Electron Emission Induced by Resonant Coherent Ion-Surface Interaction at Grazing Incidence

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A new spectroscopy based on the resonant coherently induced electron loss to the continuum in ion-surface scattering under grazing incidence is proposed. A series of peaks, corresponding to the energy differences determined by the resonant interaction with the rows of atoms in the surface, is predicted to appear in the energy distribution of electrons emitted from electronic states bound to the probe. Calculations for MeV He^+ ions scattered at a W(001) surface along the ⟨100⟩ direction with a glancing angle of 0–2 mrad show a total yield close to 1.

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The resonant coherent interaction of a swift ion channeled through the bulk with the rows of atoms in a solid is known to produce intra-atomic transitions in the probe when the transition energy is a multiple of $\Delta E_1 = 2\pi v \hbar/d$, where d is the spacing of the atoms in the rows and v is the velocity of the ion [1–5]. This effect, first predicted by Okorokov [1] and experimentally observed in different ways [2,3], has been used to obtain valuable information on the bulk dynamical screening of atomic states [2,4,5]. It could also be employed to investigate the role played by the surface dynamical screening acting on ions incident on a surface.

In this Letter we propose the detection of the resonant coherent excitation (RCE) of fast hydrogenlike ions interacting with an oriented crystal surface under grazing-incidence conditions, through the emission of the bound electron to the continuum with well-defined energies and around a preferential direction. The basic requirement to have RCE is that the probe interacts with the surface under grazing incidence with respect to a special direction of the crystal. High velocities are considered in this work ($v > 2$ a.u.), so that other processes like direct resonant and Auger loss do not contribute significantly [5].

The RCE rate is calculated in the parallel-motion approximation. The ion experiences a periodic perturbation of frequency $\Delta E_1/\hbar$ originating in the solid atoms which are disposed on the surface and equally separated by a distance d along the direction of the motion. When this perturbation induces a RCE in the bound electron the transition energy must be a multiple of ΔE_1, that is, $\Delta E_n = 2\pi n v \hbar/d$, where $n = 1,2,\ldots$ labels different harmonics. As in many resonance phenomena one expects that the transition probability decreases with n. For sufficiently high velocities ΔE_1 exceeds the ionization energy of the probe and the electron can be emitted to the continuum with large enough probability. For He^+ ions moving parallel with the ⟨100⟩ direction of a W crystal that condition is fulfilled if $v > 1.9$ a.u.

The ion trajectory introduces a slowly varying dependence upon the time of the ion-surface separation. The dynamics of the ion is governed by the surface potential, made up of two different contributions: the long-distance interaction with the electron gas of the solid, which we will refer to as the induced potential (IP), and the short-range periodic interaction with the target ion cores, referred to as the crystal potential (CP). The oscillatory components of the latter are responsible for the RCE. The lateral deflection of the probe and the corrugation of the surface in the direction of the motion are neglected, so that the trajectory, classically calculated from the surface potential, is determined by the angle of incidence φ and the impact parameter y, defined as the distance to the topmost row of atoms measured along the direction parallel with the surface. Results directly comparable with experimental findings are approximated by averaging over y.

The IP has been calculated using the well-known specular reflection model [6,7] with the plasmon-pole dielectric function [8] to describe the response of the bulk material (in Ref. [9] the main results are shown concerning the surface wake potential as an extension of the bulk wake potential [5,10]). The CP is obtained from the Molière approximation to the Thomas-Fermi potential [11], successfully used to calculate trajectories of ions reflected at surfaces with very small normal energy [12]. Moreover, the interaction of the bound electron with the target atoms is assumed to be well described by this approximation [13].

An efficient RCE requires that the ion travels along a sufficiently large number of solid atom spacings, q, before significantly changing its z position in terms of the screening length of the CP, a, i.e., $q\varphi \ll a/d$. For ions traveling along the ⟨100⟩ direction of W one has $q\varphi \ll 35$ mrad. Furthermore, from the uncertainty principle of Heisenberg the transition energy is well defined only if $2\pi nq \gg 1$. These conditions may be simultaneously fulfilled by available experimental techniques of beam orientation and collimation allowing angles of incidence in the range of mrad [14]. The uncertainty in the component of the velocity parallel to the surface and perpendicular to the ion rows must satisfy similar conditions. In addition, a tilted beam originates a slow modulation, caused by the crossing of parallel chains of atoms, superimposed on the fast modulation responsible for the RCE. This results in the splitting of each frequency $\Delta E_n/\hbar$ into "sideband" frequencies separated by $\approx \varphi \Delta E_n/\hbar$, as pointed out by Kupfer, Gabriel, and Burgdörfer [15].

Let us first estimate the order of magnitude of the RCE yield. Assuming conservation of energy in the normal motion and expressing it at the turning point one obtains

$$eZ_1 V_0 \approx \frac{M}{2}(v\varphi)^2 + Z_1^2 \frac{\hbar v_B \pi \omega_s}{4v},$$

where v_B is the Bohr velocity, V_0 is the CP at the turning point, Z_1 and M are the charge and mass of the projectile, ω_s is the classical surface plasma frequency, and the second term on the right-hand side is the image potential acting on the probe at the surface [16]. The latter accounts for the acceleration produced in the ion by interaction with the electron gas of the solid and it dominates when φ is small. The bound electron sees the rows of atoms in the solid as scattering centers separated by a distance d. Summing up the contributions coming from all of them one obtains the oscillatory components of the CP. The amplitude of the fundamental mode of frequency $\Delta E_1/\hbar$ is found to decay exponentially with the ion-surface distance z according to $V_1(z) \propto \exp(-az)$, where $a = (\alpha^{-2} + 4\pi^2 d^{-2})^{1/2}$. In the apex of the trajectory, where the probe is traveling much closer than d to a row of atoms, the interatomic interaction is alternatively turned on and off when the ion passes over an atom and in between two atoms. Consequently, the amplitude of the fundamental mode approximately coincides with the average potential in the apex, V_0. Moreover, if the contribution of higher harmonics is neglected, the transition rate is of the order of $w(z) \approx (e^2/m_e \hbar v_B) V_1^2(z)$. The transition yield is obtained by integration of the transition rate over the trajectory that, in the simplest model, is approximated by a straight line reflected at the turning point. In that case the total transition yield reduces to

$$\Gamma = 1 - \exp\left(-\frac{(eV_0)^2}{m_e \hbar v_B v \varphi a}\right),$$

where m_e is the electron mass. For He^+ ions incident on W with glancing angle $\varphi = 1$ mrad with respect to the ⟨100⟩ direction, one gets $1-\Gamma = 2.8\times10^{-9}$, 0.016, and 1.9×10^{-3} when the velocity is $v = 2$, 5, and 8 a.u. and the energy of the emitted electrons in the rest frame of the probe for $n=1$ is 2.8, 88.6, and 174.4 eV, respectively.

For the sake of simplicity we will consider an ion moving along the ⟨100⟩ direction of the (001) surface of a cubic crystal of lattice constant d. The energies of the emitted electrons are well above the vacuum level, so that one can use orthogonal plane waves as final states of momentum $\mathbf{k}$, $|\tilde{\mathbf{k}}\rangle$. They are orthogonal to the initial bound state $|0\rangle$, whose energy ε_0 depends upon z through the shift due to interaction with the surface, which has been calculated from the IP and the CP. Using first-order time-dependent perturbation theory the differential RCE rate for the transition energy ΔE_n is found to be

$$\frac{dw_n}{d\Omega} = \frac{a_0^5 e^2 V k}{(2\pi)^2 \hbar v_B} \times \sum_{G_y, H_y} \langle \tilde{\mathbf{k}} | v^*_{\mathbf{G},z} e^{-i\mathbf{G}\cdot\mathbf{R}} | 0 \rangle \langle 0 | v_{\mathbf{G}+\mathbf{H},z} e^{i(\mathbf{G}+\mathbf{H})\cdot\mathbf{R}} | \tilde{\mathbf{k}} \rangle e^{iH_y y}, \qquad (1)$$

where a_0 is the Bohr radius, $k = [2m_e(\varepsilon_0 + \Delta E_n)]^{1/2}$ is the momentum of the emitted electron in the rest frame of the ion, $\mathbf{G} = (2\pi n/d, G_y)$, $\mathbf{H} = (0, H_y)$, G_y and H_y are multiples of $2\pi/d$, V is the normalization volume, $d\Omega$ is the element of solid angle, and $v_{\mathbf{G},z}$ is the 2D Fourier transform of the CP acting on the electron (a similar expression is found in the bulk [5,17]).

The angular dependence of the RCE rate, calculated according to Eq. (1), is shown in Fig. 1 for 2.5-MeV He^+

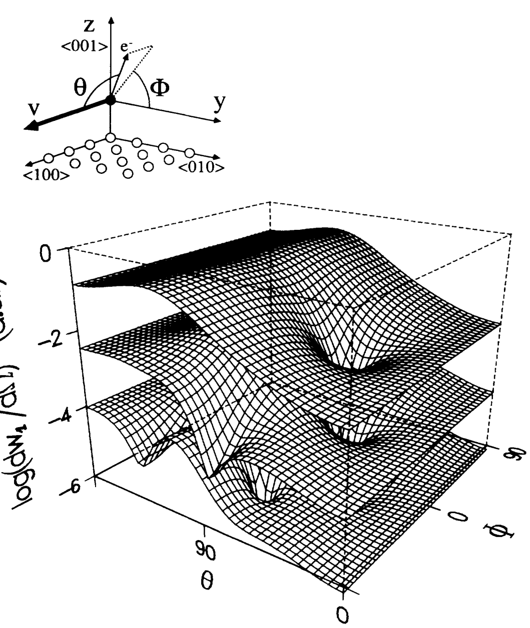

FIG. 1. Differential RCE rate (in atomic units) of 2.5-MeV He^+ ions in their ground state moving parallel to the ⟨100⟩ direction of a W(001) surface, expressed in the rest frame of the ion according to Eq. (1), for $y=0$ and $n=1$ when $z=1.5$ a.u. (upper sheet), 2.5 a.u. (intermediate sheet), and 3.5 a.u. (lower sheet), as a function of the direction of emission. The inset provides the key for understanding the angles (θ, Φ) used in the figure: θ is the polar angle with respect to the direction of motion and Φ is the azimuthal angle in the plane $(\hat{\mathbf{y}}, \hat{\mathbf{z}})$.

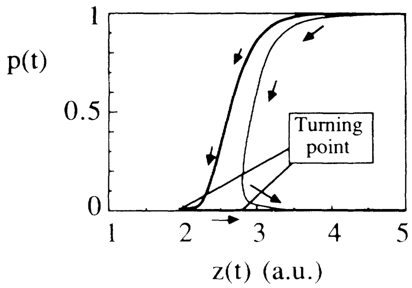

FIG. 2. Probability of having survived up to the time t against RCE of He^+ ions moving under the same conditions as in Fig. 1, with asymptotic glancing angle of incidence $\varphi=0$ mrad (thin curve) and $\varphi=1.5$ mrad (thick curve) above a row of atoms ($y=0$), as a function of the distance to the last atomic layer of the crystal, z, in the incoming (upper portion of the curves) and outgoing (lower portion) parts of the trajectory. Glancing trajectories get a z dependence due to the induced forces acting on the ion charge. Both p and the z coordinate of the ion depend on time. The arrows indicate the temporal evolution.

ions moving close to W as a function of the direction of emission (θ,Φ) in the rest frame of the particle for $n=1$, $y=0$, and $z=1.5$, 2.5, and 3.5 a.u. (see inset). The angular distribution is found to be symmetric with respect to $\Phi=0$, due to the spherical symmetry that characterizes the initial state. The preferential direction of emission is approximately given by $\theta\approx 130°$. The backward emission is 2 orders of magnitude larger than the forward emission.

The occupancy of the initial state $p(t)$ (i.e., the probability of having survived up to the time t) is obtained by integration of the equation $dp/dt=-pw$ along the trajectory. Figure 2 shows this quantity for two different angles of incidence: $\varphi=0$ and $\varphi=1.5$ mrad. The yield of emission is larger in the latter because the probe penetrates deeper inside the solid in that case, but it is almost 1 in both cases.

The differential transition yield, given by

$$\frac{d\Gamma_n}{d\Omega}=\int_{-\infty}^{\infty}dt\,p(t)\frac{dw_n}{d\Omega}\,, \tag{2}$$

is shown in Fig. 3 for $n=1$ and $n=2$ as a function of the direction of emission in the frame moving with the ion. The forward emission is almost negligible. The electrons are preferably emitted with an angle $\theta\approx 120°$ with respect to the ion velocity. In the laboratory frame this angle turns out to be $\approx 31°$ (51°) and the electron final energy is 255 eV (293 eV) for $n=1$ ($n=2$) for 2.5-MeV He^+ projectiles.

In conclusion, the resonant coherent excitation of MeV He^+ ions reflected on an oriented crystal with a glancing angle of incidence of the order of mrad has been shown to produce emission of electrons bound to the ions with well-defined energies and about a preferential direction, the yield of emission being almost 1. The initial state is

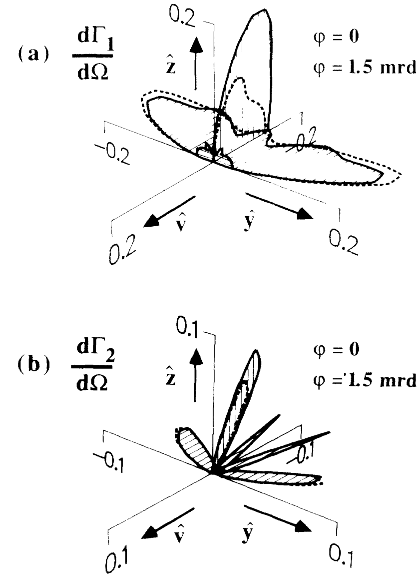

FIG. 3. (a) Angular dependence of the total yield of emission produced within the frame of the moving ion, according to Eq. (2), for the harmonic $n=1$ in the case of He^+ ions moving under the conditions stated in Fig. 1 with glancing angle of incidence $\varphi=0$ mrad (dashed curves) and 1.5 mrad (continuous curves). The distance to the origin represents $d\Gamma_1/d\Omega$ for each direction. The yield is represented in the three planes defined by the directions $(\hat{\mathbf{v}},\hat{\mathbf{y}})$, $(\hat{\mathbf{v}},\hat{\mathbf{z}})$, and $(\hat{\mathbf{y}},\hat{\mathbf{z}})$ (the vectors $\hat{\mathbf{v}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ have been included in the figure). (b) The same as (a) for $n=2$.

energy shifted by both the crystal potential and the velocity-dependent interaction with the electron gas of the solid. This offers the possibility of experimentally studying surface dynamical screening of atomic states in the vicinity of crystal surfaces.

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