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Extension and applications of switching model: Range theory, multiple scattering model of Goudsmit–Saunderson, and lateral spread treatment of Marwick–Sigmund

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ABSTRACT

The switching model (PSM) developed in the previous paper is extended to obtain an "extended switching model (ESM). In the ESM, the mixt electronic-and-nuclear energy-loss region, in addition to the electronic and nuclear energy-loss regions in PSM, is taken into account analytically and appropriately. This model is combined with a small-angle multiple scattering range theory considering both nuclear and electronic stopping effects developed by Marwick–Sigmund and Valdes–Arista to formulate a improved range theory. The ESM is also combined with the multiple scattering theory with non-small angle approximation by Goudsmit–Saunderson. Furthermore, we applied ESM to lateral spread model of Marwick–Sigmund. Numerical calculations of the entire distribution functions including one of the mixt region are roughly and approximately possible. However, exact numerical calculation may be impossible. Consequently, several preliminary numerical calculations of the electronic, mixt, and nuclear regions are performed to examine their underlying behavior with respect to the incident energy, the scattering angle, the outgoing projectile intensity, and the target thickness. We show the numerical results not only of PSM and but also of ESM. Both numerical results are shown in the present paper for the first time. Since the theoretical relations are constructed using reduced variables, the calculations are made only on the case of C colliding on C.

1. Introduction

When a particle (electron, atom, ion, *etc.*) beam with non-relativistic energy penetrates into an amorphous target matter, each particle undergoes successions of elastic and inelastic scattering collisions. The particle changes its direction and losses kinetic energy via such multiple scattering collisions and finally losses all of its kinetic energy. The distance from the incident point to the point of final stop is called "range" or "penetration depth" (Lindhard et al., 1963; Winterbon et al., 1968; Schiott, 1966; Sanders, 1968; Sigmund et al., 1971). From theoretical point of view, the range is therefore one of physical quantities defined in the framework of the multiple scattering collision theory. Term "range theory" used in this paper means that in the field of beam-target interaction.

The important energy loss processes in scattering collisions at non-relativistic energies are considered to be (a) momentum transfer between projectile and target nuclei in elastic scattering collisions and (b) electronic excitation of projectile and target atoms in inelastic collisions. One of problems when we aim to make the multiple scattering theory more precise is how to insert the elastic (nuclear) and inelastic (electronic) energy-loss effects into the theory. It has been established that the elastic energy loss effect dominates at lower projectile energies and the inelastic one dominates at higher energies. It follows then that there is an intermediate mixt region where the two energy loss effects are both non-negligible. In the range theory that covers a high incident energy to zero, it is highly required to treat the mixt region appropriately.

Several theoretical studies of the range were reported in 1960′s to 1970′s by Lindhard et al. (1963), Winterbon et al. (1968), Schiott (1966), Sanders (1968), Sigmund et al. (1971). Lindhard et al. take both nuclear and electronic stopping effects into consideration. Winterbon et al. treated only nuclear stopping effect. They made many numerical tables. Schiott treated light projectile and target matters composed of heavy atoms. Sanders improved the treatment of Lindhard et al. by means of power law potential cross-section. Sigmund et al. developed range theory by considering the electronic energy loss effect only, calculated numerically, and tabulated the results in detail. Sigmund has written a short review in 2004 (Sigmund, 2004). A more recent detailed review by Sigmund is available in a textbook published in 2014 (Sigmund, 2014).

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The range theory mentioned above is based on theoretical studies of multiple-scattering collisions. Such multiple-scattering theories date back to 1940 when Goudsmit and Saunderson (GS) (Goudsmit and Saunderson, 1940) considered an electron beam incident on a matter and constructed the multiple scattering model that does not rely upon small angle approximation. More than thirty years later, Sigmund and Winterbon (1974), Meyer (1971) developed the small angle multiple scattering theory, which is important for incident beams of atomic and ionic species. Although earlier theoretical studies of the small-angle multiple scattering were reviewed by Scott (1963) in 1963, extensive reviews including recent studies have been given by Sigmund (2004); Sigmund, 2014. Energy dependent small angle multiple scattering theories were constructed by Valdes and Arista, (1994) and later by Ikegami, 2013. Moreover, lateral spread models were derived by Marwick–Sigmund (Marwick and Sigmund, 1975) and by Ikegami (2013). Furthermore, Mekhtiche and Khalal–Kouache (Mekhtiche and Khalal, Kouache, 2016) obtained energy loss dependent angular distributions based on VA and on mean energy of projectile in targets.

Contents in the present paper are as follows. In the next section, theoretical background is briefly described based on (Ikegami, 2013; Valdes and Arista, 1994; Marwick and Sigmund, 1975; Kaneko, 1990; Lindhard et al., 1963; Winterbon et al., 1970; Schiott, 1966; Sanders, 1968; Sigmund et al., 1971; Goudsmit and Saunderson, 1940; Sigmund, 2004; Sigmund, 2014; Sigmund and Winterbon, 1974; Meyer, 1971; Scott, 1963; Ikegami, 2013; Valdes and Arista, 1994; Marwick and Sigmund, 1975; Mekhtiche and Khalal, Kouache, 2016; Kaneko, 1990; Lindhard et al., 1968. In Section 3, the present theoretical treatments are given. In Section 3.1., the switching model reported in the previous paper (Ikegami, 2013) named "previous switching model (PSM)" is extended to obtain improved one, hereafter named "extended switching model (ESM)". In 3.2., the ESM is combined with previous theories (Ikegami, 2013; Valdes and Arista, 1994; Marwick and Sigmund, 1975) to formulate the present range theory. In 3.3. and 3.4., ESM is applied to improve GS multiple scattering collision theory. Moreover, in 3.5., ESM is applied to lateral spread model. Section 4 is devoted to some numerical calculations and discussion. Because the previous paper (Ikegami, 2013) have not given numerical results of PSM, the present paper gives numerical results of PSM as well as those of ESM. A summary and conclusions are given in Section 5.

In the following, the distribution of atoms in the target is assumed to be random and homogeneous (i.e. amorphous), and recoil terms are neglected in the present range theory.

2. Theoretical background

2.1. Valdes–Arista Model, and Marwick–Sigmund Treatment

As is mentioned above, Sigmund and Winterbon (SW) developed the multiple scattering theory for the small scattering angles in 1974 (Sigmund and Winterbon, 1974). However, they did not consider any energy-loss effects in the theory. Marwick and Sigmund (MS) (Marwick and Sigmund, 1975) derived in 1975 a formula of lateral spread at a penetration depth expressed by reduced variables. These two theoretical studies have established base of a number of subsequent theoretical studies. In addition, use of the reduced variables has allowed us to compare among different projectile-target combinations. Valdes and Arista (VA) developed in 1994 the small angle multiple scattering theory taking into account the electronic energy loss effect for the first time (Valdes and Arista, 1994). The MS and VA treatments will be used to construct the present range model in Section 3.2.

2.2. Switching model for small angle multiple scattering theory

Ikegami (2013) developed switching model to establish small angle multiple scattering theory where both nuclear and electronic energy-loss effects are considered in one formula. The switching model is like that a target is divided into two layers; the one layer is dominated by nuclear energy-loss effect and another one is dominated by electronic energy-loss effect, and the existence of mixt region is neglected. Although this switching model was derived by rather rough approximation, it might be useful in that it is exactly solvable. In Section 3.1., the switching model will be improved to make possible to consider the mixt region.

2.3. Inelastic and elastic energy loss effects

In this subsection, formulation of the inelastic and elastic energy loss effects is described briefly. These energy-loss effects have been taken in previous theories in the form of ratio $\mu = E(x)/E_0$, where $E(x)$ is the projectile energy in the laboratory system at penetration depth x in the target, and E_0 is the incident energy.

In the velocity proportional region, which corresponds to the lower-energy side of convex-type excitation cross-section curve, the energy of projectile in solid affected by the inelastic energy loss is written by

$$E(x) = E_0 - S(E_0)x + \frac{1}{2}S(E_0)\frac{dS(E_0)}{dE_0}x^2, \tag{1a}$$

where, $S(E)$ is the stopping force.

Kaneko has developed the electronic stopping formula for the velocity proportional region (Kaneko, 1990). Here, as in the previous study (Ikegami, 2013), Kaneko's electronic stopping force is employed to get the formula of the ratio μ_e. By dividing the both sides of Eq. (1a) by E_0 and by introducing reduced variables τ and β_i (see below), we obtain

$$\begin{aligned}\mu_e &= \frac{\beta_1(\tau)}{\beta_0} = \frac{E_1(\tau)}{E_0} \\ &= -I_1\kappa_{ke}\tau + \tfrac{1}{2}I_2\kappa_{ke}^2\tau^2 + 1,\end{aligned} \tag{1b}$$

where

$$\beta_i = \frac{E_i a}{2Z_1Z_2e^2}\ (i = 0,\ 1), \tag{2a}$$

$$\tau = \pi a^2 N x, \tag{2b}$$

$$I_1 = \frac{v_i}{E_0\pi a^2 N}, \tag{3}$$

$$I_2 = \frac{1}{mE_0(\pi a^2 N)^2}, \tag{4}$$

$$\begin{aligned}\kappa_{ke} = {}& 16\pi N\ (k_F a_B)\left(\frac{1}{v_B}\right)Z_1^{2/3}N_{free}A^4\ (m_e v_B^2 a_B^2) \\ & \times \{1 - 4\chi^2 + \chi^4[6\ln\left(1+\frac{\pi v_F}{v_B}\right) \\ & - 2\pi v_F/(\pi v_F + v_B)]\},\end{aligned} \tag{5}$$

$$\chi^2 = \frac{v_B}{\pi v_F}, \tag{6}$$

and

$$A = 0.56/(1 - 0.511Z_1^{-2/3}r_s^{-1}). \tag{7}$$

Here, Z_1 and Z_2 are the atomic number of projectile and target atom, respectively, m is the projectile mass, and N is the number of target atoms per unit volume. Parameters τ is the reduced target thickness, β_1 and β_0 in Eq. (1b) are the reduced projectile energies corresponding to E_1 and E_0, respectively. Parameter α is a screening length of Lindhard (Lindhard et al., 1968), v_i is the initial velocity of incident atom, v_B is the Bohr velocity, a_B is the Bohr radius, and r_s is defined by the formula $r_s = (3/4\pi n_e)^{1/3}/a_B$. The quantity m_e is the mass of electron. The quantity n_e is the electron density in target slab, N_{free} is the number of the free electrons per atom, k_F is the Fermi wave number, v_F is the Fermi velocity, and κ_{ke} is a constant. Furthermore, please see the side note at