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The analytical differential cross section of elastic scattering of atoms aimed to be used in Monte Carlo modeling of propagation of fast particles in matter

E.G. Sheikin

Coddan Technologies LLC, 22 Beloostrovskaya Str., Saint Petersburg 197342, Russia
Saint-Petersburg State University, Ulyanovskaya 3, Petrodvoretz, Saint Petersburg 198504, Russia

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ABSTRACT

The analytical differential cross section (DCS) of elastic scattering of atoms that reproduces the stopping power and the straggling of energy loss is proposed. Analytical expressions derived from the DCS for diffusion σ_d and viscosity σ_v cross sections of elastic collisions of atoms are in good agreement with known cross sections of ^{38}Ar-^{40}Ar and H-Li collisions obtained from quantum mechanical simulations. The Monte Carlo modeling of the transport of sputtered Cu atoms in Ar and implantation of Bi ions in B and C materials made using the proposed DCS demonstrates its accuracy in the modeling of elastic collisions.

1. Introduction

Elastic collisions of fast atoms or ions with atoms of matter effect significantly both on the energy and on the direction of their motion in mater. Therefore in many processes such as the transport of sputtered atoms in gas discharges, the passage of ions through solids or gases the elastic scattering of fast particles (atoms or ions) by atoms of matter effects significantly on the energy and the spatial distribution of the particles both in a volume and on a surface they are impinge on. Monte Carlo (MC) methods are widely used for modeling of the propagation of fast particles in matter [1–11]. Individual collisions of particles in MC simulations are usually modeled using a DCS. The most accurate description of elastic collisions of atoms using a real interaction potential is time consuming hence in MC simulations some simplified approaches are often used to model elastic collisions. The DCS corresponding to the Variable Hard Spheres (VHS) model [12] are widely used in the MC modeling of elastic collisions of atoms [4–6]. But it should be emphasized that in the VHS model the elastic scattering is isotropic in the center-of-mass system [12] that is not conform to the scattering in the case of a real interaction potential and can result in significant incorrectness of the modeling [13].

Let us note that in the MC modeling of elastic collisions of electrons in matter more sophisticated analytical DCSs are used [14–17]. In [15], the modified Wentzel distribution that reproduces three moments of a real DCS: the total cross section, the first and the second transport cross sections is used in simulations. In [16] it is shown that the reproduction of the total cross-section by the DCS is not as important in the modeling as the reproduction of the first and the second transport cross sections. This conclusion agrees with theoretical results of [18]. The DCS developed in [16,17] that reproduces the first and the second transport cross sections is easy for using in the MC modeling and provides good agreement of MC simulations with experiment.

In our paper we extend the range of application of the DCS of [16,17] to be used in the modeling of elastic collisions of atoms. The analytical DCS for elastic scattering of atoms will reproduce the stopping power and the energy-loss straggling because it is these parameters that are important for the description of the propagation of atoms in matter [19].

2. Theory

Let us define the DCS for elastic scattering of atoms by the following analytical expression:

E-mail address: egsh@li.ru

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$$\frac{d\sigma}{d\Omega} = \sigma_0 \frac{p+1}{4\pi}\left(\frac{1+\cos\chi}{2}\right)^p, \quad (1)$$

here χ is the scattering angle in the center-of-mass coordinate system, $d\Omega = 2\pi \sin\chi d\chi$ is the solid angle element. Parameters p and σ_0 in Eq. (1) are considered as fitting parameters. It is evident that the DCS with $p = 0$ corresponds to isotropic scattering, while $p >> 1$ corresponds to strongly anisotropic scattering. Parameters p and σ_0 can be defined using known moments of a real DCS. In [17,20] the DCS defined by Eq. (1) was used for modeling of elastic scattering of electrons by atoms and the fitting parameters p and σ_0 were derived through the first and the second transport cross sections. In the case of atomic collisions the stopping power and the energy-loss straggling parameters are used to describe the propagation of atoms or ions in matter [19,21–23]. That is why the DCS given by Eq. (1) should reproduce the stopping power and the energy-loss straggling to be suitable for the modeling of elastic collisions of atoms.

The stopping cross section S_n, and the straggling parameter W of the energy loss can be defined by the following equations [19]:

$$S_n = \int T d\sigma \quad (2)$$

$$W = \int T^2 d\sigma$$

where $T = T_{\max}(\sin(\chi/2))^2$ [24] is the energy loss of the incident particle in elastic collision with target atoms, $T_{\max} = E\frac{4m_1m_2}{(m_1+m_2)^2}$ is the maximal energy loss, E is the energy of the incident particle in the laboratory coordinate system, m_1 and m_2 are the masses of the incident particle and the target atom respectively. Substituting Eq. (1) into Eq. (2) we obtain the nuclear stopping cross-section and the straggling parameter in the following form:

$$S_n = T_{\max}\frac{\sigma_0}{p+2} \quad (3)$$

$$W = T_{\max}^2 \frac{2\sigma_0}{(p+2)(p+3)}$$

Solving Eqs. (3) we express the parameters σ_0 and p through S_n and W:

$$\begin{aligned} p &= \tfrac{2S_nT_{\max}}{W} - 3 \\ \sigma_0 &= \tfrac{S_n}{T_{\max}}\left(\tfrac{2S_nT_{\max}}{W} - 1\right) \end{aligned} \quad (4)$$

Undoubtedly, the DCS defined by Eq. (1) with parameters p and σ_0 calculated from Eq. (4) correctly reproduces both the stopping power and the energy-loss straggling of atoms in elastic collisions. In principle, experimentally determined S_n and W can be used for the calculation of the parameters p and σ_0, but experimental data are quite restricted. The required parameters can be estimated from numerical simulations of elastic scattering of atoms using an appropriate interatomic potential. In [25] the stopping power and the energy-loss straggling functions were calculated for several interatomic potentials in the form of the screened Coulomb potential:

$$V(r) = \frac{Z_1Z_2e^2}{r}\Phi(r/a), \quad (5)$$

where Z_1 and Z_2 are the atomic numbers of the incident particle and the target atom respectively, e is the electron charge, r is the distance between colliding particles, Φ is the screening function, a is the screening length. The screening function $\Phi(r/a)$ is often approximated by the relation: $\Phi(r/a) = \sum_{i=1}^{n} c_i \exp(-d_i r/a)$. Different potentials characterized by different screening functions and different screening lengths are used in the modeling of atomic collisions [24,26]. In our paper we will consider only two potentials: the Moliere potential [25] using the Firsov screening length $a = a_F = 0.8853a_0/(\sqrt{Z_1} + \sqrt{Z_2})^{2/3}$ and the ZBL potential [24] with the universal screening length $a = a_U = 0.8853a_0/\left(Z_1^{0.23} + Z_2^{0.23}\right)$, where a_0 is the Bohr radius. These two potentials are widely used in the MC modeling of the transport of sputtered atoms [3,13] and ion implantation [10,11].

As in [25] we introduce the reduced energy ε defined by the expression:

$$\varepsilon = \frac{aE_c}{Z_1Z_2e^2} \quad (6)$$

where $E_c = Em_2/(m_1 + m_2)$ is the energy of the particle in the center-of-mass system. The reduced stopping cross section $s_n(\varepsilon)$ and the reduced energy loss straggling $\omega(\varepsilon)$ can be expressed through $S_n(E)$ and $W(E)$ by the following relations [25]:

$$\begin{aligned} s_n &= \frac{m_1+m_2}{m_1}\frac{1}{4\pi a Z_1Z_2e^2}S_n \\ \omega &= \frac{1}{\pi}\left(\frac{m_1+m_2}{4Z_1Z_2e^2m_1}\right)^2 W \end{aligned} \quad (7)$$

Using Eqs. (6) and (7) we can rewrite parameters σ_0 and p defined by Eq. (4) through the reduced parameters $s_n(\varepsilon)$ and $\omega(\varepsilon)$ in the following form:

$$\begin{aligned} p(\varepsilon) &= \frac{2\varepsilon s_n(\varepsilon)}{\omega(\varepsilon)} - 3 \\ \sigma_0(\varepsilon) &= \pi a^2 \cdot \frac{s_n(\varepsilon)}{\varepsilon}\cdot\left(\frac{2\varepsilon s_n(\varepsilon)}{\omega(\varepsilon)} - 1\right) \end{aligned} \quad (8)$$

In [25] the parameters $s_n(\varepsilon)$ and $\omega(\varepsilon)$ were computed for the set of screened Coulomb potentials in the range of $10^{-4} \leqslant \varepsilon \leqslant 10$. Thus we can assume that fitting functions for $s_n(\varepsilon)$ and $\omega(\varepsilon)$ proposed in [25] are valid only at $\varepsilon \geqslant 10^{-4}$. It is easy to estimate from Eq. (6) that in the case of collisions of Cu with Ar atoms the reduced energy $\varepsilon = 10^{-4}$ corresponds to the energy of Cu atom E = 18.82 eV. This value exceeds the peak energy in the energy distributions of sputtered atoms [27]. Consequently, the use of the DCS defined by Eqs. (1) and (8) for the modeling of elastic collisions of sputtered atoms requires the functions $s_n(\varepsilon)$ and $\omega(\varepsilon)$ to be specified not only at $\varepsilon \geqslant 10^{-4}$ but also at $\varepsilon \ll 10^{-4}$. We simulated $s_n(\varepsilon)$ and $\omega(\varepsilon)$ in a wide range of energies: $10^{-7} \leqslant \varepsilon \leqslant 100$, using the same approach as in [25]. Results of our simulations of $s_n(\varepsilon)$ and $\omega(\varepsilon)$ and fitting functions $s_n(\varepsilon) = 0.5\ln(1+\varepsilon)/(\varepsilon + A\varepsilon^B)$ and $\omega(\varepsilon) = 1/(4 + A\varepsilon^{-B} + C\varepsilon^{-D})$ from [25] are presented in Figs. 1 and 2 for the Moliere potential. It is seen from the figures that the fitting functions of [25] really provide accurate values of $s_n(\varepsilon)$ and $\omega(\varepsilon)$ only at $\varepsilon > 10^{-4}$.Parameters σ_0 and p simulated from Eq. (8) through the parameters $s_n(\varepsilon)$ and $\omega(\varepsilon)$ for the Moliere and the ZBL potentials are shown in Figs. 3 and 4. It is seen from Figs. 3 and 4 that σ_0 is decreasing function of ε while the p parameter is increasing function of ε. The parameters σ_0 and p defined from the ZBL and the Moliere potentials differ significantly only at $\varepsilon < 1$. Parameters σ_0 and p shown in Figs. 3 and 4 were fitted by the series $\exp\left(\sum_{i=0}^{n} b_i(\ln(\varepsilon))^i\right)$. Coefficients b_i corresponding to $\sigma_0/\pi a^2$ and p parameters defined from the ZBL and the Molier potentials are listed in Table 1. The number of coefficients in the series is chosen to provide the desired precision of the fitting function. In our case the maximal deviation of the fitting function from the parameters σ_0 and p is less than 3% in the energy range $10^{-7} \leqslant \varepsilon \leqslant 100$.The simple analytical expression of the DCS given by Eq. (1) allows one to obtain analytical formulae for diffusion σ_d and viscosity σ_ν cross-sections that are derived through a DCS by the following equations [28]: