J. Phys.: Condens. Matter 5 (1993) A267–A268. Printed in the UK

Resonant coherent excitation to the continuum in grazing ion–surface collisions

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Abstract. An extension of the Okorokov effect to the case in which the ion moves near an oriented surface and the electron is ejected into the continuum is considered. The effect of the screening of the initial electronic bound state on the final electron energy is analysed.

The resonant coherent excitation (RCE) of bound electron states on ions channelled along crystalline directions in a solid is well established (Okorokov 1965, Datz *et al* 1978). Ions at grazing incidence on a crystal surface undergo surface channelling, hence a surface type of RCE has also been proposed (Kupfer *et al* 1981, Kawai and Kawai 1988). Recently, we have studied RCE from bound to continuum states of a hydrogenic ion travelling along an atomic row of a crystal surface (García de Abajo *et al* 1992). The ion–surface interaction has two contributions: the induced potential $V_{IP}(z)$ from the electron polarization generated by the ion nuclear and electronic charges (Echenique *et al* 1990), and the crystal potential $V_{CP}(z)$ from the lattice of atomic cores with tightly bound electrons (z is chosen normal to the surface). V_{CP} is the provider of the harmonic terms of frequency $2\pi nv/d$, where v is the ion velocity, d the atomic spacing and n the order of the harmonic (well defined frequencies require ions travelling within a few mrad from the row direction). Their amplitude decay with the distance to the surface approximately as $V_{CP}^{(n)}(z) = V_0 \exp(-az)$ with $a = \sqrt{(\lambda^{-2} + 4\pi n^2 d^{-2})}$, where λ and V_0 are the screening length and amplitude of the isolated atom potential. The oscillating terms cancel out in the definition of the ion trajectory, which is approximated as that of a structureless classical charge.

For an He (1s) ion of $v > 1.9$ au moving along the (100) direction of W ($d = 5.98$ au), RCE proceeds to final continuum states. Using a first-order approximation to the transition amplitude, it is seen that the transition rate $w(y, z)$ is small (y is the impact parameter with respect to a top-most row of solid atoms measured on the surface). Hence, the population $p(t)$ of the 1s state can be assumed to obey the relation $dp/dt = wp$. Due to the long time of ion–surface interaction in the incoming trajectory, $p(t_0) \simeq 0$ for $\phi \leqslant 1$ mrad, with t_0 defining the apex and ϕ the angle of incidence of the trajectory. This means that RCE is produced with probability equal to one, at least when other transitions are neglected. Furthermore, it mainly happens on the incoming part of the trajectory, so that hard close collisions and surface imperfections are not going to degrade or unmask the effect.

Transition energies are given by $\Delta E = 2\pi nv/d$. Therefore, a number of final continuum states (for $n = 1, 2, \ldots$) are populated. The dominating transition corresponds to $n = 1$. The final energy of the emitted electron depends on the binding of the initial 1s orbital, which is modified by the interaction with the surface. Since the crystal potential V_{CP} decays

0953-8984/93/ SA0267+02$07.50

exponentially with z, it will affect the binding close to the apex of the trajectory. On the other hand, V_{IP} recreates the classical induced potential away from the surface: $V_{IP} = 3/4z$ for $z > v/\omega_s$ (ω_s is the surface plasmon frequency), and this shift in the 1s binding should be appreciable. At smaller values of z the induced potential becomes non-local, the electron self-energy saturates to $-\pi\omega_s/4v$ and its interaction with the ion-induced polarization will become highly non-local (Echenique and Pendry 1975).

The transition rate along the trajectory depends on the velocity and angle of incidence of the ions; consequently, the energy at the peak in the distribution of emitted electrons also depends on ϕ and v, and allows one to determine the changes of binding energy of the initial electron state due to the crystal and induced potentials. The dependence on velocity is present only for V_{IP}.

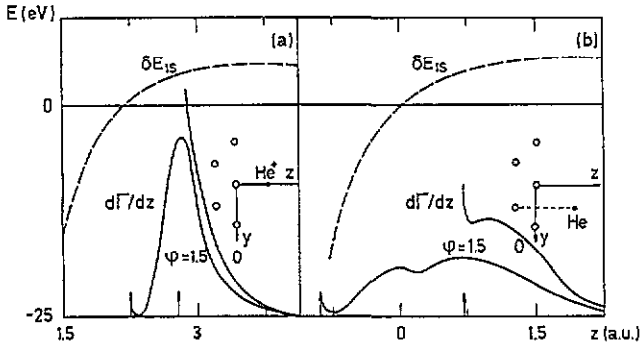

Figure 1. Broken lines: shift of the energy of He^+ (1s) as a function of the coordinate z: (a) for impact parameter $y = 0$, (b) is shown for $y = d/2$. At the bottom of the figure the transition rate $d\Gamma/dz$ is shown for $\phi = 0$ and 1.5 mrad. Arrows indicate the turning points for the trajectories.

We show in figure 1 energy shifts for two values of ϕ, and the corresponding transition rates $d\Gamma/dz = w(y, z)[p_{inc}(z) + p_{out}(z)]/v_z$ that give the number of electrons emitted per unit normal distance z travelled by the ion; the incoming p_{inc} and outgoing p_{out} populations of the ground state along the trajectory are considered for an ion moving with normal velocity v_z. Integration of the energy shift weighted by the transition rate $d\Gamma/dz$ gives the average value of the energy at the resonance in the distribution of emitted electrons; this value is shifted 3–5 eV from that given by the binding of He^+ (1s), for $0 < y < d/2$.

In conclusion, we point out that electrons emitted by RCE should present not only specific angular distributions (García de Abajo *et al* 1992), but also characteristic energies that allow the study of the action of surface potentials on atomic bound states.

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