Nuclear Instruments and Methods in Physics Research B 269 (2011) 981–984

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Molecular dynamics study of kinetic electron emission induced by slow sodium ions incident on gold surfaces

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ARTICLE INFO

Article history:
Received 31 July 2010
Received in revised form 10 December 2010
Available online 17 December 2010

Keywords:
Impact phenomena (including electron spectra and sputtering)
Theories and models of many-electron systems
Electronic stopping

ABSTRACT

Electron excitation and emission phenomena, due to Na^+ ion impact on Au (1 0 0) surfaces, are studied at incident projectile energies below the threshold for kinetic electron emission. The trajectories and velocities of the projectile and the target atoms are simulated with molecular dynamics. This information are used to calculate the energy loss by electronic stopping as a series of discrete events, localized in space and time, that are treated as sources of excitation energy. The diffusion of the energy deposited by the projectile into the solid is converted into electron yield as proposed by Duvenbeck and coworkers [14]. The results show similar trends to available experimental data.

1. Introduction

Electron excitation and electron emission are among the main consequences of the interaction of a charged ion, or a neutral atom, impinging on a solid surface. These processes are activated either at the expense of the internal energy or the kinetic energy of the projectile. Correspondingly, the mechanisms of the electron emission fall into the two categories of potential electron emission (PEE) [1] and kinetic electron emission (KEE) [2]. While PEE is in principle understood, the basic features of KEE are still a matter of debate, particularly at low incident energy. Two well-known KEE channels are projectile–electron collisions [3] and electron promotion in close atom–atom contacts [4]. Both these processes are subject to a threshold condition, namely they are not possible if the kinetic energy of the projectile is lower than a threshold value. Also PEE is a threshold phenomenon: electron emission may occur if the potential energy carried by the projectile exceeds the minimum energy needed for a target electron to overcome the surface barrier [5]. Then, PEE can be excluded if one uses alkali metal ions to probe sufficiently high work function surfaces. Several experiments, in projectile–target systems where the contribution of PEE is absent or negligible, have measured electron emission yields below the KEE thresholds [6,7].

These "*sub-threshold*" processes have been intensively investigated [6–9], although a satisfactory explanation is still lacking. Several existing theoretical models suffer from two main limitations: on the one hand, they approximate the excitation mechanism to many effective, one-electron processes [8,9]. On the other hand, they do not take into account the detailed motion of the projectiles and the target atoms [7–9].

Concerning the first issue, one electron treatments of electron emission have found several difficulties in explaining the sub-threshold electron yields [6,7], which suggests that many-electron excitations play a non-negligible role in these processes. A phenomenological many electron approach in excellent agreement with experiments is provided by the hot spot model by Sroubek and coworkers [10,11].

As for the second point, the effective atom-electron potential, used in many electron emission calculations [6] does not take into account the specific trajectories of target atoms in the solids during the projectile–surface interaction; in most cases, this potential is only representative of an 'average' interaction on all the possible collision cascades generated by the projectile**.** A more accurate treatment requires molecular dynamics (MD) to calculate the classical trajectories and velocities of the projectile and the target atoms. This information may be used in quantum dynamical calculations to predict the electron emission properties of the systems [12].

Here, we propose an attempt to extend the basic idea of the hot spot model using MD simulations. The system under investigation is Na scattering from Au(1 0 0), which allows us to exclude PEE as possible emission mechanism. In addition, we consider initial projectile energies in the range of 0.1 to 2.0 keV, so that we can neglect excitations due to direct atom–electron collisions and electron promotion in close atomic encounters [6].

The organization of the paper is as follows: in Section 2 we briefly outline the characteristics of the hot spot model; in

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doi:10.1016/j.nimb.2010.12.046

Section 3, we present calculations of the energy loss of the moving atoms in the solid, discussing its relationships to available experimental electron yields [13]; in Section 4 we use a model for energy diffusion [14] and electron emission to calculate the electron yield from our MD simulations, and we compare the results to the experiments of Ref. [13].

2. Hot spot model

The basic idea inherent the hot spot model is that surface electrons are excited with the energy deposited by the incident particle. This energy, assumed to be equal to the energy loss of the projectile due to electronic stopping, produces a broadening of the one-electron energy distribution of target states. Then, electron emission is possible if the broadening is sufficiently large to allow an electron at the Fermi energy to be excited above the vacuum level. However, in the sub-threshold regime the energy distribution of excited electrons is so narrow that emission processes are possible only if the excitation energy is confined, for a sufficiently long time δt, in a region of atomic length r_e. In the free electron gas approximation, the Lindhard–Sharff–Schiøtt (LSS) formulation of electronic stopping [15] leads to the simple expression

$$\Gamma = A \exp\left[-\frac{\phi}{Bv}\right], \tag{1}$$

for the electron yield [10], in which ϕ is the substrate work function, v the initial velocity of the projectile, and A and B are two characteristic parameters of the projectile–substrate system. The advantage of Eq. (1) is that it predicts an exponential behavior of the electron yield with the inverse velocity of the projectile; such a trend has been experimentally observed in several laboratories for various particle substrate systems. Indeed, the model function (1) can be easily applied to measurements via some adjustments of A and B [16]. The main problem, however, lies in the definition of A and B that depend critically on δt and r_e, as well as on the electronic stopping power S_e, the substrate density of states at the Fermi level, and the heat capacity. In Fig. 1, we show how the hot spot model correctly reproduces the measured electron emission yields of Au [13] and of two different surfaces of Ru [7], following the impact of Na^+ ions. The solid lines are obtained by fixing B to 1.08 au and adjusting A by fitting Eq. (1) to data. Interestingly enough, the choice of a common value for B is justified because the variation of δt and r_e, for both Au and Ru, is somewhat compensated by the change in the stopping power and the heat capacity (see also discussion in Ref. [16]).

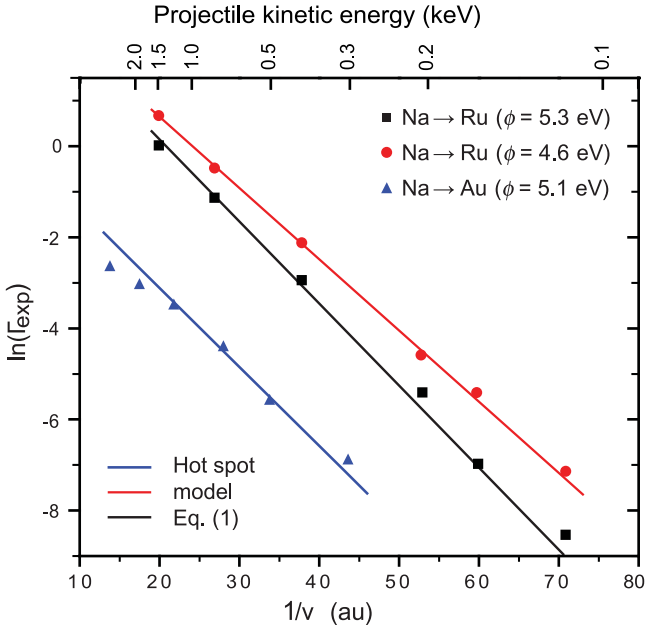

Fig. 1. Natural logarithm of electron yield, ln Γ, versus the inverse velocity for the Na^+ ions impinging on Ru [10] and Au [13] surfaces. The top horizontal axes represents the initial projectile kinetic energy, E_{in} (in keV). Solid lines are obtained from the hot spot model as discussed in the text.

In the hot spot model, the projectile is the only source of excitation, while the contribution of the surface atoms in the collision cascade area is neglected. Indeed, in Eq. (1) all the possible effects of the collision cascade on the projectile motion are averaged out, the impinging particle following an approximate straight line in a charged frictional medium [10]. The idea of the present work is to use MD in the computation of the trajectories and velocities of all moving atoms, thus, estimating the energy deposited in the solid by the impinging atom and its diffusion through the medium.

3. Molecular dynamics simulations and energy deposition

We simulate the impact of a Na^+ ion on a (1 0 0) FCC cluster of ~4000 Au atoms, arranged on 14 layers, fixing the position of the outermost atoms of each layer to improve the stability of the cluster. With the impinging particle at normal incidence, we sample the initial kinetic energy in the range of 0.1–2.0 keV. We select 28 different impact points, uniformly distributed along the regions of maximum symmetry of the (1 0 0) plane, and we observe the collision cascade for time scales of 100 fs. We calculate the trajectories of both the projectile and the target atoms with a standard molecular dynamics code, in which the equations of motion are computed by means of the velocity-Verlet algorithm [17]. The interatomic potentials have the form of the Karolewski composite potential [18], for the Au–Au interaction, and the Ziegler–Biersack–Littmark (ZBL) potential [19], for the Na–Au interaction. The contribution of the electronic stopping is included using the LSS theory.

The classical motion of all moving atoms allows us to calculate the energy loss due to electronic friction; the latter is treated as a series of discrete events where each atom i loses an energy

$$\Delta E_i = K_{LSS} \boldsymbol{v}_i \cdot \Delta \boldsymbol{r}_i \tag{2}$$

between two consecutive time steps. In Eq. (2), $\boldsymbol{v}_i$ is the average velocity and $\Delta \boldsymbol{r}_i$ the average displacement of the i atom, located at $\boldsymbol{r}_i$, when the observation time is t_i; the constant K_{LSS}, specific of the LSS approach, depends on the characteristics of the moving atom and the electronic substrate [20]. The individual energy loss events are localized in space and time, thus their space–time distributions may be approximated to Dirac's delta functions:

$$S_i(\boldsymbol{r}, t) = \Delta E_i \delta(\boldsymbol{r} - \boldsymbol{r}_i)\delta(t - t_i) \tag{3}$$

The sum of all contributions (2), averaged over the 28 impact points of the MD simulation, leads to the total energy loss E_{LSS} due to electronic stopping, for a given incident energy. The logarithm of this quantity is reported in Fig. 2, as function of the inverse initial velocity of the projectile, in order to ease direct comparison with the electron yield of Fig. 1. As a further analysis, we consider the total energy loss for events that take place within the first 4, 7, and 10 atomic layers of the Au cluster, respectively. The logarithmic distributions of the four series of points are linearly correlated. Their slope decreases as the number of layers included in the calculation increases. This behavior indicates that E_{LSS} follows the same law as the electron yield, namely:

$$E_{LSS} = \alpha \exp\left[-\beta \frac{1}{v}\right] \tag{4}$$

where the parameters α and β are easily estimated by fitting the model function of Eq. (4) to the data of Fig. 2. In particular, the