Resonant neutralization of ions scattered from surfaces in the intermediate-velocity regime

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We report on a theoretical investigation of the resonant neutralization of ions scattered from solid surfaces in the intermediate-velocity regime (a few tens of keV per nucleon). We also propose a general formula for the resonant neutralization probability of ions which asymptotically conforms with the fixed-ion approximation at low velocity and with the first perturbation theory at high velocity.

I. INTRODUCTION

Theoretical studies of the charge-exchange scattering of an atom or an ion at a solid surface have been going on for a long time. In early investigations, of which Hagstrum's work[1] is the most typical, the ion-surface encounter is treated as a quasistatic process and a neutralization rate is calculated on the basis of the so-called fixed-ion approximation.[1,2] However, there are some problems. The fixed-ion approximation is not appropriate for the calculation of the electron-transfer probability involving levels above the Fermi level, for example, ionization of the sputtered atoms,[3] or excited-states formation of the atoms leaving from the solid surface.[4] Because these are essentially nonadiabatic phenomena, the electronic system experiences explicitly time-dependent perturbation as a result of the classical motion of the projectile. More precisely, a quantum phase evolution plays an important role, which has been addressed by Trubnikov and Yavlinskii.[2] Recently, several authors[5-8] have calculated resonant neutralization probabilities of the low-energy ions as a nonadiabatic process. Their interests, however, are restricted to the very low-energy case.

On the other hand, electron capture occurs from a core level of target atoms in the high-velocity regime, where first perturbation theory may be employed and the incident particle has an equilibrium charge state in the bulk.[9,10] Therefore we can compare a charge-exchange cross section to gas-phase results and also we may calculate it by means of the binary encounter model.

In the intermediate-velocity regime ($v \approx v_B$, where v is the velocity of the incident ion and v_B is the Bohr velocity), as the ion moves at velocities comparable to electron velocities in the solid, the adiabatic picture breaks down and quantum-mechanical energy uncertainty becomes important as a result of finite interaction time. However, the ion captures electrons from the conduction or valence bands as is the case with the slow ion, in which case the binary encounter model is not appropriate. Therefore we can use neither the fixed-ion approximation nor first perturbation theory, which complicates calculation of the neutral fraction in such a velocity regime. But this velocity regime has become increasingly important in ion-beam crystallography.[11] Recently, excellent experimental studies have been carried out by Haight et al.[12] Their results

show that He ions capture electrons from the valence band of Si at the surface by means of the resonant tunneling process. But there have been no theoretical studies in this regime yet.

It is the purpose of the present paper to calculate the resonant neutralization probabilities of the ions which cross the solid surface from bulk to vacuum with intermediate velocity and to discuss some dynamical effects which cannot be found in Hagstrum's formula. And then we will propose a general formula of the resonant neutralization at the solid surface which asymptotically conforms with the fixed ion approximation in the low-velocity limit and with first perturbation theory in the high-velocity limit.

The formalism is developed in Sec. II, where a general formula is proposed, and is compared with the fixed ion model and with first perturbation theory. In Sec. III, dynamic effects are discussed in detail using a very simple model.

II. FORMALISM

The model used here is the same as that of Brako and Newns.[7] The moving atom is assumed to have a valence state or a certain excited state Ψ_a of energy ϵ_a which lies near the Fermi level ϵ_F and interacts with the states Ψ_k of energy ϵ_k in a conduction band or a valence band. The nuclear motion is treated classically and separated from any electronic processes, so a Hamiltonian of the electron system becomes time-dependent parametrically through the trajectory of the ion. Therefore, we employ the time-dependent Anderson-Newns Hamiltonian,[6,7]

$$H = \epsilon_a c_a^\dagger c_a + \sum_k \epsilon_k c_k^\dagger c_k + \sum_k [V_k^*(t)c_a^\dagger c_k + V_k(t)c_k^\dagger c_a] , \quad (1)$$

where $c_a^\dagger$ and $c_k^\dagger$ are electron creation operators for states Ψ_a and Ψ_k. The energy ϵ_a is generally dependent on the position of the moving ion but I neglect it for simplicity. If the ion moves linearly with a velocity v, the wave function $\Psi_a(\mathbf{r}, t)$ in the laboratory system of coordinate is equal to

$$\Psi_a(\mathbf{r},t)$$

$$=\Phi_a(\mathbf{r}-\mathbf{v}t)\exp\left[-\frac{i}{\hbar}\epsilon_0 t\right]\exp\left[\frac{i}{\hbar}(m\mathbf{v}\cdot\mathbf{r}-\tfrac{1}{2}mv^2 t)\right] ,$$

$$(2)$$

where ϵ_0 is the energy of the state $\Phi_a(\mathbf{r})$ freezed at surface where electrons experience not only an ion-core potential but also an image potential and a surface dipole barrier. It is very difficult to determine ϵ_0 for each kind of incident particles. So, ϵ_0 is an unknown parameter in this paper. But the energy level ϵ_a in the laboratory system should be written as

$$\epsilon_a=\epsilon_0+\tfrac{1}{2}mv^2 . \tag{3}$$

Consequently, both the transition matrix V_k and the energy level ϵ_a depend on the velocity of the ion, an idea introduced by Trubnikov and Yavlinskii.[4]

Using this Hamiltonian, the Heisenberg equations of motion become

$$i\hbar\dot{b}_a(t)=\sum_k V_k^*(t)\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t_0)\right]b_k(t) , \tag{4}$$

$$i\hbar\dot{b}_k(t)=V_k(t)\exp\left[\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t_0)\right]b_a(t) , \tag{5}$$

where we have defined

$$b_\nu(t)=c_\nu(t)\exp\left[\frac{i}{\hbar}\epsilon_\nu(t-t_0)\right] \quad (\nu=a,k) , \tag{6}$$

and time t_0 refers to the system before the ion came into interaction with the solid surface. Equation (5) is solved to give

$$b_k(t)=-\frac{i}{\hbar}\int_{t_0}^t V_k(t')\exp\left[\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t'-t_0)\right]b_a(t')dt'$$

$$+b_k(t_0) . \tag{7}$$

And then, substituting Eq. (7) into Eq. (4), we can obtain

$$i\hbar\dot{b}_a(t)=-\frac{i}{\hbar}\int\sum_k V_k^*(t)V_k(t')\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t')\right]b_a(t')dt'+\sum_k V_k(t)\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t_0)\right]b_k(t_0) . \tag{8}$$

It is difficult to solve Eq. (8), so we must employ an approximation at this stage. Brako and Newns[7] solved it approximately in the case where the energy band is infinitely wide, but their final results were restricted to the low-energy case. Therefore, we employ another approximation applicable to the higher-energy case and to the narrow-band case. To solve this integrodifferential equation (8) approximately, we expand the operator $b_a(t')$ around the time t, which leads to

$$i\hbar\dot{b}_a(t)=\sum_k V_k(t)\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t_0)\right]b_k(t_0)-\frac{i}{\hbar}\int_{t_0}^t\sum_k V_k^*(t)V_k(t')\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t')\right]dt'b_a(t)$$

$$-\frac{i}{\hbar}\int_{t_0}^t(t'-t)\sum_k V_k^*(t)V_k(t')\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t')\right]dt'\dot{b}_a(t)+\cdots . \tag{9}$$

If the ion moves so fast that the condition,

$$\left|\frac{1}{\hbar^2}\int_{t_0}^t(t'-t)\sum_k V_k^*(t)V_k(t')\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t')\right]dt'\right|\ll 1 , \tag{10}$$

is valid, we can neglect the expanded terms except the zeroth-order one, which we call the local-time approximation.[13] Accordingly, Eq. (8) becomes

$$i\hbar\dot{b}_a(t)=\Gamma(t)b_a(t)+\sum_k V_k(t)\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t_0)\right]b_k(t_0) , \tag{11}$$

where

$$\Gamma(t)=-\frac{i}{\hbar}\int_{t_0}^t\sum_k V_k^*(t)V_k(t')\exp\left[-\frac{i}{\hbar}(\epsilon_k-\epsilon_a)(t-t')\right]dt' . \tag{12}$$

Equation (12) is the time-dependent self-energy, whose imaginary part gives us the effective transition rate discussed by Moyer and Orvek,[8] and whose real part is the time-dependent valence energy. This self-energy depends not only on events occurring at a time t, but also on the motion of the atom; in other words it approximately reflects a quantum phase evolution which brings about quantum-mechanical energy uncertainty as a result of the finite interaction time.

Equation (11) may be solved to give

$$b_a(t) = -\frac{i}{\hbar} \int_{t_0}^t \sum_k V_k(t') \exp\left[-\frac{i}{\hbar}(\epsilon_k - \epsilon_a)(t'-t_0)\right] \exp\left[-\frac{i}{\hbar}\int_{t'}^t \Gamma(\tau)d\tau\right] dt' b_k(t_0) + \exp\left[-\frac{i}{\hbar}\int_{t_0}^t \Gamma(\tau)d\tau\right] b_a(t_0) .$$

(13)

And then we obtain the occupation numbers of the state Ψ_a as follows:

$$n_a(t) = \frac{2}{\hbar^2} \mathrm{Re}\left[\int_{t_0}^t dt_2 \int_{t_0}^{t_2} \sum_k n_k(t_0) V_k^*(t_2) V_k(t_1) \exp\left[-\frac{i}{\hbar}(\epsilon_k - \epsilon_a)(t_1 - t_2)\right]\exp\left[-\frac{i}{\hbar}\int_{t_1}^{t_2}\Gamma(\tau)d\tau\right]\right.$$

$$\left.\times \exp\left[\frac{2}{\hbar}\int_{t_2}^t \mathrm{Im}\Gamma(\tau)d\tau\right]dt_1\right] + n_a(t_0)\exp\left[\frac{2}{\hbar}\int_{t_0}^t \mathrm{Im}\Gamma(\tau)d\tau\right] .$$

(14)

With the local-time approximation, the second exponential function of integrand in Eq. (14) should be taken as unity. Accordingly, Eq. (14) becomes

$$n_a(t) = n_a(t_0)\exp\left[-\int_{t_0}^t P(\tau)d\tau\right]$$

$$+ \int_{t_0}^t Q(t')\exp\left[-\int_{t'}^t P(\tau)d\tau\right]dt' ,$$

(15)

where

$$P(t) = -\frac{2}{\hbar}\mathrm{Im}\Gamma(t), \text{ and } Q(t) = -\frac{2}{\hbar}\mathrm{Im}\Gamma'(t) ,$$

(16)

and $\Gamma'(t)$ is defined by

$$\Gamma'(t) = -\frac{i}{\hbar}\int_{t_0}^t \sum_k n_k(t_0) V_k^*(t) V_k(t')$$

$$\times \exp\left[-\frac{i}{\hbar}(\epsilon_k - \epsilon_a)(t - t')\right]dt' .$$

(17)

Looking at the first term of Eq. (15), which gives the survival probability of the initial state before the atom came into the interaction with the solid surface, we may conclude that $Q(t)$ corresponds to the hopping rate from solid to atom, and that $P(t) - Q(t)$ may be regarded as the hopping rate from atom to solid. Indeed, Eq. (15) satisfies the following rate equation[14]

$$\dot{n}_a(t) = Q(t)[1 - n_a(t)] - [P(t) - Q(t)]n_a(t) .$$

(18)

A similar but semiclassical rate equation is adopted in the low-velocity regime.[2,14] But both $P(t)$ and $Q(t)$ have oscillatory behavior as a result of the quantum mechanical fluctuations, therefore they are meaningful only when they are integrated over the time t.[8] Then why are $P(t)$ and $Q(t)$ unlike? It is because an electron can hop above the Fermi level, getting energy from the atomic motion, which is not possible in Hagstrum's formulation. In other words, it is possible for the atom to pick up an electron even though ϵ_a is above ϵ_F, and also to put it off into an empty state in the conduction band even if ϵ_a is below ϵ_F. Letting $t \to \infty$, we obtain a neutral fraction from Eq. (15). Here we assume that the ion comes from the bulk to the surface, begins to interact with a surface atom at a time t_0 and leaves from the surface after the collision. Then we need the occupation numbers in the bulk as an initial condition. In the high-velocity regime, the initial state $n_a(t_0)$ may be zero because the electron-loss cross section is very large. On the other hand, the time integral of $P(t)$ is very large in the low-velocity regime because the atom interacts with the surface for a long time. Accordingly, the first term vanishes in both cases. But in the intermediate velocity regime, the initial-state occupation $n_a(t_0)$ is an unknown factor. Recent experimental data[12] shows that He ions are neutralized at the surface by means of resonant tunneling process and retain no memory within the solid. So, the first term of Eq. (15) will be hereafter neglected. Consequently, the neutralization probability becomes as follows

$$n_a = \int_{-\infty}^{+\infty} Q(t')\exp\left[-\int_{t'}^{+\infty} P(\tau)d\tau\right]dt' .$$

(19)

In the high-velocity case, $P(t)$ may be very small. Therefore, the exponential function may be taken unity. Equation (19) becomes

$$n_a(t) = \int_{t_0}^t Q(\tau)d\tau$$

$$= -\mathrm{Re}\left[\frac{2}{\hbar^2}\int_{t_0}^t dt_1 \int_{t_0}^t dt_2 \sum_k n_k(t_0)V_k^*(t_1)V_k(t_2)\exp\left[-\frac{i}{\hbar}(\epsilon_k - \epsilon_a)(t_1 - t_2)\right]\right] ,$$

(20)

which coincides exactly with the result of the first-order perturbation theory.[8]

If the ion moves very slowly and ϵ_F lies much higher than ϵ_a, the two transition rates $P(t)$ and $Q(t)$ are nearly equal, so Eq. (19) is approximately written as

$$n_a(\infty) = 1 - \exp\left[-\int_{-\infty}^{+\infty} P(\tau)d\tau\right] ,$$

(21)

which is the same results of the fixed ion approximation. But if ϵ_a lies near ϵ_F, the fixed-ion approximation will not be valid, because $Q(t)$ is much different from $P(t)$ even

though the ion moves very slowly.[7] In this way, we can show that Eq. (15) or Eq. (19) is valid over a wide range of ion velocities.

III. MODEL CALCULATION AND DISCUSSION

In this section we simplify Eq. (19) using a crude model. First we assume that the time variation of $V_k(t)$ does not depend on wave number k, so that $V_k(t)$ can be written as[6]

$$V_k(t) = V_k u(t) . \tag{22}$$

The function $u(t)$ gives us the time-variation of the interaction. And the linear Doppler shift, which was introduced by van Wunnik et al.,[15] is generally included in the transition matrix V_k. Then Eqs. (16) become

$$P(t) = \frac{2}{\hbar} \int d\epsilon \Delta(\epsilon) \int_{t_0}^{t} u(t)u(t')\cos[(\epsilon - \epsilon_a)(t - t')/\hbar]dt' , \tag{23}$$

$$Q(t) = \frac{2}{\hbar} \int d\epsilon \Delta(\epsilon) f(\epsilon, T)$$

$$\times \int_{t_0}^{t} u(t)u(t')\cos[(\epsilon - \epsilon_q)(t - t')/\hbar]dt' ,$$

where

$$\Delta(\epsilon) = \frac{\pi}{\hbar} \sum_k |V_k|^2 \delta(\epsilon - \epsilon_k) \tag{24}$$

is the usual transition probability or the life-time broadening, but in our case it generally depends upon the ion velocity through the electron translational factor.[15,16] And

$$f(\epsilon, T) = \frac{1}{1 + \exp[(\epsilon - \mu/k_B T)]} \tag{25}$$

is the Fermi-Dirac function.

In the alkali-metal case we can employ the free-electron-gas model to calculate the matrix elements, but in the transition-metal or the covalent-solid cases electron capture depends on the detailed electron-density distribution because electron capture will occur closer to the surface atom at high velocity.[12] In this case the electronic states Ψ_k should be projected to a certain atomic orbital Ψ_d such as a d electronic state and so Eq. (24) is rewritten as follows

$$\Delta(\epsilon) = \frac{\pi}{\hbar} |V_d|^2 \rho_d(\epsilon) , \tag{26}$$

where $\rho_d(\epsilon)$ is the projected density of states defined as

$$\rho_d(\epsilon) = \sum_k |\langle \Psi_d | \Psi_k \rangle|^2 \delta(\epsilon - \epsilon_k) , \tag{27}$$

in which we are taking account of both the band structure and the local electronic structure. Using this approximation, we can employ the binary-collision picture including the band structure of the solid.

Roughly speaking, the results are characterized by an interaction time [a width of $u(t)$ in time] and insensitive to the detailed time variation of $u(t)$ because the time integrals in Eqs. (23) give us a width of the quantum mechanical energy uncertainty and nothing more. Therefore we choose

$$u(t) = \exp(-\gamma |t|) \quad (\gamma = v/\alpha) , \tag{28}$$

where α is an interaction length. Equation (28) is not only reasonable physically but convenient for integration. Using this time variation, Eqs. (23) become

$$P(t) = 2 \int \Delta(\epsilon)g(\epsilon)d\epsilon e^{-2\gamma|t|} + 4 \int \Delta(\epsilon)g(\epsilon)\{\cos[(\epsilon - \epsilon_a)t/\hbar] - e^{-\gamma|t|}\}d\epsilon e^{-\gamma|t|}\Theta(t) ,$$

$$Q(t) = 2 \int \Delta(\epsilon)g(\epsilon)f(\epsilon, T)d\epsilon e^{-2\gamma|t|} + 4 \int \Delta(\epsilon)g(\epsilon)f(\epsilon, T)\{\cos[(\epsilon - \epsilon_a)t/\hbar] - e^{-\gamma|t|}\}d\epsilon e^{-\gamma|t|}\Theta(t) , \tag{29}$$

where $\Theta(t)$ is the step function, and

$$g(\epsilon) = \frac{1}{\pi} \frac{\hbar\gamma}{(\epsilon - \epsilon_a)^2 + (\hbar\gamma)^2} \tag{30}$$

gives us a width of the energy uncertainty. To compare the present result with the fixed-ion model, we will neglect the second term of Eq. (29) which has oscillatory behavior as a result of the quantum-mechanical phase evolution. However we must give notice that this simplification will not change the qualitative feature, but the oscillation is numerically not so small in the high-energy case.[8] Consequently, we obtain very simple expressions for the transition rates which can be compared with the results of the fixed-ion approximation as follows:

$$P(t) = Ae^{-2\gamma|t|}, \quad A = 2 \int \Delta(\epsilon)g(\epsilon)d\epsilon , \tag{31}$$

$$Q(t) = A'e^{-2\gamma|t|}, \quad A' = 2 \int \Delta(\epsilon)g(\epsilon)f(\epsilon, T)d\epsilon ,$$

and Eq. (19) becomes

$$n_a(\infty) = \frac{A'}{A} \left[1 - \exp\left[-\frac{2A}{\gamma} \right] \right] . \tag{32}$$

We now further assume that the density of states in the solid is independent of energy within the finite-band width, which leads to

$$A = 2\Delta \int_{\epsilon_b}^{\epsilon_t} g(\epsilon)d\epsilon, \quad A' = 2\Delta \int_{\epsilon_b}^{\epsilon_t} g(\epsilon)f(\epsilon, T)d\epsilon , \tag{33}$$

where ϵ_t and ϵ_b are the top and the bottom of the conduction or valence bands, respectively.

In the following we consider some limiting cases at $T = 0$.

(i) If the ion velocity is so slow that $|\epsilon_F - \epsilon_a| \gg \hbar\gamma$, the energy uncertainty function can be regarded as a delta function. In this case we obtain the usual result of the fixed ion model (Hagstrum's formula):
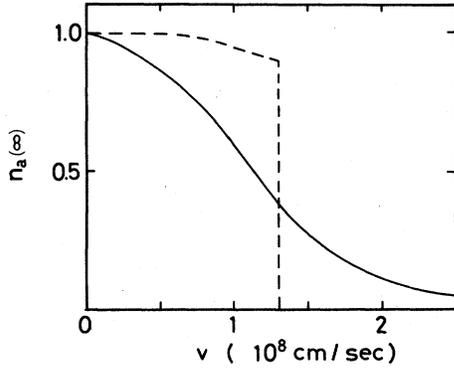
FIG. 1. Neutralization probabilities: solid line, Eq. (29); dashed line, Eq. (31), for $\epsilon_0-\epsilon_b=5$ eV, $\epsilon_F-\epsilon_b=10$ eV, $\alpha=2$ Å, and $\Delta=10$ eV.

$$n_a(\infty)=1-\exp[-2\Delta/\gamma] \; ; \tag{34}$$

but even though the ion velocity is very slow, we cannot employ this approximation in the $|\epsilon_F-\epsilon_a|\simeq\hbar\gamma$ case, in which case we should use the next approximation.

(ii) If $A/\gamma\gg1$ and $|\epsilon_a-\epsilon_b|\gg\hbar\gamma$, we obtain the very simple result

$$n_a(\infty)=\int_{\epsilon_b}^{\epsilon_F}g(\omega)d\omega \; , \tag{35}$$

which is generally applicable in the very slow case, and also in the intermediate-velocity regime according to circumstances. Indeed, substituting Eq. (30) to Eq. (35), we get

$$n_a(\infty)=\frac{1}{\pi}\{\tan^{-1}[(\epsilon_F-\epsilon_a)/\hbar\gamma]-\tan^{-1}[(\epsilon_b-\epsilon_a)/\hbar\gamma]\} \; , \tag{36}$$

which is the same as the empirical formula proposed by Haight et al.[12]

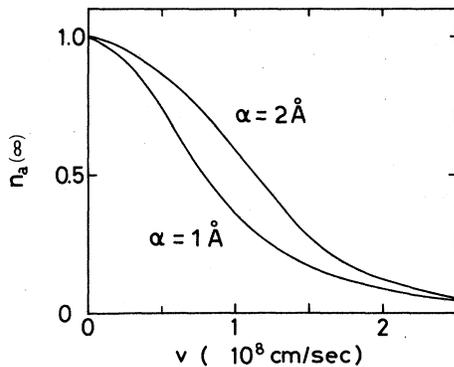(iii) At high velocity, Eq. (33) becomes

$$n_a(\infty)=A'/\gamma \; . \tag{37}$$

FIG. 2. Neutralization probabilities for $\epsilon_0-\epsilon_b=5$ eV, $\epsilon_F-\epsilon_a=10$ eV, $\Delta=10$ eV, $\alpha=1$ Å (lower curve), $\alpha=2$ Å (upper curve).
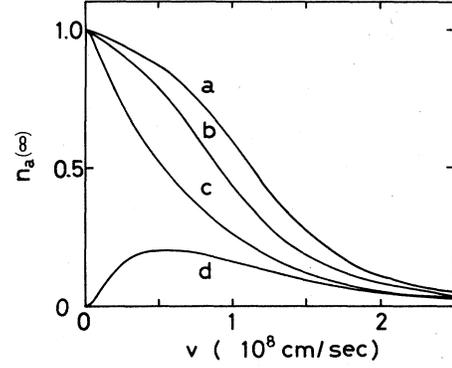

FIG. 3. Neutralization probabilities for $\epsilon_F-\epsilon_b=10$ eV, $\Delta=10$ eV, $\alpha=2$ Å, and $\epsilon_0-\epsilon_b=$(a) 5 eV, (b) 7 eV, (c) 9 eV, (d) 11 eV.

In Figs. 1–3, the calculated curves using Eqs. (32) and (33) are shown where we assume that $\Delta(\epsilon)$ is independent of the ion velocity (consequently, the linear Doppler shift is omitted) and that the bandwidth is infinite like an electron-gas model. In Fig. 1 the solid curve shows the present result for the neutralization probability [Eq. (32)] and the dashed curve shows the fixed-ion model [Eq. (34)]. The probabilities decreases rapidly with increasing ion velocity because the energy level ϵ_a is shifted up far above the Fermi energy by the electron translation factor. And another important parameter is the interaction time or length in the intermediate-velocity regime as we can see in Fig. 2. Finally, Fig. 3 shows the neutralization probabilities for the various energy levels ϵ_0. If the energy level ϵ_0 is above the Fermi energy, the calculated curve has a maximum in the dependence of the ion velocity. An application of the present result to the negative hydrogen formation is shown in Ref. 17. We will report on detailed numerical analyses of Eq. (19) for various situations in future.

IV. CONCLUDING REMARKS

In this paper, we have calculated the probability for resonant neutralization of an ion at surfaces in the intermediate-velocity regime. The result obtained conforms asymptotically with the result of the fixed-ion model at low velocity and with the result of first-order perturbation theory at the high velocity. In the intermediate-velocity regime, energy uncertainty plays an important role in consequence of the finite time of the interaction which cannot be seen in the fixed-ion approximation. This energy uncertainty makes it possible for an ion to pick up an electron inelastically; in other words the electron hops up above the Fermi level getting some energy from the kinetic energy of the energetic ion.

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