Secondary Electron Emission from a Solid Surface by Ion Impact

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A theoretical model calculation has been performed for the electron yield from a Au surface by slow He^+, Ne^+, Ar^+, and Xe^+ ions. Analysis was made on the basis of the conventional three step model: (1) the primary excitation of electrons by an ion, (2) the transport of excited electrons to a surface, and (3) the overcome of the surface potential barrier. In the first step, the inner-shell excitation process is parameterized in connection with the Firsov theory. In the second step, use is made of the electron gas model in estimating the inelastic processes.

The third process is described in quantum-mechanical manner. Comparison of the calculated results with the data shows agreement qualitatively.

1. Introduction

Since the phenomena of secondary electron emission were discovered in the beginning of this century, it has been a growing field[1]. So far, two mechanisms were known to govern the secondary electron emission process.[2,3] One is the kinetic process and the other is the potential process. The former is the conversion of kinetic energy possessed by the primary ions into that of excited electrons via Coulomb interaction. This process becomes deminant when the kinetic energy is rather high. Roughly speaking, the total yield of secondary electrons is proportional to the energy deposition rate, or, the electronic stopping power.[4] As a typical feature, there exists the threshold kinetic energy E_{th} of the projectile. For example, E_{th} for excitation of conduction electrons is given by $E_{th} = (1/2)Mv_{th}$ with

$$v_{th} = [v_f^2/4 + \phi/2m]^{1/2} - v_f/2 \tag{1}$$

Here v_f, m, M and ϕ denote the Fermi velocity, the electron rest mass, the mass of a projectile, and the work function, respectively.

On the other hand, the latter becomes a main process when the projectiles are highly ionized at small kinetic energies. In this case, the total yield of secondary electrons is qualitatively proportional to the total potential energy carried by the ion.[2] Recently, a novel experimental technique enabled us to obtain emission statistics,[5,6] Winter et al.[5] measured the total yield induced by ions at low velocities, which cover the

threshold energy for the kinetic process. Their result shows evidence of the existence of E_{th} in light-ion-target combinations, while at the same time no clear threshold was found up to very low incident-energies of heavy ions. The latter implies the possibility of inner-shell excitation.

The aim of this paper is to calculate the total yield of secondary electrons induced by low-velocity heavy ions in order to investigate the possibility of inner-shell excitation. Throughout the paper, m, e, $\hbar$, a_0, and v_0 are the electron rest mass, the elementary charge, the Planck constant divided by 2π, the Bohr radius, and the Bohr velocity, respectively.

2. Theoretical model

The emission process is considered as a conventional three-step model,[7-9] Namely, (1) the creation of excited electrons inside a solid target by primary ions, (2) the propagation of those electrons from the created point to the metal surface, and (3) the overcome of the surface-barrier potential. In this paper, the case is considered where the primary ions are incident normally on the solid surface.

2.1 Internal excitation of electrons

As a first process, we here treat the inner-shell excitation by means of statistical method. In atomic collisions in solids, many-body problem should be dealt in general. However, this excitation process can be considered in the frame of two-body scattering problem. We put a base on the Firsov's statistical theory[10] which might be a crude model but is convenient to see the overall feature of the low-velocity electronic stopping as functions of Z_1 (atomic number of a projectile), Z_2 (that of a target atom), and v (velocity of a projectile).

As the impinging ions collide with target atoms, the target electrons will be excited via the coupling of atomic orbitals.

It follows the inner-shell excitation. Even at low energies, it will be possible for several orbitals to take part in the coupling. As a consequence of this excitation, the kinetic energy of the excited electrons is distributed and finally a local thermal-equilibrium will be attained in a macroscopically small region. Based on this assumption, the energy distribution of the internally excited electrons per unit primary ion path, d/dz (dN/dE), is described as

$$d/dz(dN/dE) = A \exp(-B E). \tag{2}$$

In the above, B is the inverse of the local thermal temperature. In order to determine A and B, we prepare two relations. One is the number of excited electrons per unit primary path, denoted by I, and the other is the excitation energy per unit path by the primary ions, denoted by J. In explicit forms, I and J are described using eq. (2) as

$$I = \int d/dz(dN/dE)\, dE = A/B, \tag{3}$$

$$J = \int d/dz(dN/dE)\, EdE = A/B^2. \tag{4}$$

The quantity J is just the electronic stopping power of a material. Then we determine A and B to connect with the Firsov's result. Hereafter a brief description of the Firsov model is given. In a close collision of a projectile with a target atom, the electron cloud of both systems overlap each other and the flux of electrons flows into the collision partner. This means the exchange of electron flux, namely, the exchange of momentum between two systems. The force $\boldsymbol{F}'$ acting on the partner atom via this mechanism is given by

$$\boldsymbol{F} = \pm m\ \dot{\boldsymbol{R}} \int_s n(\boldsymbol{r})v(\boldsymbol{r})/4\, dS, \tag{5}$$

where $\boldsymbol{R}$ denotes the position vector of internuclear separation, and n $(\boldsymbol{r})$ and $v(\boldsymbol{r})$ are the local electron density and the local velocity of electrons at position $\boldsymbol{r}$. The integral is over the so-called Firsov plane placed on a midpoint of two nucleus.
Then the work W derived by this force $\boldsymbol{F}$ becomes

$$W = \int \boldsymbol{F} \cdot d\boldsymbol{R}. \tag{6}$$

The local density and the local velocity of electrons denoted by n $(\boldsymbol{r})$ and $v(\boldsymbol{r})$, respectively, are connected with each other by means of the Thomas-Fermi statistical theory as follows:

$$\begin{aligned} v(\boldsymbol{r}) &= (3/4)v_f(\boldsymbol{r}) \\ v_f(\boldsymbol{r}) &= (\hbar/m)[3\pi^2 n(\boldsymbol{r})]^{1/3}. \end{aligned} \tag{7}$$

Using the potential ψ $(\boldsymbol{r})$, we have

$$n(\boldsymbol{r}) = 1/(3\pi^2)[(m/\hbar)\{2\ e\ \psi(\boldsymbol{r})\}^{1/2}]^3. \tag{8}$$

Thus assuming a straight-line trajectory, the work W can be expressed as a function of impact parameter b in the following:

$$W(b) = \frac{m^2 e^2 v}{3\pi^2 \hbar^3} \int_{-\infty}^{\infty} dx\ 2\pi \int_0^{\infty} d\rho\rho\{\psi([R^2/4+\rho^2]^{1/2})\}^2. \tag{9}$$

with $R^2 = b^2 + x^2$. The function form ψ $(\boldsymbol{r})$ is taken to be

$$\psi(\boldsymbol{r}) = e(Z_1+Z_2)(1/r)\chi(r/a_{TF}), \tag{10}$$

where χ (x) is the Thomas-Fermi screening function. The Thomas-Fermi screening constant $a_{TF} = 0.8853a_0 \Big/ (Z_1+Z_2)^{-1/3}$. The expression (10) means a statistical Thomas-Fermi potential in the limit of the united atom. By multiplying $2\pi\ b$ and integrating over b, we have the total stopping cross section σ. When σ is multiplied by the number density N_0 of target atoms, it reduces to the quantity J defined in eq. (4). Namely, we have

$$N_o 2\pi \int_0^\infty db\ b\ W(b) = J \tag{11}$$

On the other hand, the number of excited electrons as a function of b, $N_e(b)$, in such collisions is estimated by

$$N_e(b) = \int_{-\infty}^{\infty} dx \int_S dS\ n(\boldsymbol{r}). \tag{12}$$

Therefore, integration of $N_0 \times N_e(b)$ over b leads to the number of excited electrons per unit lenght, corresponding to the quantity I in eq. (3). Then we also have

$$N_0\ 2\pi \int_0^\infty db\ b\ N_e(b) = I. \tag{13}$$

Thus, coupling of eqs. (3) and (4) with (11) and (13) determines the values of A and B.

To determine A and B is just a problem in this section and hereby the energy distribution of excited electrons inside a solid is parameterized with a suitable connection with the Firsov's result.

2.2 Transport of the excited electrons to a surface and overcome of surface potential.

As a second process we discuss here the electron transport.

Let $P(E', E, z, \theta)$ represent the transport probability of excited secondaries moving on a straight-line trajectory with angle θ from the point of creation with energy E' to the surface with energy E. In general, elastic and inelastic propagations are both possible, and they are physically independent.

Then first we treat them separately and finally sum up both contributions to the total yield.

The elastic propagation is described by

$$P_{el}(E', E, z, \theta) = \exp(-z/\lambda(E)\cos\theta)\delta(E-E') \tag{14}$$

where $\lambda(E)$ denotes the inelastic mean free path of secondary electrons with the neglect of angular spread. This relation corresponds to the so-called escape probability model.

On the other hand, the inelastic propagation is derived on the basis of the continuous slowing-down approximation (CSDA) as follows:

$$P_{inel}(E', E, z, \theta) = \delta(E-y(x)) \tag{15}$$

where $y(x)$ is the solution of the equation

$$x = z/\cos\theta = \int_{E'}^{y} dE/S(E) \tag{16}$$

as a function of $x(=z/\cos\theta)$. Here S(E) is the electronic stopping power. The inelas-

tic quantities, $\lambda(E)$ and $S(E)$, are computed for the degenerate electron-gas model,[7,8] in which the individual and the collective (plasmon) excitation are both included.

Let us move to transmission of the surface barrier potential.
According to the classical picture, the transmission probability is always unity as long as the kinetic energy E exceeds the potential barrier $U(=E_f+\phi)$. However, in the quantum mechanical picture, this probability is still less than unity even for cases of $E > U$ since the reflection effect at the surface is significant.[11] We adopt a quantum mechanical manner. At the same time, the emission angle θ is restricted to a region $0 \leqq \theta \leqq \theta_c$, where θ_c is the critical angle defined by $\theta_c = \cos^{-1}\{(E_f+\phi)/E\}$.

2.3 Energy distribution and total yield.

Using the above mentioned quantities and the models, the energy distribution of excited secondary electrons outside a solid surface can be finally obtained in the following analytical form:[7]

$$d\gamma/dE = [(d^2N/dEdz)\ \lambda(E)+(dN/dz)/S(E)] \times(1/3)\alpha^3(2+\alpha)/(1+\alpha)^2 \tag{17}$$

with $\alpha = \{E/(E+E_f+\phi)\}^{1/2}$. In these equations, the kinetic energy E of the emitted electrons is measured from the vacuum level. The contribution of the first and the second term in the square brackets of (17) correspond to the elastic and inelastic process, respectively.

The yield of emitted electrons is straightforwardly estimated by integrating $d\gamma/dE$ over E.

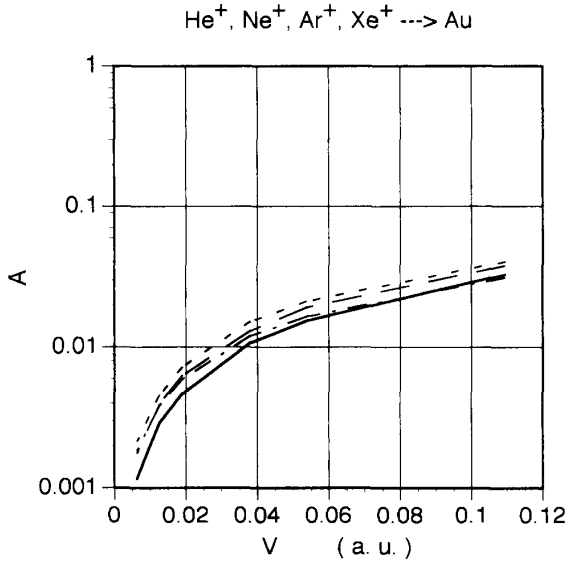

Fig. 1 The values of A as a function of v (in units of $v_0 = 2.19\times 10^8$cm/s) for He^+(———), Ne^+(— — —), Ar^+(- - - - -) and Xe^+(— - — - —) incidence on Au.

$$\gamma = \int_0^{Emax} (d\gamma/dE)dE. \tag{18}$$

Usually, the upper limit E_{max} is taken to be about 50 eV.

3. Results and discussion

Figure 1 and 2 show the values of A and B determined in the described method for

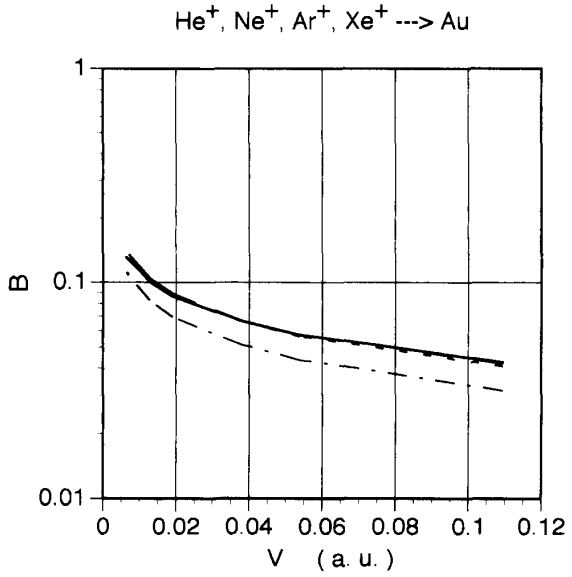

Fig. 2 The values of B as a function of v in units of v_0 for He^+, Ar^+ and Xe^+ incidence on Au. Legends are the same as in fig. 1.

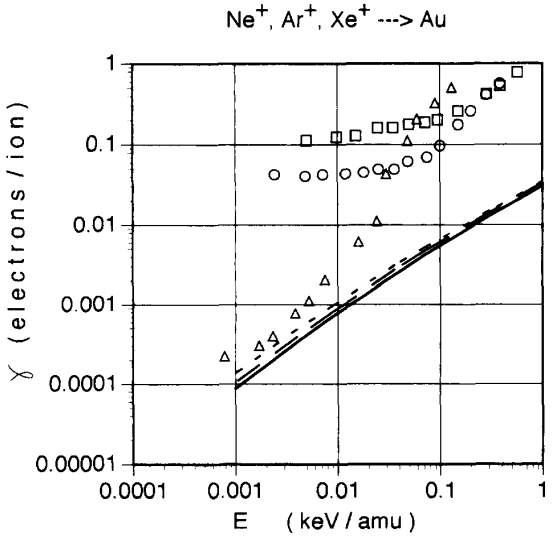

Fig. 3 The yield of secondary electrons emitted from Au surface : calculation (——— ; Ne^+, —— ; Ar^+, – – – – ; Xe^+) and the data (□ ; Ne^+, ○ ; Ar^+, △ ; Xe^+) [ref. 5] ,

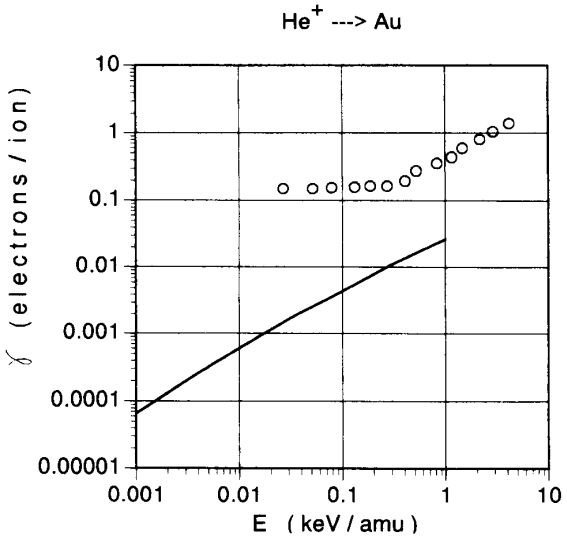

Fig. 4 The yield of secondary electrons emitted from Au surface : calculation (——— ; He^+) and the data (○ ; He^+) [ref. 5] ,

the projectile (He^+, Ne^+, Ar^+, and Xe^+)- target (Au) combinations as a function of impact velocity in atomic units. A typical feature is that the values of A is increasing with velocity but those of B is decreasing. The former can be interpreted as the increase of the total number of excited electrons by incident ions. On the other hand, the latter means that the number of excited electrons with higher energies is more increasing with velocity than that with lower energies. One will find that the heavier the ion is, the larger A is and the smaller B is. Figures 3 and 4 show the calculated yield of secondary electrons emitted from Au surface by He^+, Ne^+, Ar^+, and Xe^+ ions with energy $E(0.001\ keV/amu \leqq E \leqq 1keV/amu)$. Apart from the values of A and B, $\lambda(E)$ and $S(E)$ in eq. (17) are calculated for a degenerate electron gas model[7,8] characterized by $r_s = 3.01$ for Au. The solid state property of Au is that $E_f = 5.53eV$, $\phi = 4.9eV$. In the case of the low-energy Xe^+ incidence the calculated result is in good agreement with the experimental data, while in other cases agreement is not so good. The independence of the yield on energy shown in the data for He^+, Ne^+ and Ar^+ ions at low energies is due to the contribution of potential emission process. In our calculation, this process is not taken into account so that in this sense disagreement is inevitable. As the energy increases, the yield for Xe^+ incidence is also increasing more rapidly than the calculated one. The reason has not been made clear and it is a future problem to be solved.

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