0}	6.91×10^{0}
100	1.10×10^{2}	4.85×10^{1}	4.55×10^{1}	4.63×10^{1}	1.41×10^{1}	1.04×10^{1}	1.22×10^{1}	6.85×10^{0}	1.23×10^{1}	8.73×10^{0}
200	1.13×10^{2}	5.52×10^{1}	5.32×10^{1}	5.17×10^{1}	1.78×10^{1}	1.43×10^{1}	1.56×10^{1}	8.89×10^{0}	1.74×10^{1}	1.22×10^{1}
500	9.52×10^{1}	5.45×10^{1}	5.35×10^{1}	5.06×10^{1}	2.05×10^{1}	1.78×10^{1}	1.81×10^{1}	1.09×10^{1}	2.09×10^{1}	1.54×10^{1}
750	8.26×10^{1}	5.03×10^{1}	4.98×10^{1}	4.73×10^{1}	2.05×10^{1}	1.82×10^{1}	1.84×10^{1}	1.14×10^{1}	2.12×10^{1}	1.58×10^{1}
1 keV/n	7.21×10^{1}	4.67×10^{1}	4.65×10^{1}	4.43×10^{1}	2.01×10^{1}	1.80×10^{1}	1.80×10^{1}	1.15×10^{1}	2.08×10^{1}	1.58×10^{1}
2	4.98×10^{1}	3.61×10^{1}	3.64×10^{1}	3.47×10^{1}	1.79×10^{1}	1.63×10^{1}	1.63×10^{1}	1.10×10^{1}	1.86×10^{1}	1.44×10^{1}
5	2.69×10^{1}	2.21×10^{1}	2.26×10^{1}	2.18×10^{1}	1.30×10^{1}	1.20×10^{1}	1.20×10^{1}	8.83×10^{0}	1.34×10^{1}	1.08×10^{1}
7.5	1.99×10^{1}	1.70×10^{1}	1.77×10^{1}	1.71×10^{1}	1.07×10^{1}	9.94×10^{0}	1.00×10^{1}	7.56×10^{0}	1.10×10^{1}	9.04×10^{0}
10	1.58×10^{1}	1.40×10^{1}	1.46×10^{1}	1.42×10^{1}	9.14×10^{0}	8.52×10^{0}	8.60×10^{0}	6.69×10^{0}	9.35×10^{0}	7.78×10^{0}
20	8.83×10^{0}	8.46×10^{0}	8.80×10^{0}	8.70×10^{0}	6.01×10^{0}	5.62×10^{0}	5.68×10^{0}	4.64×10^{0}	6.08×10^{0}	5.17×10^{0}
50	3.91×10^{0}	4.02×10^{0}	4.26×10^{0}	4.25×10^{0}	3.16×10^{0}	2.95×10^{0}	3.02×10^{0}	2.59×10^{0}	3.15×10^{0}	2.74×10^{0}
75	2.68×10^{0}	2.88×10^{0}	3.02×10^{0}	3.04×10^{0}	2.32×10^{0}	2.16×10^{0}	2.22×10^{0}	1.94×10^{0}	2.29×10^{0}	2.03×10^{0}
100	2.05×10^{0}	2.22×10^{0}	2.36×10^{0}	2.39×10^{0}	1.85×10^{0}	1.72×10^{0}	1.78×10^{0}	1.57×10^{0}	1.82×10^{0}	1.63×10^{0}
200	1.06×10^{0}	1.19×10^{0}	1.26×10^{0}	1.29×10^{0}	1.05×10^{0}	9.76×10^{-1}	1.02×10^{0}	9.17×10^{-1}	1.02×10^{0}	9.25×10^{-1}
500	4.34×10^{-1}	5.07×10^{-1}	5.46×10^{-1}	5.60×10^{-1}	4.79×10^{-1}	4.46×10^{-1}	4.63×10^{-1}	4.30×10^{-1}	4.64×10^{-1}	4.20×10^{-1}
750	2.92×10^{-1}	3.45×10^{-1}	3.66×10^{-1}	3.79×10^{-1}	3.31×10^{-1}	3.11×10^{-1}	3.24×10^{-1}	3.04×10^{-1}	3.22×10^{-1}	2.93×10^{-1}
1 MeV/n	2.17×10^{-1}	2.63×10^{-1}	2.79×10^{-1}	2.90×10^{-1}	2.56×10^{-1}	2.37×10^{-1}	2.51×10^{-1}	2.35×10^{-1}	2.49×10^{-1}	2.27×10^{-1}
2	1.11×10^{-1}	1.33×10^{-1}	1.42×10^{-1}	1.48×10^{-1}	1.35×10^{-1}	1.26×10^{-1}	1.33×10^{-1}	1.28×10^{-1}	1.29×10^{-1}	1.19×10^{-1}
3	7.29×10^{-2}	9.02×10^{-2}	9.56×10^{-2}	1.01×10^{-1}	9.23×10^{-2}	8.62×10^{-2}	9.11×10^{-2}	8.76×10^{-2}	8.84×10^{-2}	8.18×10^{-2}
5	4.41×10^{-2}	5.53×10^{-2}	5.86×10^{-2}	6.21×10^{-2}	5.76×10^{-2}	5.38×10^{-2}	5.71×10^{-2}	5.50×10^{-2}	5.49×10^{-2}	5.10×10^{-2}
6	3.76×10^{-2}	4.63×10^{-2}	4.92×10^{-2}	5.24×10^{-2}	4.89×10^{-2}	4.57×10^{-2}	4.82×10^{-2}	4.74×10^{-2}	4.64×10^{-2}	4.39×10^{-2}
8	2.81×10^{-2}	3.53×10^{-2}	3.82×10^{-2}	4.02×10^{-2}	3.87×10^{-2}	3.64×10^{-2}	3.78×10^{-2}	3.71×10^{-2}	3.72×10^{-2}	3.46×10^{-2}
10	2.26×10^{-2}	2.97×10^{-2}	3.15×10^{-2}	3.35×10^{-2}	3.27×10^{-2}	3.08×10^{-2}	3.25×10^{-2}	3.16×10^{-2}	3.13×10^{-2}	2.99×10^{-2}
20	1.23×10^{-2}	1.73×10^{-2}	1.84×10^{-2}	1.95×10^{-2}	2.15×10^{-2}	2.04×10^{-2}	2.14×10^{-2}	2.08×10^{-2}	2.08×10^{-2}	2.00×10^{-2}
30	8.47×10^{-3}	1.26×10^{-2}	1.39×10^{-2}	1.46×10^{-2}	1.73×10^{-2}	1.65×10^{-2}	1.72×10^{-2}	1.69×10^{-3}	1.65×10^{-2}	1.59×10^{-2}
50	5.28×10^{-3}	8.91×10^{-3}	9.61×10^{-3}	1.03×10^{-2}	1.32×10^{-2}	1.31×10^{-2}	1.32×10^{-2}	1.31×10^{-2}	1.27×10^{-2}	1.27×10^{-2}
70	3.82×10^{-3}	6.89×10^{-3}	7.47×10^{-3}	8.05×10^{-3}	1.14×10^{-2}	1.12×10^{-2}	1.13×10^{-2}	1.17×10^{-2}	1.09×10^{-2}	1.11×10^{-2}
100	2.76×10^{-3}	5.28×10^{-3}	5.82×10^{-3}	6.17×10^{-3}	1.00×10^{-2}	1.01×10^{-2}	1.01×10^{-2}	1.17×10^{-2}	9.61×10^{-3}	1.03×10^{-2}
200	1.54×10^{-3}	3.37×10^{-3}	3.79×10^{-3}	4.18×10^{-3}	8.43×10^{-3}	8.67×10^{-3}	8.89×10^{-3}	1.13×10^{-2}	7.90×10^{-3}	9.20×10^{-3}
300	1.11×10^{-3}	2.83×10^{-3}	3.10×10^{-3}	3.58×10^{-3}	7.78×10^{-3}	8.34×10^{-3}	8.32×10^{-3}	1.13×10^{-2}	7.19×10^{-3}	8.78×10^{-3}
500	7.90×10^{-4}	2.31×10^{-3}	2.57×10^{-3}	2.89×10^{-3}	7.33×10^{-3}	7.82×10^{-3}	7.80×10^{-3}	1.13×10^{-2}	6.88×10^{-3}	8.13×10^{-3}
700	6.93×10^{-4}	2.00×10^{-3}	2.41×10^{-3}	2.51×10^{-3}	6.95×10^{-3}	7.17×10^{-3}	7.38×10^{-3}	1.11×10^{-2}	6.50×10^{-3}	7.80×10^{-3}
1000	5.42×10^{-4}	1.95×10^{-3}	2.22×10^{-3}	2.41×10^{-3}	6.48×10^{-3}	6.89×10^{-3}	6.90×10^{-3}	1.09×10^{-2}	6.33×10^{-3}	7.13×10^{-3}

IV. CONCLUSIONS

A computational method developed for proton NIEL was extended to the calculation of alpha particle NIEL. The new data fills a significant gap in existing NIEL calculations. In addition, it allows evaluation of the relative damage of alpha particles and protons in the space environment.

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