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Induced charge in ion–metal surface collisions

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ABSTRACT

When an ion arrives at the metal surface, it produces an induced charge that affects formation of the ion–metal system electron states. The state promotion in a dipole field is discussed and measured electron energy spectra produced in multiply ion–metal collisions are explained using this model. The paper presents the results of calculating the electron density distribution of induced charge near the metal surface in the classical approach and also, quantum mechanically, with a variation model of a Density Functional Theory approximation. In the both cases the spatial cloud of induced charge is oblate parallel to the metal surface; in quantum mechanical solution the cloud is also shifted towards the approaching ion.

1. Introduction

The effect of ion- or electron-induced charge on field-emission phenomena were studied in many papers where the main attention was given to the potential barrier shape that determines the surface field-emission properties [1].

In describing the multi charged ions neutralization in colliding with metal surface, the model proposed in [2] is widely used, which stipulates that electron capture by the multicharged ion with charge Z is explained by disappearance of the potential barrier separating the projectile ion and metal ions from each other and predicts that ion states with binding energies close to the electron binding energy in the metal conduction band (i.e., states with principal quantum numbers $n = 4$–6 (for $Z = 5,6$) are preferably occupied. But in some cases experimental spectra of Auger electrons emitted in multiply charged ion–metal collisions show that deep states with $n = 2,3$ are occupied. In Section 2 we have discussed the effect of state promotion in a dipole field, which produces a strong reconstruction of states during a collision; the cases when this model is applicable have been discussed. In Section 3, the observed electron energy spectra have been analyzed by using the theoretical models.

Since the induced charge forms a spatial cloud of electrons, it cannot be regarded as a point charge. In Section 4, a formula for spatial distribution of the induced charge cloud in the classical approach has been obtained, while in Section 5 the approximation of Density Functional theory has been used for this purpose. In Section 6, we have estimated the internuclear distances for which the approximation of the point induced charge should be refined.

2. Dipole model describing the state reconstruction in multicharged ion–metal collisions

In our paper [3] we showed that in the process of collision, when the ion-surface distance R gradually decreases, the states are being significantly reconstructed in the field of the dipole consisting of an ion with charge Z and induced charge $(-Z)$ (see Fig. 1 [3]).

As it is known, the dipole field does not contain bound states at small inter-nuclei distances. Therefore, the specific effect taking place in R decreasing is state promotion (binding energy decrease) of terms formed at $R \to \infty$ from deeply bound multicharged ion states with $n = 1$–3. All the ionic states are promoted. The field of incoming ion "marks" the nearest atom of the metal, and its states begin splitting from the conduction band. The dipole field also affects the states formed from the metal atoms, causing their Stark splitting and reconstruction. Occupation of the multicharged ion states takes place when those promoted states cross the levels formed from metal atoms. The probability of transition at crossing point R_c is defined by the Landau–Zener model [4]:

$$P = exp\{-2\pi H_{12}^2/(\Delta F v)\}, \quad (1)$$

where P is the transition probability in a single pass through the crossing point, H_{12} is the matrix element describing the levels splitting at R_c, ΔF is the difference in level slopes at crossing point R_c, and v is the collision velocity.

Quantity H_{12} may be estimated by using the formula suggested in [5]:

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$$H_{12} = 9,13Z^{-1/2}exp\{-1,324R_cZ^{-1/2}(2I_m)^{-1/2}\} \quad (2)$$

Here R_c is the crossing point location, I_m is the electron binding energy in metal, atomic units are used. Usually, the off-diagonal element is approximated by half the energy difference of the levels at the distance of the crossing. Landau–Zener model is not applicable with the limits for $R_c \to 0$ and $R_c \to \infty$. In these cases we need to change the model of state coupling.

Each intersection takes place twice: in the incoming and outcoming parts of the particle trajectory. Therefore, the transition probability is $W = 2P(1-P)$. Crossings at large R_c do not cause electron capture, since in this case $P = 1$, and crossings are "missed". At small R_c $P \to 0$. Thus, only crossings with $P = 0.1$–0.9 are efficient. There is an open question: could this double passing will occur as levels are different on the ingoing and outgoing parts of the trajectory due to the neutralization? But if we have only one passing of crossing we still need to have H_{12} or level splitting at crossing point large enough to obtain the probability of transition $P = 0.1$–0.9. We have estimated [6] the transition probabilities at level crossings for the case of C^{5+}–Ni collisions at the collision energy of 150 eV discussed in Section 3, and found out that the electron capture is to occur in the states formed at $R \to \infty$ from states with $n = 2,3$.

Thus, the state promotion model changes our understanding of initially occupied autoionizing states. The differences in the 'state promotion model' and 'side feeding model' are as follows: (i) the 'state promotion model' involves the state reconstruction while the 'side feeding model' usually ignores it; (ii) probabilities of electron capture at level crossing are much higher than that in the 'side feeding model' where electrons are captured from deep states of metal atoms.

The 'over-barrier' model predicts complete neutralization of incoming ions. In this case the proposed 'state promotion' model does not work. In the case of partial neutralization the state promotion still exists. It is possible to introduce universal coordinates $R(Z)Z = R(Z = 1)$ and $E_i(Z)/Z^2 = E_i(Z = 1)$; for this purpose, it is sufficient to rescale the axes in Fig. 1. For every initial charge of a projectile ion, we need to consider the subset of states associated with each value of ion charge.

Reconstruction of the states under the influence of the dipole field always takes place in the initial part of the ion trajectory. The neutralization becomes less pronounced also in the case of the increase in the collision velocity. Cases are also known when hard collision with the surface atom results in particle deflection by a large angle with simultaneous formation of one or two vacancies in the inner electron shells. These vacancies can live till the particle escape from the surface. Subsequent Auger decay of the vacancies leads to occurrence of multicharged ions leaving the surface. In this case, the dipole model can be used for the outgoing part of the trajectory.

3. Comparison with experimental data

The predicted effect of occupying deep states with $n = 2,3$ in the case of interaction with metal ions with $Z = 5,6$ is confirmed by the measured Auger electron spectra [6] (Fig. 2) where lines corresponding to Auger transitions from states $2s^2$–1s, 2s2p–1s, $2p^2$–1s predominate, while no transitions from higher states are observed.

The line position in the observed energy spectrum informs that the Auger decay of K-vacancy takes place when the L shell accommodates 2–4 satellite electrons [7]. Their presence could not be explained by a cascade of Coster–Cronicg transitions with $\Delta n = 1$ because they are too slow as compared with the calculated Auger decay rate for K-vacancy [8,9]. Therefore, the experimental electron energy spectra for the case under consideration confirm our conclusion about the existence of an additional mechanism for electron capture to the deeply bound states with $n = 2,3$ due to which the L-vacancies are filled more completely in ion–metal collisions as compared with the model considering only over-barrier transitions.

For better fitting of experimental data, the authors of the over-barrier model also included in the model the state reconstruction [10].

4. Electron density distribution in the ion–metal interaction: classical approach

It is evident that, when the ion approaches the metal, not a point charge is induced in it but a certain electron cloud near the surface. Thorough consideration of the real electron density

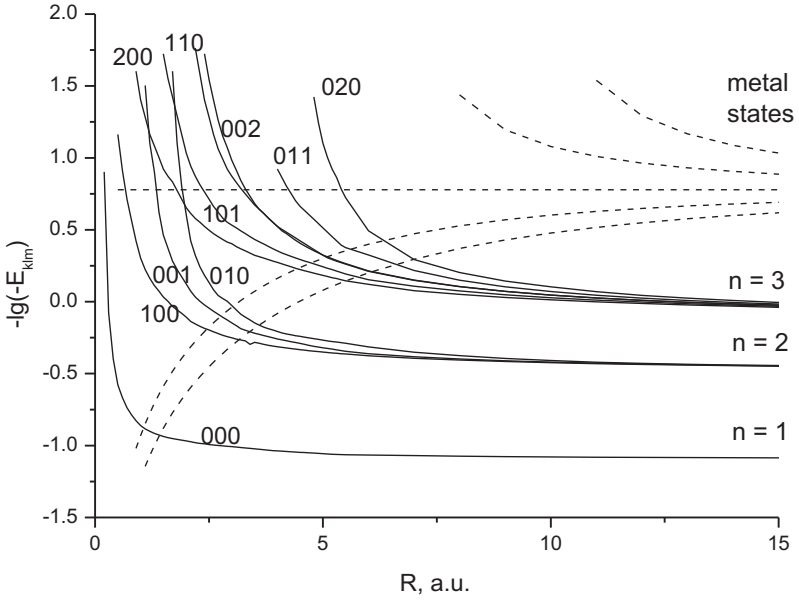

Fig. 1. States versus inter-nuclei distance R in the dipole field of centers with $Z = 5$. Crossing points R_c mentioned in the text are those where solid lines cross dash lines. At these points electron transitions occur.