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Calculation of electron-beam induced displacement in thin films by using parameter-reduced formulas

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ABSTRACT

Based on the Mott cross sections of relativistic electron collisions with atoms, we calculate displacement creation by electron beams of arbitrary energies (up to 100 MeV) in thin films of arbitrary atomic numbers (up to Z = 90). In a comparison with Mont Carlo full damage cascade simulations, we find that total number of displacements in a film can be accurately estimated as the product of average displacements created per collision and average collision numbers in the film. To calculate average displacements per electron-atom collision, energy transfer from Mott cross section is combined with NRT model. To calculate collision numbers, mean deflection angles and multi-scattering theory are combined to extract collision number dependence on film thickness. For each key parameter, parameter-reduced formulas are obtained from data fitting. The fitting formulas provide a quick and accurate method to estimate radiation damage caused by electron beams.

1. Introduction

Radiation damage by electron beams cannot be avoided in e-beam based characterization techniques including transmission electron microscopy (TEM) and scanning electron microscopy (SEM). Displacement creation can extend to much lower energy range when atoms' thermal vibration taken into consideration [1,2]. Unique radiation effects by TEM analysis beam has led to intentional beam modification technique. To name a few examples, electron beams can weld carbon nanotubes [3], and convert carbon onions into diamond [4], and induce nanocrsytallization in amorphous metallic glasses [5].

The displacements creation and radiation effects in Si [6], Ge [7], compound semiconductors [8], pyrolytic graphite [9], single-crystal graphite [10], and carbon-based nanostructures [11–13], have been well documented. Prediction of e-beam induced damage can be tracked back to 1960s by researchers at Oak Ridge National Laboratory [14]. Monte Carlo simulation codes such as CASINO has been developed to predict electron trajectories [15]. Most recently, DEEPER (Damage creation and particle transport in matter) code has been developed to provide a full capability to simulate distributions of electrons, energy deposition, and displacements [16].

Quantitative estimation of e-beam damage requires prolonged computation time for statistical accuracy, due to small electron scattering cross sections for significant momentum transfer. Hence, the present study is motivated to develop a method to quickly estimate displacement creation by electron beams of a wide energy range. Such knowledge is critically needed in transmission electron microscopy (TEM) analysis to optimize/minimize electron fluence or analysis time for damage control. The knowledge is also useful for irradiation studies which intentionally use electron beams for modification.

2. Modeling procedure, numerical calculation and fitting

The present study is limited to a relatively thin specimen in which beam dispersion is not significant after beam penetration. One such example is TEM specimens which are typically about 50 nm to 200 nm thick. The key approach of damage calculation is to find average number of collisions in films, n_C, and average number of displacements created per collision, $\overline{N_d}$. Hence the total displacements per electron, N_{Total}, is approximately the product of these two parameters:

$$N_{Total} = n_C \cdot \bar{N}_d \tag{1}$$

The average number of collisions can be expressed as:

$$n_C = \frac{D}{\lambda} \tag{2}$$

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where D is the film thickness and λ is the mean free flying path, which is given by

$$\lambda = \frac{A}{\rho N_A \sigma_T} \tag{3}$$

where A is the atomic number, ρ is the density, N_A is the Avogadro number, and σ_T is the total elastic scattering cross section.

2.1. Mott cross section

Mott model has been developed to describe electron-atom scattering for relativistic electrons [17]. One drawback of the Mott model is numerical calculations which involve infinite series of Legendre expansions. Towards a simplified expression without losing accuracy, Mott differential cross section is often expressed by adding a screening factor to a Rutherford differential cross section, as given by [18–20]

$$\frac{d\sigma_{Mott}}{d\Omega} = R_{Mott} \times \frac{d\sigma_{Ruth}}{d\Omega} \times [1 - F_e(q)]^2 \tag{4}$$

$$R_{Mott} = \sum_{j=0}^{4} \alpha_j(Z,\beta)(1-\cos\theta)^{\frac{j}{2}} \tag{5}$$

$$\alpha_j(Z,\beta) = \sum_{k=1}^{6} b_{kj}(Z)(\beta - \overline{\beta})^{k-1} \tag{6}$$

where Z is the atomic number, β is the velocity of electrons in the unit of speed of light, b_{kj} is coefficient obtained from fitting [20]. The second term in Eq. (4) is the Rutherford differential cross section for a point charge, which is given by [18]:

$$\frac{d\sigma_{Ruth}}{d\Omega} = (Z \times r_e)^2 \times \left(\frac{1-\beta^2}{\beta^4}\right) \times \frac{1}{(1-\cos\theta)^2} \tag{7}$$

where classic electron radiation $r_e = 2.817938 \times 10^{-13}$ cm. The third term in Eq. (4) is the screening factor, which is given by [21]:

$$F_e(q) = \sum_{i=1}^{3} A_i \frac{[h\alpha_i/(2\pi)]^2}{[h\alpha_i/(2\pi)]^2 + q^2} \tag{8}$$

where h is the Plank constant, a_i is fitting parameters and q is momentum transfer calculated by:

$$q = 2 \times \beta \times \gamma \times m_e \times c \times \sin\frac{\theta}{2} \tag{9}$$

where $\gamma = (1-\beta^2)^{-1/2}$ and m_e is the mass at rest of electron.

The total Mott cross section, σ_{Mott}, can be obtained by numerical integration of Eq. (4). The present study calculate σ_{Mott} for elements from Z = 1 to Z = 92 and for energy from 100 keV to 100 MeV. Through comparisons with all numerical results, we find the following formula which give the best fitting with minimized errors (valid from Z = 1 to Z = 92).

$$\sigma_{\text{Mott}}(\mu\text{m}^2) = \begin{cases} \frac{1.14\times10^{-12}}{\beta^{2*\left(0.9+\frac{Z}{A-Z}\right)}}[(Z-Z_0)*Z]^k & Z > 2 \\ \frac{1.14\times10^{-12}}{\beta^{3.8}}Z^{2.035} & Z = 2 \\ \frac{1.14\times10^{-12}}{\beta^2} & Z = 1 \end{cases} \tag{10}$$

where A is the atomic mass number of target atoms. k is a parameter calculated by:

$$k = A_1 e^{-\frac{Z-Z_0}{t_1}} + A_2 e^{-\frac{Z-Z_0}{t_2}} + y_0 \tag{11}$$

where Z_0, A_1, A_2, t_1, t_2 and y_0 are all fitting parameters. These parameters need to be divided into 7 groups to describe the complexity from the periodic table, and are provided in Table 1.

The above fitting makes it possible to quickly calculate σ_{Mott} without numerical calculations. Fig. 1 compares the exact results from the numerical calculations by using Eqs. (4)–(9) and the fitting-obtained results by using Eqs. (10) and (11), for elements randomly selected from Z = 1 to Z = 92 and bombarding electrons for energies ranging 100 keV to 100 MeV. All solid lines are fitting obtained results. The cross sections decrease with increasing energies and begin to be saturated at the energy of about 1000 keV and beyond. Fitting results are in good agreements with numerical calculation results. Small deviation is observed only for high Z mass at low energy range. As to be shown, such small deviation at low energy region plays an ignorable role in influencing damage calculation since the threshold e-beam energy for displacement creation is typically higher than 1 MeV for high Z atoms.

2.2. Displacement creation per electron collision

For every elastic collision governed by Coulomb force, displacements are created once energy transfer from an electron collision is larger than the displacement threshold energy, E_d. The energy transfer from relativistic electron to a static atom, E_t, is calculated by [22]:

$$E_t = \frac{[(E_k + m_e c^2)\sin^2\theta + Mc^2(1-\cos\theta)]E_k(E_k + 2m_e c^2)}{(E_k + Mc^2)^2 - E_k(E_k + 2m_e c^2)\cos^2\theta} \tag{12}$$

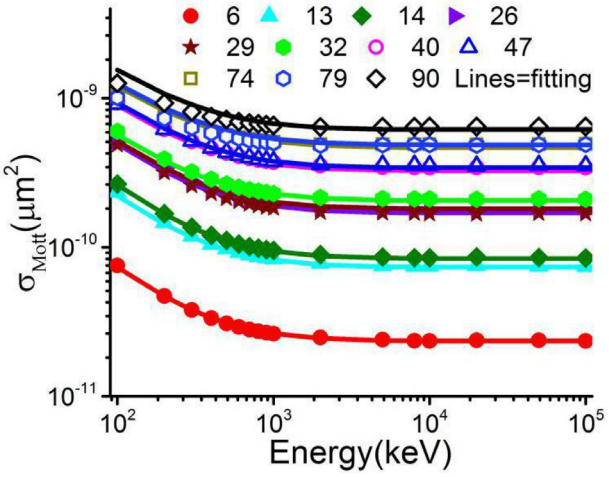

Fig. 1. Comparison of results from numerical calculations and fitting for different atomic mass numbers. The fitting is obtained by parameter reduced formula of Eq. (10).

Table 1
Fitting parameters to calculate the total Mott cross sections using Eqs. (10) and (11).

Group	Z_0	A_1	t_1	A_2	t_2	y_0
1 ($3 \leqslant Z \leqslant 10$)	2	4.67586	0.47096	1.14154	2.96433	0.66093
2 ($11 \leqslant Z \leqslant 18$)	10	3.49801	0.34041	0.65818	3.8001	0.84258
3 ($19 \leqslant Z \leqslant 36$)	18	0.81231	0.69343	0.77947	4.14312	0.82741
4 ($37 \leqslant Z \leqslant 54$)	36	0.9401	0.58233	0.62479	4.74957	0.86197
5 ($55 \leqslant Z \leqslant 80$)	54	0.64261	1.23424	0.5252	9.4171	0.76334
6 ($81 \leqslant Z \leqslant 86$)	80	0.63494	0.59416	0.4875	3.42972	0.90325
7 ($87 \leqslant Z \leqslant 92$)	86	0.617	0.64265	0.50989	4.5773	0.85768