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Deposition and re-emission of potential energy – extended dynamical COB simulation

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Abstract. We present results of a numerical computer simulation based on the extended dynamical classical over the barrier model (EDCOM). To get an energy balance for the transferred potential energy of the highly charged ions (HCIs) to the solid surface, we apply an additional extension of the model evaluating the energy loss of Auger electrons which are generated during the relaxation of the HCI. From the results of the simulation we can distinguish between the potential energy deposited in the nuclear system due to image charge acceleration of the incoming HCI and the potential energy which is released over Auger processes. Further, we break down this energy into that which is deposited in the solid and that which is re-emitted due to escaping secondary electrons.

1. Introduction
The interaction of a slow HCI with solid surfaces is characterized by a very small interaction zone of about 1–10 nm$^2$ on the surface and a few angstroms in depth. The energy which is released during the relaxation process of an HCI can exceed several 100 keV without considering the kinetic energy. This amount of energy, called potential energy, is stored in the ion during the ionization process as the sum of the ionization energy. The relaxation mechanisms are combined with the emission of secondary particles like electrons, neutral atoms, ions and X-ray. The sum of the energy released in these emission channels is only around 10% to 20% of the total potential energy of the HCI. A few experiments [1,2] were also tried to determine the amount of the deposited potential energy into the surface. However, a full understanding of the mechanism of the energy deposition is lacking. To compare these experimental results with theory, the well known extended dynamical classical over the barrier model (EDCOM) [3,4], can be used. We extended this model to get an energetic balance of the transferred energy, additional to the current very good agreement with experiments evaluating the total electron yield [3] and the equilibrium charge state in surface channeling experiment [6].

2. Numerical EDCOM simulation
An HCI approaching the surface feels the force with the self image charge created in the solid. The consequence is an electrostatic potential, which accelerates the ion to the surface. This depends on the ion charge state and on the distance of the ion to the surface. Active electrons, those electrons which can leave the solid or the HCI, are also influenced by the image potential of the HCI. Further, the total potential which is felt by the active electron is a superposition
of the screened atomic potential of the ion, the image charge potential of the ion and the self image charge potential of the active electron. It can be written in atomic units as:

\[ V_{\text{tot}} = V_{\text{ion}} + V_{\text{img,ion}} + V_{\text{img,el}} = \frac{-q}{\sqrt{x^2 + (z - R)^2}} + \frac{-q}{\sqrt{x^2 + (z + R)^2}} - \frac{1}{4\pi} \]  

(1)

Thereby \( R \) is the distance of the ion to the surface. The position vector in cylindrical coordinates is then \( \vec{R} = 0\hat{\rho} + R\hat{z} \). The position vector of the active electron is described by \( \vec{r} = x\hat{\rho} + z\hat{z} \).

The numerical calculation has to include two main aspects. The first is the calculation of the time dependent rate equation for the population of the energy levels of the HCI:

\[ \frac{dn_n}{dt} = \Gamma_{RN}^n - a_n\Gamma_{RI}^n + \sum_{n' > n} \Gamma_{AI,-\text{gain}}^n - \sum_{n' < n} \Gamma_{AI,-\text{loss}}^n + \Gamma_{SF}^n + a_n\Gamma_{PO}^n , \]

(2)

and second the Newton equation of motion:

\[ \Delta \vec{v} = \frac{\vec{F}(q, \vec{R})}{m_{\text{ion}}} \Delta t , \]

(3)

with the forces consisting of the attractive image charge force and the repulsive force generated by the Thomas-Fermi potential:

\[ \vec{F}(q, \vec{R}) = -\left( \frac{q(R)}{2(R - z_{n_m})} \right)^2 \hat{e}_z + \vec{F}_{\text{TFM}}(\vec{R}) . \]

\( z_{n_m} \) is the position of the image plane. The rates in the equation 2 represent the resonant neutralization \( \Gamma_{RN}^n \), the resonant ionization \( \Gamma_{RI}^n \), the gain and loss rates due to Auger relaxation \( \Gamma_{AI,-\text{gain}}^n \) and \( \Gamma_{AI,-\text{loss}}^n \), and the side feeding and peel off rates \( \Gamma_{SF}^n \), \( \Gamma_{PO}^n \). The modeling direction of the rates and the numerical procedure are described in detail elsewhere [3-5]. With these concepts one is able to describe the formation of hollow atoms several atomic units in front of the surface, to predict the time dependent relaxation of the HCI, to estimate the energy gain and to obtain energy dispersive electron yields which are in good agreement with experimental data [3].

3. Extensions for an energy balance

To calculate the fragmentation of the potential energy we evaluate the kinetic energy of the secondary electrons. The electrons emitted during Auger relaxation processes are stored in discrete energy intervals. Depending on the position of the ion, the released energy conserved in the kinetic energy of the electrons has to be divided into two parts. One part is the re-emitted energy due to secondary electrons emission. The other is the energy retained in the solid due to electron scattering and energy loss processes. As long as the position of the HCI is above the surface we assume that 50% of the electrons penetrate the surface and 50% can leave the surface. The corresponding energy is obtained by summing the number of electrons multiplied by their energy

\[ E_{\text{dep}} = E_{\text{re}} = 0.5 \sum_i N_{\text{Auger}}(E_i) E_i \]

(5)

\( E_i \) is the kinetic energy of the electrons stored in the ith energy interval. If the position of the ion is below the surface we introduce an attenuation of all electrons which are moving toward the surface due to scattering. The electrons which penetrate the solid deposit all their kinetic energy in the solid. The electrons traveling through the solid to the surface are attenuated
dependent upon the kinetic energy of the electrons and the emission depth. For the attenuation we adopt a model developed by Cumpson and Seah [7] for inelastic scattering corrections in AES and XPS of over layer-substrate experiments. They present an exponential relation of the attenuation coefficient $K$ and the emission depth $d$:

$$K(E, d) = e^{-d/\lambda(E)}$$  \hspace{1cm} (6)

Further the characteristic attenuation length $\lambda(E)$ depends on the kinetic energy $E$ of the electron. It can be expressed by equation 7, where $a$ is the lattice constant and $Z$ the atomic number of the target.

$$\lambda(E) = 0.31 a^{3/2} \frac{E}{Z^{0.45} \ln(E/27) + 3}$$  \hspace{1cm} (7)

The amount of deposited and re-emitted potential energy can be written as:

$$E_{\text{dep}} = 0.5N_{\text{Auger}} + 0.5N_{\text{Auger}} (1 - K),$$  \hspace{1cm} (8)

$$E_{\text{re}} = 0.5N_{\text{Auger}} K.$$  \hspace{1cm} (9)

4. Numerical results and comparison with experimental data

First the energy gain due to the image charge acceleration is compared with experimental results already presented in the literature. Figure 1 shows the energy gain for an HCI in the self image charge potential in front of a solid surface for varying charge states. The calculated values (stars) are compared with experimental values published by Lemell [8] (triangles) and Burgdörfer [9] (circles). Additionally the analytic function of the COB model [4] is plotted, which is known to be a lowest estimation. The numerical values are in acceptable agreement with the experimental data. In figure 2 the image charge energy gain as a function of the incident energy of the ion in the range of 100 eV up to 1000 eV is shown. As one can see the calculated energy gain remains almost constant at 45 eV using Ar$^{9+}$ interacting with a copper surface. Therefore, we can conclude that the image charge gain is independent of the primary kinetic energy in this range. This is an important requirement for the calorimetric measurements [2], which are
based on the extrapolation to zero kinetic energy. The most important result of the numerical model is the prediction of the energy fragmentation. That is, how much of the potential energy released over Auger processes remains in the solid, how much is converted into kinetic energy and how much is re-emitted over secondary electrons. These results are presented in figure 3 where the different parts of the total potential energy over different charge states of Argon ions are plotted. First we focus on the separation between the energy released over Auger processes (upward triangles) and the energy converted into kinetic energy (downward triangles). One can see that only around 5% of the total energy is converted into kinetic energy. This value is nearly constant with variation of the charge state. Conversely around 90% of the total potential energy is released via Auger electrons. Again this value remains nearly constant with the charge state. Further the energy released during Auger relaxation splits again into a retained part (squares) and a re-emitted part (circles). In figure 3 one can see that these fractions of the potential energy also remain constant with changing charge state. The atomic energy levels of the HCI are calculated inclusive the image charge interaction using first order of perturbation theory. For high charge states ($\text{Ar}^{9+}$) or small distances to the surface the perturbation of the image potential may be too large, so that the part of energy transferred over Auger electrons decreases slightly. In conclusion, we have described a way to extend the EDCOM model to get an energy balance of the fragmentation of the potential energy in HCI surface interaction. The model assumes that all the potential energy stored in the HCI is released over Auger processes. Depending on the position of the electron emission, the energy is retained in the solid due to elastic electron scattering. In this model we can further distinguish between potential energy deposited in the electronic system of the solid due to electron transfer and deposited via nuclear collisions due to image charge acceleration.

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