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SIMULATION AND VERIFICATION OF DPA IN MATERIALS*†

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Abstract

A recent implementation and verification of consistent modeling of displacements per atom (DPA) in the MARS15 code are described for high-energy particles and heavy ions.

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1. Introduction

Radiation damage is displacement of atoms from their equilibrium position in a crystalline lattice due to irradiation with formation of interstitial atoms and vacancies in the lattice. Resulting deterioration of material (critical) properties is measured – in the most universal way – as a function of displacements per target atom (DPA). DPA is a strong function of projectile type, energy and charge as well as material properties including its temperature. The phenomenon becomes very serious for high-intensity beams especially for high-charge heavy ions ($\sim z^2$), being identified, for example at FRIB and FAIR, as one of the critical issues, limiting lifetime of targets to as low as a few weeks. A recent implementation of consistent DPA modeling into the MARS15 code [1] and its verification are described in this paper.

2. DPA Modeling in MARS15 Code

A model used in the MARS15 code for DPA calculations in electromagnetic processes [2] has been extended to an arbitrary projectile of energy ranging from 1 keV to 10 TeV. A primary knock-on atom (PKA) created in nuclear collisions can generate a cascade of atomic displacements. This is taken into account via damage function ν(T). DPA is expressed in terms of damage cross section σ_d :

$$\sigma_d(E) = \int_{T_d}^{T_{\max}} \frac{d\sigma(E,T)}{dT} \nu(T)\, dT,$$

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where E is kinetic energy of the projectile, T is kinetic energy transferred to the recoil atom, T_d is the displacement energy, and T_{max} is the highest recoil energy according to kinematics. In a modified Kinchin-Pease model [3], ν(T) is zero at $T<T_d$, unity at $T_d <T<2.5T_d$, and $k(T)E_d/2T_d$ at $2.5T_d <T$, where E_d is "damage" energy available to generate atomic displacements by elastic collisions (Fig. 1). T_d is an irregular function of atomic number (~40 eV). The displacement efficiency, k(T), introduced as a result of simulation studies on evolution of atomic displacement cascades [4], drops from 1.4 to 0.3 once the PKA energy is increased from 0.1 to 100 keV, and exhibits a weak dependence on target material and temperature.

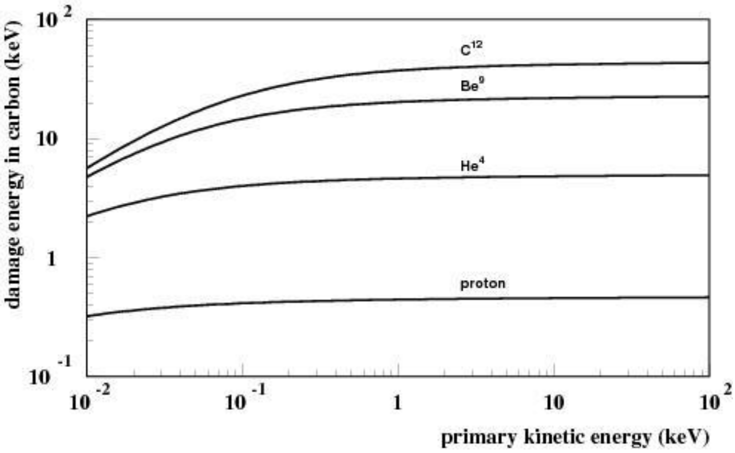

Figure 1. Damage energy E_d versus PKA energy.

For electromagnetic elastic (Coulomb) scattering, the Rutherford cross-section with Mott corrections and nuclear form-factors (a factor of two effect) are used in our model. Resulting displacement cross-sections due to Coulomb scattering are shown in Fig. 2 for various projectiles on silicon and carbon targets. For elementary particles, energy dependence of σ_d disappears above 2-3 GeV, while it continues to higher energies for heavy ions. For projectiles heavier than a proton, σ_d grows with a projectile charge z as z^2/β^2 at $\gamma\beta > 0.01$, where β is a projectile velocity. All products of elastic and inelastic nuclear interactions as well as Coulomb elastic scattering of transported charged particles (hadrons, electrons, muons and heavy ions) from 1 keV to 10 TeV contribute to DPA in the MARS15 model.

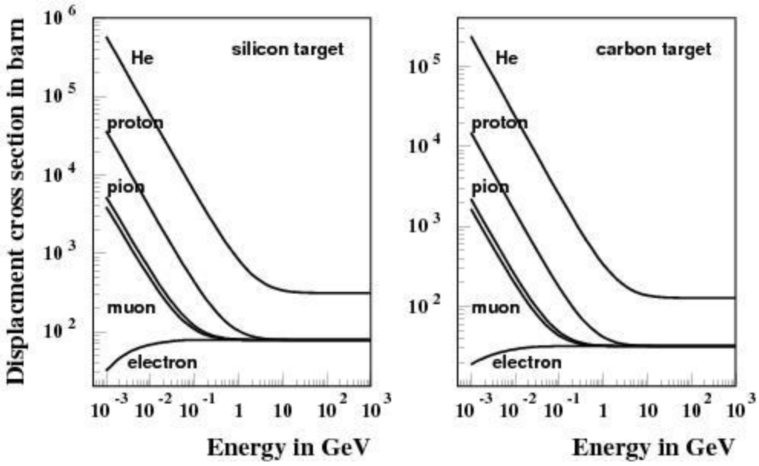

Figure 2. Displacement cross-section in silicon and carbon for various projectiles.

3. DPA Calculation Comparison

In this section, results on DPA calculated with the new MARS15 model for three cases are compared with those obtained with other DPA-capable codes, SRIM/TRIM, PHITS and MCNPX. The first case is a 1-GeV proton beam of 1-cm^2 area on a 3-mm thick iron target. SRIM, PHITS and MCNPX results are courtesy of Susana Reyes. As one can see in Table 1, there is a quite substantial difference between the predictions, with SRIM giving a very small value and the MARS15 result being a factor of 2.6 to 2.9 above those by PHITS and MCNPX. Calculated with MARS15 contributions to DPA of physics processes are as follows: 75.5% nuclear inelastic, 16% nuclear elastic, 2.75% electromagnetic elastic, 5.5% low-energy neutrons, and 0.25% electrons. The dominance of nuclear interactions in this case explains the above differences.

Table 1. DPA for 1-GeV protons on 3-mm iron.

Code	SRIM	PHITS	MCNPX	MARS15
DPA/pot	1.18e-22	2.96e-21	3.35e-21	8.73e-21

The second case is a 0.32-GeV/u Uranium beam of 9-cm^2 area on a 1-mm thick beryllium target. SRIM and PHITS results are again a courtesy of Susana Reyes. Table 2 shows that SRIM and MARS15 results are now very close to each other, while those calculated with PHITS are a factor of 70 lower. Calculated with MARS15 contributions to DPA of physics processes are as follows: 0.3% nuclear inelastic, 99.06% electromagnetic elastic, 0.02% low-energy neutrons, and 0.62% electrons. The dominant role of Coulomb scattering in this case explains the similarity of the SRIM and MARS15 predictions.

Table 2. DPA for 0.32-GeV/u Uranium on 1-mm beryllium target.

Code	SRIM	PHITS	MARS15
DPA/pot	2.97e-20	5.02e-22	2.13e-20

The third case is a 0.13-GeV/u Germanium beam of 0.004-cm^2 area on a 1.2-mm thick tungsten target. TRIM and PHITS results are a courtesy of Yosuke Iwamoto. Table 3 gives calculated DPA values in the first hundred microns of the target. The difference between TRIM and MARS15 needs to be understood.

Table 3. Entrance DPA for 0.13-GeV/u Germanium on 1.2-mm tungsten target.

Code	TRIM	PHITS	MARS15
DPA/pot	8.04e-16	1.25e-17	1.43e-16

4. BLIP Beam Tests for 0.7-MW NuMI/LBNE Target

A majority of data on radiation damage is available for reactor neutrons. Studies with hundred MeV protons [5] have revealed that a threshold of about 0.2 DPA exists for carbon composites and graphite. MARS15 studies helped realize that the BLIP beam tests with 0.165-GeV protons can emulate the NuMI neutrino target situation for a 120-GeV proton beam (Table 4). It turns out that despite a substantial difference in the beam energies in these cases, nuclear interactions and Coulomb scattering contribute about the same way (45-50% each) to the peak DPA in thick graphite targets irradiated at these two facilities.

Table 4. Peak DPA in POCO graphite targets at BLIP and NuMI.

Target	E_p (GeV)	Beam σ (mm)	N_p (1/yr)	DPA (1/yr)
NuMI	120	1.1	4.0e20	0.45
BLIP	0.165	4.23	1.12e22	1.5

References

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