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RADIATION DAMAGE DUE TO ELECTROMAGNETIC SHOWERS*†

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Abstract

Radiation-induced damage due to atomic displacements is essential to correctly predict the behavior of materials in nuclear reactors and at charged-particle accelerators. Traditionally the damage due to hadrons was of major interest. The recent increased interest in high-energy lepton colliders gave rise to the problem of prediction of radiation damage due to electromagnetic showers in a wide energy range – from a few hundred keV and up to a few hundred GeV. The report describes results of an electron- and positron-induced displacement cross section evaluation. It is based on detailed lepton-nucleus cross sections, realistic nuclear form-factors and a modified Kinchin-Pease damage model. Numerical data on displacement cross sections for various target nuclei is presented.

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Introduction

Radiation-induced damage due to atomic displacements is essential to correctly predict the behavior of materials in nuclear reactors and at charged-particle accelerators. Traditionally the damage due to hadrons was of major concern. It was shown recently that in a high-flux nuclear reactor the radiation damage to structural materials due to electromagnetic showers (EMS) is not negligible and can be comparable to that due to neutrons [1]. For nuclear reactors usually coupled neutron-gamma transport calculations are performed while secondary electrons and positrons are considered to be deposited locally. Therefore, gamma-induced displacement cross sections were evaluated that take into account the electron- and positron-nucleus interactions implicitly [1-2]. Another essential feature of the studies is that, being based on the second Born approximation, the cross section evaluations were not performed for target nuclei heavier than iron. This study deals with an evaluation of electron- and positron-induced displacement cross sections because for high-energy accelerators electron and positron transport is modeled explicitly. The energy region for this evaluation is extended well above the level of 10–15 MeV which is characteristic of nuclear reactors. At high energies the finite size of nuclei becomes important and a nuclear form-factor is taken into account. In addition, the Mott electron-nucleus cross section is employed [3], so that the study is not limited by the second Born approximation and target nuclei heavier than iron are accounted for.

Formalism

A displacement of an atom from its equilibrium position in a crystalline lattice due to irradiation gives rise to a production of an interstitial atom and a vacancy in the lattice which is a *radiation damage* [4].The number of atomic displacements per target atom (DPA) due to irradiation is expressed in terms of damage cross section, σ_d, as follows:

$$\sigma_d(E) = \int_{T_d}^{T_{\max}} \frac{d\sigma(E,T)}{dT} \nu(T) dT, \tag{1}$$

where E is kinetic energy of the projectile (electron or positron), T is kinetic energy transferred to the recoil atom, T_d is the displacement energy–the minimal transferred kinetic energy required to produce a displaced atom, $T_{\max}$ is the highest possible–from the standpoint of kinematics–kinetic energy transferred to the recoil atom, $d\sigma / dT$ is an elastic scattering cross section of the projectile, $\nu(T)$ is the damage function which takes into account the multiplicity of the displaced atoms in the cascade generated by the primary knock-on atom (PKA) of energy T [4-5]. The displacement energy depends on target material and various authors use slightly different datasets. The data on T_d used in this study is given in Table 1.

According to relativistic kinematics, the maximal kinetic energy of a PKA is expressed as follows:

$$T_{\max} = \frac{2E\left(2m_e c^2 + E\right)}{Mc^2 + \frac{m_e^2}{M}c^2 + 2\left(m_e c^2 + E\right)}, \tag{2}$$

where m_e and M are the rest masses of the projectile and target, respectively, and c is the speed of light. The minimal projectile kinetic energy, $E_{\min}$, required to displace an atom in lattice from its equilibrium position can be derived from Eq. (2) and is expressed as follows:

$$E_{\min} = m_e c^2 \sqrt{\left(1 - \frac{T_d}{2m_e c^2}\right)^2 + \frac{T_d}{2m_e c^2}\left(1 + \frac{m_e}{M}\right)\cdot\left(1 + \frac{M}{m_e}\right)} - \left(m_e c^2 - \frac{T_d}{2}\right). \qquad (3)$$

The numerical data on $E_{\min}$ shown in Figure 1 reveals high sensitivity of the data to the displacement energy.

Table 1. The displacement energies, T_d, used in the study

Target atomic number, Z	T_d (eV)
13	25
22	30
29	30
41	60
42	60
73	90
74	90
82	25
All others	40

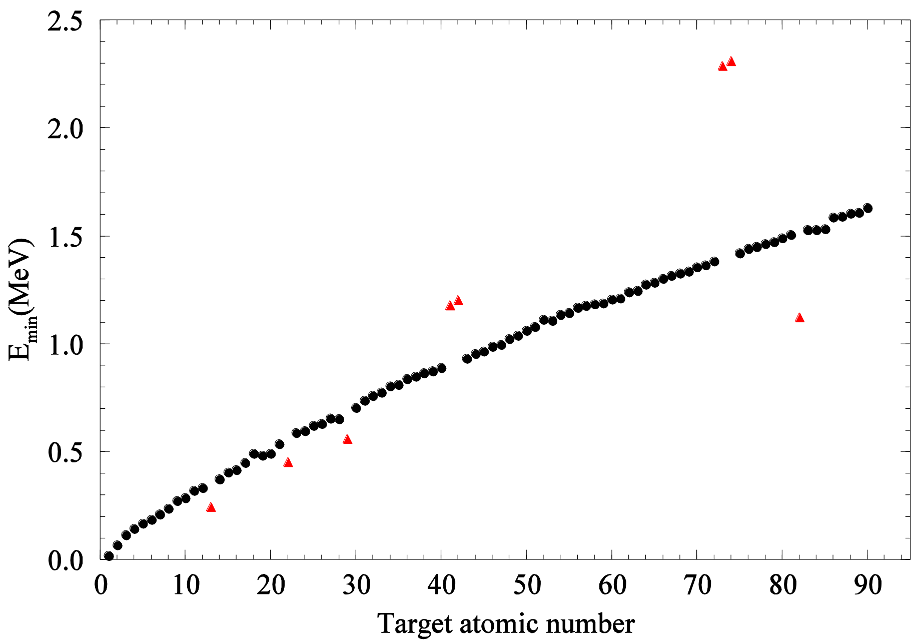

Figure 1. Minimal electron kinetic energy, $E_{\min}$, required to produce a lattice displacement according to Eq. (3). Circles correspond to target nuclei with T_d = 40 eV while triangles refer to nuclei with other displacement energies.

Elastic scattering cross sections

At energies above several keV the results of a detailed fitting to the Mott electron-nucleus cross section, σ_M , are used [3]. Namely, the authors performed the fitting to the ratio of σ_M / σ_R , where σ_R is Rutherford cross section, for almost entire periodic table with the average error less than 1% as compared to exact values of σ_M . The McKinley-Feshbach cross section, σ_{MF}, was derived in the second Born approximation [6] and is valid when $(\alpha Z / \beta)^2 << 1$, where α is the fine structure constant, Z is the target nucleus atomic number, and β is the ratio of the velocity of projectile to that of light.

At high projectile energies one has to take into account a nuclear form-factor because the presence of the damage function, $\nu(T)$, in the integrand of Eq. (1) gives rise to high sensitivity of σ_d to transferred energy (see below). A symmetrized Fermi function [10] was used for form-factors of deuterium, carbon and nuclei with Z > 9. For the other nuclei a modified harmonic-oscillator model [11] was applied. A simple Gaussian nuclear form-factor with the same average radius as in the above models was considered as well. The difference in σ_{PKA} due to including nuclear screening is negligible–it is about one percent even for heavy nuclei at high energies.

In order to demonstrate the quality of the cross sections over the entire energy range, Figure 2 shows a comparison for the integral cross section of PKA production. The latter is defined as follows:

$$\sigma_{pka}(E) = \int_{T_d}^{T_{\max}} \frac{d\sigma(E,T)}{dT} dT. \tag{4}$$

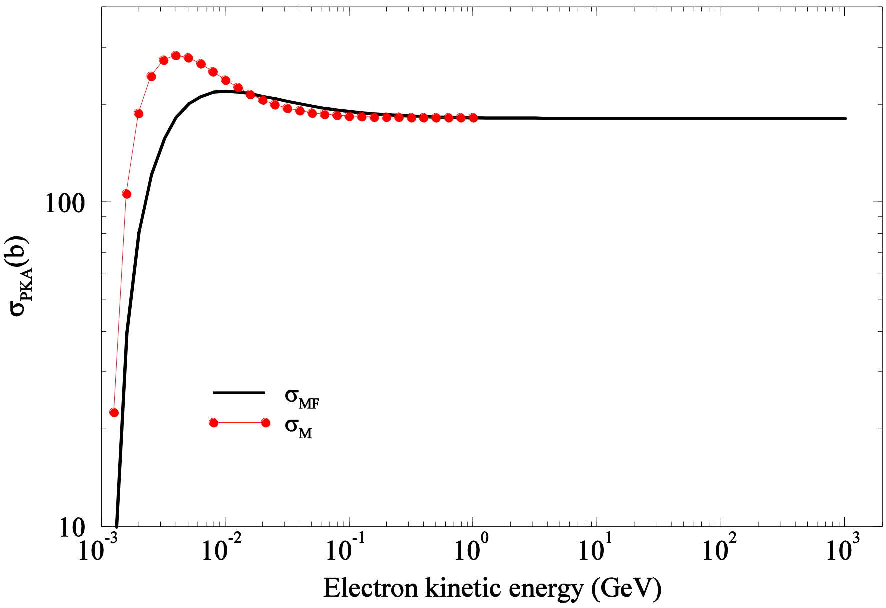

Figure 2. Integral cross section of PKA production, $\sigma_{pka,}$, calculated for a pointlike ^{207}Pb nucleus according to Mott (σ_M) and McKinley-Feshbach (σ_{MF}) formalisms.

The McKinley-Feshbach approximation is as follows:

$$\frac{d\sigma(E,T)}{dT} = \frac{\sigma_0}{\gamma^2\beta^4}\frac{\delta}{T_{\max}}\frac{1}{y^2}\left(1-\beta^2 y \pm \pi\alpha\beta Z\left[\sqrt{y}-y\right]\right), \tag{5}$$

where σ_0 is $\pi(r_0 Z)^2$, r_0 is classical electron radius, $\delta = Mc^2/(Mc^2+2E)$, $y = T\delta/T_{\max}$, and the term which includes $\pi\alpha\beta Z$ is positive for electrons and negative for positrons. The asymptotic value of σ_{pka} at $E \to \infty$ can be shown to be

$$\sigma_{pka}(\infty) = \sigma_0 \frac{2m_e}{M}\frac{m_e c^2}{T_d} \tag{6}$$

and for a ^{207}Pb target nucleus the asymptotic cross section is equal to 182 barn.

The Mott cross section is considered to be exact and at energies around 1 GeV it virtually coincides with the McKinley-Feshbach cross section. It justifies using the latter at high energies even for target nuclei heavier than iron. At energies below 10 MeV the disagreement between σ_M and σ_{MF} is about a factor of two, so that at low energies one has to use the Mott cross section. At low energies the disagreement between σ_M and σ_{MF} decreases when the target atomic number decreases and for iron the two cross sections practically–within a few percent–coincide.

Damage function

The damage function, $\nu(T)$, is the number of displaced atoms generated by a PKA of energy T. It can be expressed as follows (see [4, 5, 7, 8]):

$$\nu(T) = \begin{cases} 0 & (T < T_d) \\ 1 & (T_d \le T < 2.5T_d), \\ k(T)E_d/2T_d & (2.5T_d \le T) \end{cases} \tag{7}$$

$$E_d = \frac{T}{1+kg(\varepsilon)}, \tag{8}$$

$$k = 0.13372 Z^{2/3}/A^{1/2}, \tag{9}$$

$$\varepsilon = \frac{T}{86.931 Z^{7/3}}, \tag{10}$$

$$g(\varepsilon) = 3.4008\varepsilon^{1/6} + 0.40244\varepsilon^{3/4} + \varepsilon, \tag{11}$$

where A is the target atomic mass and the energy T in Eq. (10) is in eV. The function $k(T)$ is given by the following expression:

$$k(T) = 0.24 - 1.04\left(\frac{A_1}{X} + \frac{B_1}{X^{4/3}} + \frac{C_1}{X^{5/3}}\right), \quad (12)$$

where A_1, B_1, C_1, and X are -9.57, 17.1, -8.81, and $20T$, respectively, while T is in keV.

The function $k(T)$, called displacement efficiency, replaces the constant of 0.8 used in earlier studies [4-5]. It was introduced as a result of simulation studies on evolution of atomic displacement cascades [9]. The function $k(T)$ was found to depend weakly on target material and its temperature.

At transferred energies above $2.5T_d$ the damage function reveals some growth with T. Therefore, taking into account the nuclear form-factor, $F(q^2)$, is important to correctly predict the damage cross section at high energies. Figure 3 shows the average recoil energy of PKA for lead. For an iron target nucleus the recoil energies calculated with McKinley-Feshbach and Mott formalisms practically coincide. One can see from Figure 3 that for incident electrons with energies from 10 MeV up to 1 TeV the average transferred energy is above $2.5T_d$, so that neglecting the form-factor would significantly overestimate the damage cross section. It should be noted that average recoil energy calculated using the simple Gaussian form-factor agrees within about a percent with results obtained with more precise and complicated models.

The calculated damage cross sections with and without form-factor are shown in Figure 4. The importance of the form-factor in a wide energy region–from the onset of the effect at about 50 MeV and up to the highest energy studied–is clearly seen in the Figure 4.

Importance of correct description of the displacement efficiency $k(T)$ [12] is shown in Figure 5. For iron, starting at 100 MeV and above, the difference in σ_d due to the difference in description of the displacement efficiency is about 20%. One accepts the same Eq. (12), derived initially for iron, for all target nuclei as far as a weak dependence on material was observed [8-9].

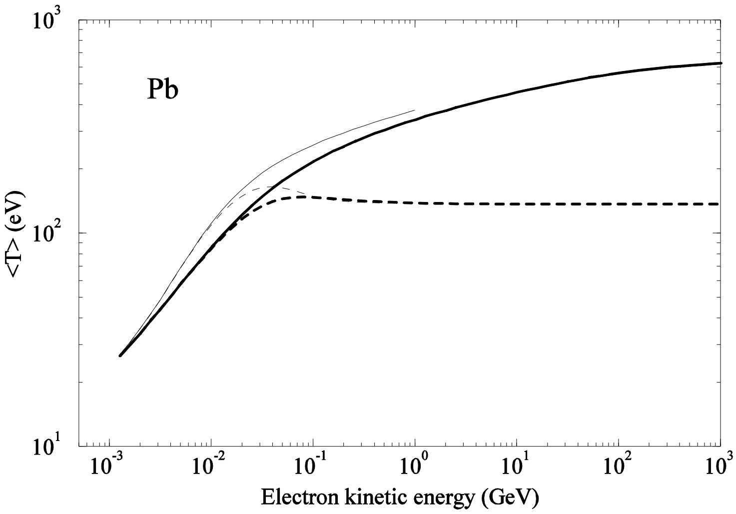

Figure 3. Average recoil energy, $< T >$, of PKA *vs* electron energy for lead. Calculations were performed with the McKinley-Feshbach (thick lines) and Mott (thin lines) cross sections for a pointlike (solid lines) and extended target nucleus (dashed lines).

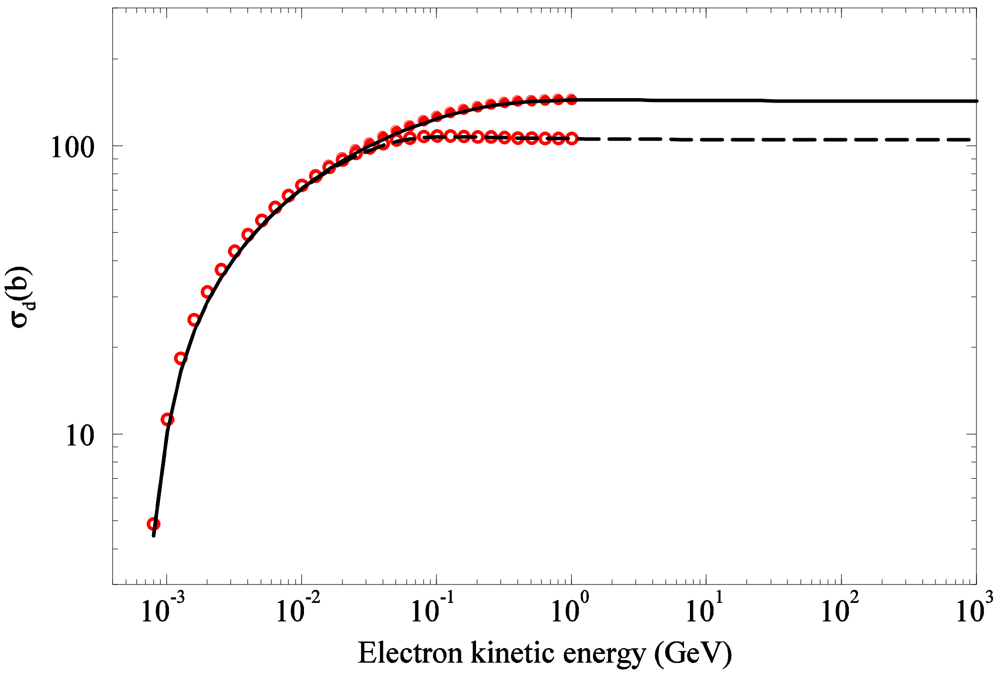

Figure 4. Damage cross sections calculated for iron with McKinley-Feshbach (lines) amd Mott (circles) cross sections for a pointlike (solid line and full circles) and extended target nucleus (dashed line and open circles). For the purpose of this comparison, the displacement function, $k(T)$, equal to 0.8 was used instead of Eq. (12).

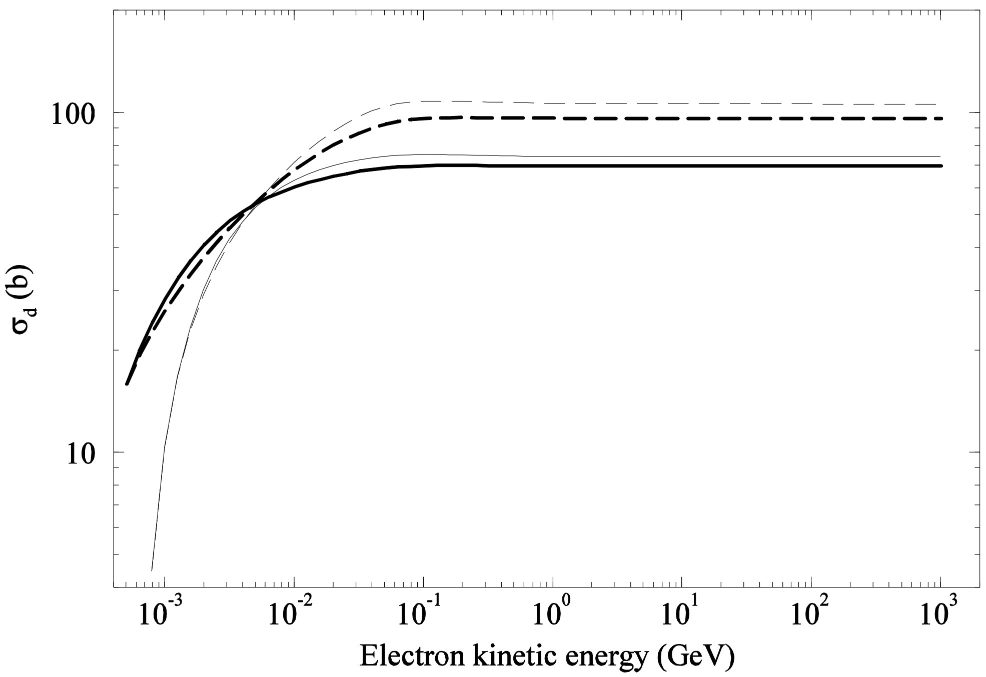

Figure 5. Damage cross section for aluminum (thick lines) and iron (thin lines) calculated with the displacement efficiency of 0.8 (dashed lines) and with Eq. (12) (solid lines).

Results

All the damage cross sections presented in this section were calculated with the realistic nuclear form-factors taken into account [10-11]. The damage cross sections for a number of target nuclei are shown in Figure 6. One can see that, due to high sensitivity of σ_d (see Eq. (1)) on the lower integration limit, the irregular displacement energies (see Table 1) give rise to significant variations in the damage cross sections. From practical standpoint it is reasonable to consider the target nuclei with $T_d = 40\,\mathrm{eV}$ and all the other nuclei separately. For the former target nuclei the dependence σ_d on target atomic number is pretty smooth if one neglects the small variations due to irregularities in atomic masses (see Figure 7. Therefore, in practical calculations for target nuclei with $T_d = 40\,\mathrm{eV}$ one can make a simple interpolation in Z. For the other nuclei separate calculations are required.

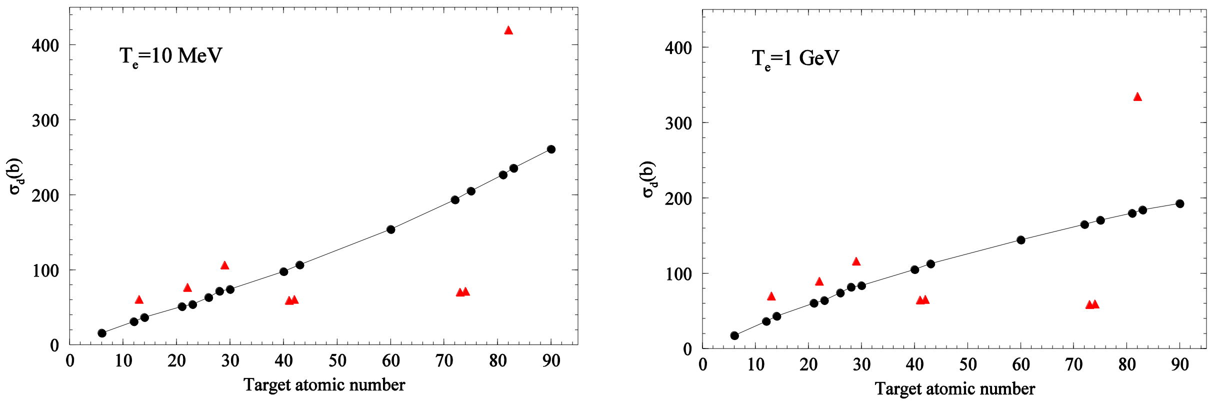

Figure 6. Calculated damage cross sections for various target nuclei and for two electron energies. The displacement function $k(T)$ from Eq. (12) was used. Circles correspond to target nuclei with $T_d = 40\,\mathrm{eV}$ while triangles refer to nuclei with other displacement energies.

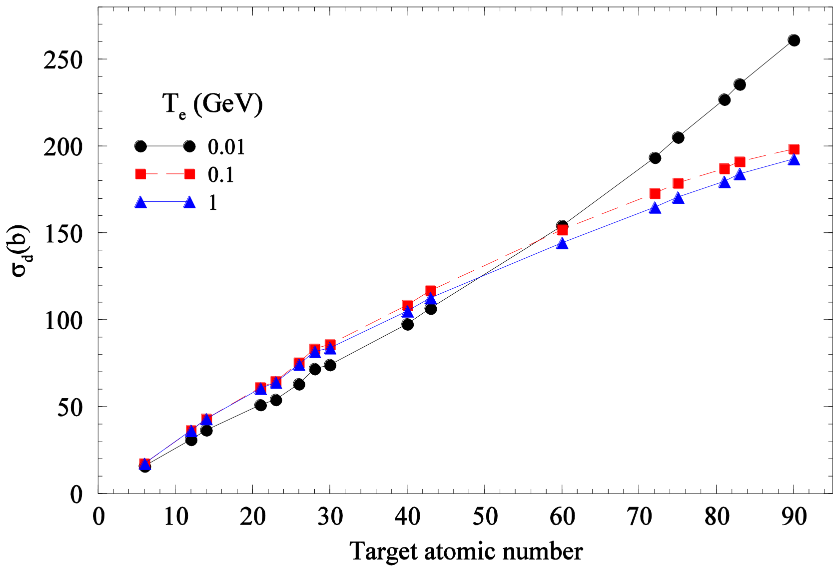

Figure 7. Damage cross sections calculated for several electron energies and for various target nuclei with $T_d = 40\,\mathrm{eV}$. The displacement function $k(T)$ from Eq. (12) was used.

Detailed fitting to the Mott cross section [3] was performed only for electrons as projectiles. Therefore, one can distinguish electrons and positrons as projectiles only when using the McKinley-Feshbach formalism [6] which means the difference can be correctly expressed only for target nuclei not heavier than iron. On the other hand, the difference is negligible at high energies–above 10 MeV for aluminum and above 100 MeV for iron (see Figure 8). As a result, one can choose the following approach in order to describe positron-induced damage cross section for target nuclei heavier than iron: (i) applying the same positron-to-electron ratios as observed for iron under 100 MeV and (ii) assuming equivalence of electron and positron damage cross sections above 100 MeV.

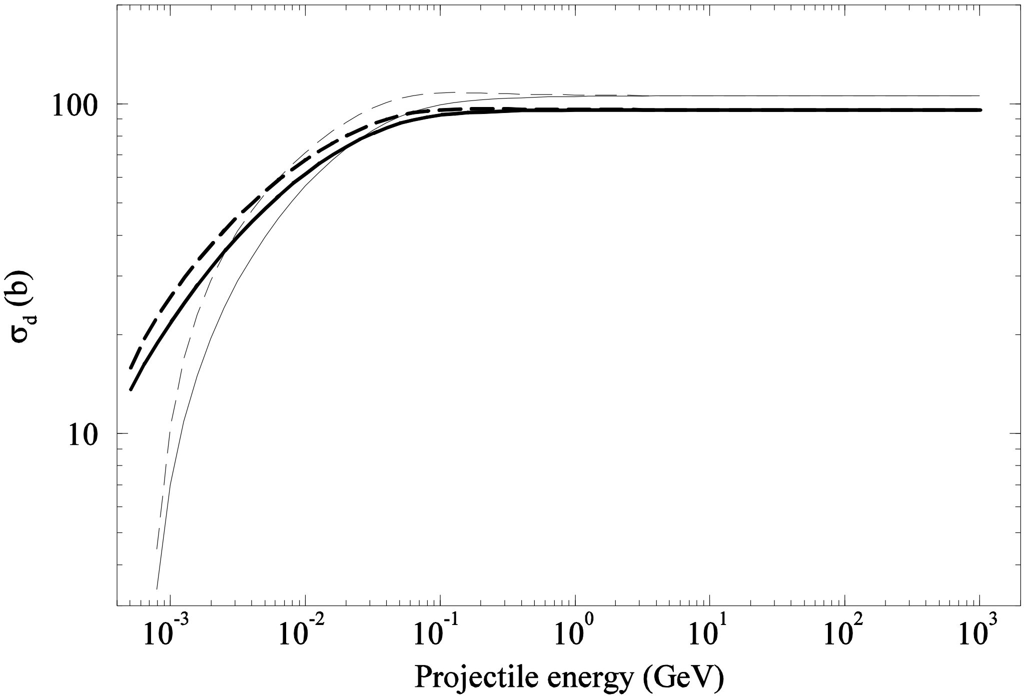

Figure 8. Calculated damage cross sections for electrons (dashed lines) and positrons (solid lines) for aluminum (thick lines) and iron (thin lines) according to Eq. (5). For the purpose of this comparison the displacement function, $k(T)$, equal to 0.8 was used instead of Eq. (12).

Conclusions

The formalism used to calculate damage cross sections due to electrons and positrons is described. It employs the following: (i) Mott electron-nucleus cross section and McKinley-Feshbach electron- and positron-nucleus cross sections; (ii) realistic nuclear form-factors; (iii) damage function according to the modified Kinchin-Pease model with a corrected displacement efficiency. Importance of taking into account the nuclear form-factor and correct displacement efficiency function is studied.

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