Vacuum/volume 44/number 9/pages 901 to 902/1993
Printed in Great Britain

0042-207X/93$6.00+.00

Electron transport simulation for the ion–electron emission problem

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The cascade model of electron transport (1–10^3 eV) in matter is proposed to solve ion–emission problems. The model needs only well-known fundamental data about the target and is free of fitting parameters. The results obtained by the Monte Carlo method using the cascade model are in agreement with experimental data in the literature.

1. Introduction

Ion interactions with metal surfaces are known to generate many electrons with energy from a few eV up to 1 keV, which determine the ion–electron emission (IEE) value.

IEE studies have two main components, firstly, the identification of the spatial and energy distribution of electrons, resulting from the ion interaction with the metal surfaces and secondly, a description of the electron transport. It is possible to solve the second part of the problem by Monte Carlo simulation of the electron trajectories, based on an elastic and inelastic electron–atom interaction calculation[1] (for the electron energy >0.5 keV) or an elastic and inelastic electron–ion, electron–Fermi gas interaction calculation[2–4] (for the other electron energies). Economy of the computer time for the fast (E ⩾ 1 keV) electrons is attained by combining the relatively few loss and angle scattering collisions; other collisions are considered individually. If the electron energy is less than ~1 keV it is possible to simulate the electron transport by considering individual elastic and inelastic electron scattering in metals, except for the description of plasmon generation. Thus, the problem of electron energy loss description (ionization, plasmon, electron-'hole' generation) is one of the basic problems. Usually two-particle collision theory is used for a description of the ionization process, but the dielectric theory is used for the electron–Fermi gas interaction description. The dielectric function (DF) obtained in the first Born approximation may be used for a description of the low energy (⩽100 eV) electron transport with the help of semi-empirical parameters, well known only for normal metals[5]. As a consequence, there is a problem of determining the computation method of integral and differential electron ionization scattering characteristics based on minimal information about metals without any semi-empirical parameters.

2. Experimental results and discussion

We propose to use the classical symmetrical binary theory of atomic collisions for a description of the electron energy losses and scattering angles of the electrons (first and second) after the atomic ionization. In this theory we assume that the test electron accelerated in an atomic field has an energy $E = E+2U_i$ before its collision with the atomic electron (where U_i is the mean kinetic energy of an electron in the ith shell and $U_i = E_f$ for the Fermi gas electrons). In addition, it is assumed that the minimum electron energy transmitted to an atom or Fermi electron is $W+U_i$ (where W is the surface potential barrier for the metal studied), but the maximum transmitted energy is considered to be E, because the electron is a classic particle in this model. The mean energy loss of the test electron under the given assumption, for example, can be described as:

$$-\frac{dE}{dx} = \sum_{i=1}^{N} \frac{\pi e^4 n}{E+2U_i}\left\{\ln\frac{E}{U_i+W} + 4\left(1-\frac{U_i+W}{E}\right)\right\}. \quad (1)$$

In this equation, e is the electron charge, n is the electron number in the ith shell, and N is the electron shell number.

The corresponding energy losses of the test electron spent in the generation of the second particle are shown in Figure 1. It can be seen, that our calculated ionization, electron-'hole' energy loss disagrees with the semi-empirical results[5] by more than a factor 2 that can be attributed to experimental error for an electron energy ⩾20 eV. This fact allows us to affirm that the symmetrical binary collision theory may be used for determination of the integral and differential (first and second) electron parameters after atom ionization and electron-'hole' excitation.

In case of the elastic electron–ion interaction simulation we suppose that ion cores are randomly distributed in medium and that the real electrical potential of every ion is spherically symmetrical and restricted to within spheres of radius $R = 0.5\ A$ (where, A is the crystal grating constant of Al)[2]. The potential

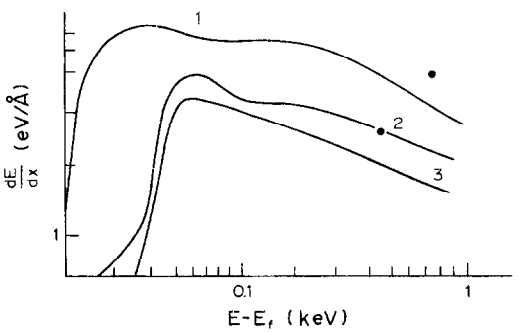

Figure 1. The mean energy loss dE/dX in Al. (1) Our results; (2) ionization and electron-'hole' excitation[5]; and (3) plasmon excitation[5].

value $V(R)$ is obtained on the basis of the Hartree–Fock functions and the Slater exchange term, considering the influence of the other ion. The accurate computation of the other phase shifts based on the Calogero method[6] is reduced to solving the differential non-linear equation:

$$\delta_l'(R) = -\frac{V(R)}{k}\left\{\cos\delta_l(R)\hat{j}_l(kR) - \sin\delta_l(R)\hat{n}_l(kR)\right\}^2, \quad (2)$$

with the band condition $\delta_l(0) = 0$, where $\hat{j}_l(kR) = kR \times j_l(kR)$, $\hat{n}_l(kR) = kR \times n_l(kR)$; $\hat{j}_l(kR)$, $n_l(kR)$ are the spherical Bessel functions of the first and second orders, k is the wave number of an incident particle (in atomic units), R is the distance between the ion core and the test electron. The obtained phase shift values

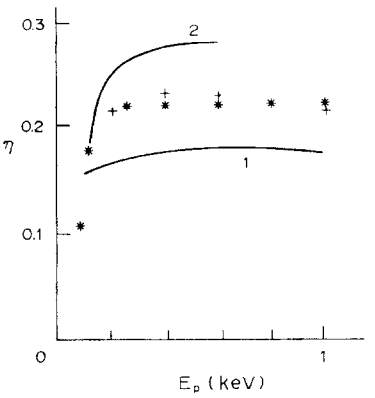

Figure 2. Variation of the backscattering coefficient η of Al with the primary electron energy E_p. (*) Experimental results[7]; (+) ref 8; and calculated values (1) this work, (2) ref 2.

are used for a computation of the integral and differential elastic electron–ion cross-sections:

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2}\left\{\sum_{l=0}^{l'}(2l+1)\exp(i\delta_l)\sin\delta_l P_l(\cos\theta)\right\}^2$$

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{l'}(2l+1)\sin^2\delta_l \quad (3)$$

where $P_l(\cos\theta)$ is the lth Legendre polynomial. The electron trajectories are simulated on the basis of this method up to the energy $\sim W$. Figure 2 shows the experimental and calculated values of the backscattering coefficient of Al with the primary electron energy E for electron–electron emission. It can be seen that calculated values are in very good agreement with the experimental ones.

This theoretical model allowed us to calculate the electron trajectories up to an electron energy $\sim W$. If the spatial and energy electron distribution obtained as a result of ion–metal surface interaction is known, the model would allow us to compute the integral and differential IEE data.

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