Near-threshold emission of electrons during grazing scattering of keV Ne atoms from an Al(111) surface

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The number of electrons emitted during grazing scattering of Ne atoms with kilo-electron-volt energies from an Al(111) surface is recorded in coincidence with the energy loss of scattered projectiles. Irrespective of the total projectile energies used, we observe a pronounced increase of total electron emission yields when the energy for motion normal to the surface exceeds about 25 eV. Based on energy loss spectra and classical computer simulations of projectile trajectories we attribute electron emission under these scattering conditions to a promotion mechanism in binary collisions between Ne and Al target atoms resulting in single and double excitations of projectiles.

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Emission of electrons induced by impact of atomic projectiles on solid surfaces is an important issue in applications related to, e.g., surface analytical tools, particle detection, or plasma wall interactions. Aside from this feature and numerous fundamental studies on this topic, a microscopic understanding of the relevant interactions mechanisms is far from being complete. For impact of atoms and ions on metal surfaces, a basic mechanism for electron excitation and emission is considered as energy transfer in binary collisions with conduction electrons.[1,2] In more detail, the emission of electrons results from a complex interplay of primary excitation, electron transport, and crossing of the vacuum-solid interface.[3] At small incidence angles with respect to the surface plane (surface channeling, i.e., steering of projectiles by atoms of the topmost crystal layer and no penetration into the bulk) we could recently show for H and He atoms that electron emission near the respective kinetic threshold is fairly well described in terms of a binary encounter model taking into account the phase space of a free electron gas.[4] For larger grazing angles of incidence and heavier noble gas atoms, electron promotion in binary collisions of atomic projectiles with target atoms was identified as relevant electron emission mechanism.[5–9].

Recently, Lörinčík and Šroubek[10] explained electron emission for collision of slow Ne atoms and ions impinging on a Au surface in terms of a nonadiabatic perturbation of the Fermi gas due to the rapid passage of projectiles through the surface. Their conclusion was based on molecular orbital correlation diagrams for Ne-Au which indicate that electron promotion is negligible for impact energies below about 3 keV. Motivated by this interesting subject, we have investigated the mechanisms of electron emission for collisions of atoms with a surface under a grazing angle of incidence. In this regime of surface scattering, projectiles are reflected in a sequence of small-angle scattering from the topmost layer of the surface with defined trajectories.[11,12] A key feature of our experimental method is based on the coincident detection of the energy loss of scattered projectiles with a specific number of emitted electrons per particle impact. This allows us to relate the total inelastic processes during the scattering event with the surface to a specific number of emitted electrons.[13] This type of translation energy spectroscopy was successfully used to reveal the relevant electronic excitation and emission processes for atom impact on surfaces of ionic crystals.[14,15]

In the experiments, Ne atoms specularly scattered from an Al(111) surface are recorded by means of a multichannelplate detector which provides the start signal for our time-of-flight (TOF) setup.[13,16] The electrons are detected by means of a surface barrier detector biased to a high voltage of 25 kV where the pulse heights are proportional to the number of emitted electrons. The experiments are performed under ultra-high vacuum conditions in the lower 10^{-11} mbar regime with a carefully prepared clean and flat Al(111) target. Details concerning our setup and experimental procedures are given elsewhere.[16] In passing we note that use of neutral projectiles eliminates contributions of potential electron emission.

In Fig. 1 we show total electron yields γ as function of projectile energy for Ne atoms scattered from an Al(111) surface under grazing angles of incidence ϕ_{in} ranging from 1.3° to 5.5°. We reveal a pronounced enhancement of γ with increasing angle combined with a shift toward smaller projectile energies. Note that in the plot of the data energies for

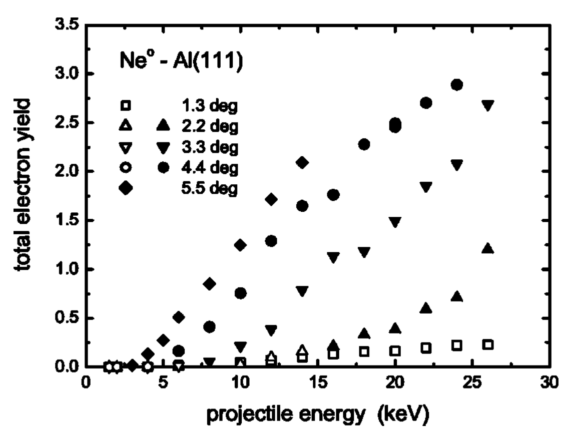

FIG. 1. Total electron yields as a function of projectile energy for scattering of Ne atoms from Al(111) under different angles of incidence Φ_{in}. Full symbols denote data for $E_z > 25$ eV.

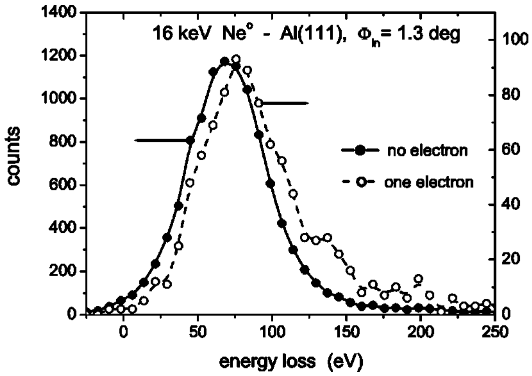

FIG. 2. TOF spectra converted to energy loss scale for scattering of 16 keV Ne atoms from Al(111) under $\phi_{in}=1.3°$. Full circles: emission of no electron (left scale), open circles: emission of one electron (right scale).

the motion normal to the surface plane E_z larger than 25 eV are represented by full symbols. Since our experiments are performed in the regime of surface channeling, E_z determines the distance of closest approach to the surface plane during the complete scattering event ("critical energy" amounts to about $E_z=220$ eV here[11]). We reveal a relatively efficient emission of electrons for normal energies exceeding about 25 eV, whereas for scattering under smaller angles and smaller E_z noticeable electron yields are only detected at higher projectile energies.

The different behavior for impact under smaller and larger E_z can be attributed to different electron emission mechanisms as concluded from TOF spectra for respective angles of incidence. Figure 2 shows TOF spectra for 16 keV Ne atoms scattered under $\phi_{in}=1.3°$, Fig. 3 spectra for 5 keV Ne atoms scattered under $\phi_{in}=5.5°$. The spectra are recorded in coincidence with the emission of no electron (full circles), one electron (open circles), and two electrons (full triangles in Fig. 3). For small angles (Fig. 2) we observe a small shift between the two spectra of about 10 eV with the shape of spectra being unchanged. This slight shift is consistent with a model of electron excitation in head-on binary encounters

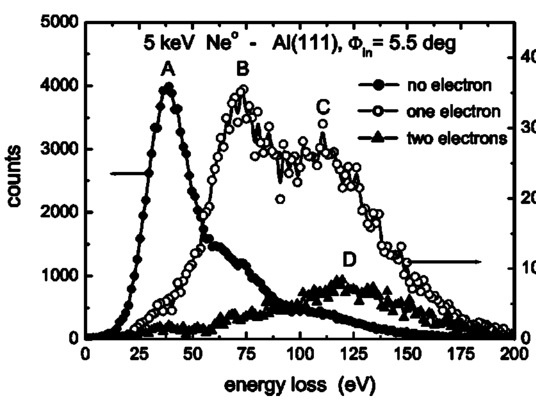

FIG. 3. TOF spectra converted to energy loss scale for scattering of 5 keV Ne atoms from Al(111) under $\phi_{in}=5.5°$. Full circles: emission of no electron (left scale), open circles: emission of one electron (right scale), full triangles: emission of two electrons (right scale).

between atomic projectile and valence electrons in the selvage of the surface.[4] The full width at half maximum of the energy distribution of the incident 16 keV He° beam amounts to 20 eV. This distribution causes small finite signals at zero and negative energy loss.

For larger angles (cf. Fig. 3) the spectra are clearly different. A striking feature of the data is a substantial shift in energy of the peaked structures in the spectrum related to the emission of one electron. Two broad peaks can be identified showing energy shifts with respect to the zero-electron spectrum of about 35 eV (peak "B") and about 75 eV (peak "C"). Such structures cannot be explained by excitations in binary encounters with valence electrons, since the maximum energy transfer to valence electrons amounts to 5.4 eV only as calculated with a Fermi momentum k_F derived for bulk electron densities of Al. From literature on this subject we identify these features as electronic excitations of Ne projectiles in binary collisions with individual Al atoms of the topmost surface layer.[17] These excitations proceed in terms of electron promotion of transient molecular orbitals (MO) formed during the collisions.[5,10,18,19] For sufficiently small impact parameters, electron promotion leads to excitation and ionization of Ne atoms in collisions with atoms in the gas phase or at a solid surface. Xu *et al.*[17] reported for collisions of Ne^+ with a polycrystalline Al surface a threshold energy of about 230 eV at $\phi_{in}=20°$; this compares well with the transverse energy of about 25 eV observed here (cf. Fig. 1).

The TOF spectrum coincident with the emission of two electrons has a clearly smaller intensity and shows a maximum (peak "D") close to peak "C" of the one electron spectrum. The tail at low energy losses is assumed to stem primarily from spurious electrons produced at slits, etc., of our setup.

For a more detailed interpretation of data one has to take into account that sufficiently small impact parameters are needed for electron promotion. For the present system we estimate from MO correlation diagrams for Ne-Al (Ref. 10) impact parameters of about 1 to 1.2 a.u., i.e., distances which can only be achieved for surface channeling of kiloelectron-volt atoms for incidence angles of several degrees. This feature has important consequences on the projectile energy loss. Peak "B" showing a lower energy loss in the one-electron spectrum in Fig. 3 is identified with the ionization of the projectile. This loss is, however, clearly higher than the ionization potential of 20.6 eV for Ne atoms. Based on computer simulations of classical trajectories for the present collision system we attribute the enhanced energy loss in the experimental data to a specific energy transfer to lattice atoms at sufficiently small impact parameters needed for electron promotion.

Figure 4 displays a calculated spectrum for the energy transfer of 5 keV Ne scattered from Al(111) under $\Phi_{in}=5.5°$. In our computer simulations trajectories of 100 000 atoms are calculated in terms of classical mechanics using pair potentials with Ziegler, Biersack, and Littmark screening[20] and taking into account thermal vibrations of lattice atoms in the Debye model.[21] The distribution for distances of closest approach to specific Al target atoms r_{min} and the resulting energy transfer is plotted in the upper part of the figure. Impact parameters amount from about 0.9 a.u. to

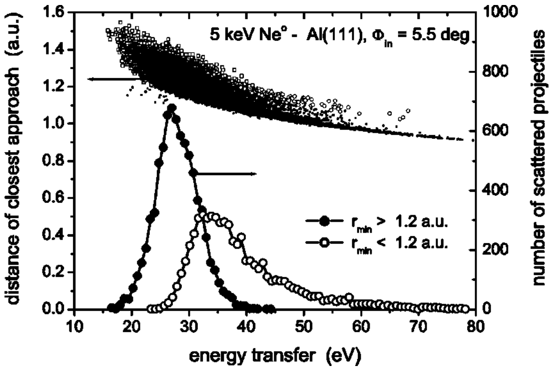

FIG. 4. Computer simulations on elastic energy transfer to Al lattice atoms for specular scattering of 5 keV Ne atoms from Al(111) under $\Phi_{in}=5.5°$. Full circles: distance of closest approach to specific Al atoms $r_{min} \geqslant 1.2$ a.u., open circles: $r_{min} < 1.2$ a.u..

about 1.5 a.u. From this distribution we generate (elastic) energy loss spectra for impact parameters smaller and larger than 1.2 a.u. which is estimated as the threshold for electron promotion of the $4f\sigma$ level to vacuum energies in the MO model. A striking feature of the two spectra is a shift in energy transfer by typically 10 eV. Thus the observed energy loss in the spectrum shown in Fig. 3 can be explained by ionization of the projectile and an enhanced energy transfer to Al lattice atoms in collision with impact parameters needed for MO promotion. These impact parameters are clearly smaller than those for scattering of projectiles without ionization (and electron emission) (cf. spectrum in Fig. 3 for emission of no electrons).

The simulations also reveal that most of the measured projectile energy loss at 5 keV related to no excitations of projectiles (peak "A") stems from elastic collisions with surface atoms. Contributions from excitations of conduction electrons of the metal are clearly smaller in this case.

The second broad feature in the spectrum related to emission of one electron (peak "C") is ascribed to double electron promotion resulting in the formation of doubly excited $2p^4\,nln'l'$ Ne** levels (excitation energies larger than about 45 eV)[5,6] and in double ionization of Ne atoms ($2p^4$ Ne^{++}) (excitation energies larger than about 63 eV). The doubly excited terms have been shown to decay via autoionization under emission of an electron.[9] Since the lifetimes of these terms are sufficiently long with respect to typical interaction times with the surface, autoionization takes place on the outgoing trajectory where a fraction of ions can survive a subsequent reneutralization.[2,5] We have studied also the charge fractions of the scattered beams and observed enhanced ion fractions for projectiles showing an energy loss attributed to this mechanism.

An interesting aspect of our study is the possibility to derive estimates on the relative contributions of the relevant excitation mechanisms by comparing intensities in the TOF spectra for emission of a specific number of electrons. From the spectra related to the emission of no, one, and two electrons we deduce from the integral intensities in Fig. 3 the probabilities for the emission of n electrons W_n and obtain a total electron emission yield

$$\gamma = \sum_{n=0}^{\infty} W_n \times n \Bigg/ \sum_{n=0}^{\infty} W_n \approx 0.2. \qquad (1)$$

We note that the method of coincident combination of TOF and electron number spectra provides also information on events related to no emission of electrons[16] so that reliable small total electron yields can be measured. As can be judged from the peaks "B," "C," and "D" in the one- and two-electron spectra in Fig. 3, the yield here results in comparable parts from single excitation with ionization and from double excitation with autoionization and double ionization.

Relating the intensities of peak "A" representing the elastic events to the rest of all spectra gives the overall fraction of electronic excitations which amounts to 50% here. Comparison of the intensities of the foot structure of peak "A" (electronic excitations related to the emission of no electron) with the peaks in the one- and two-electron spectra shows that 35% of the excitations are accompanied with emission of electrons. This analysis demonstrates the possibility of gaining specific insights concerning the interaction scenario. In view of the complexity of the relevant processes a detailed interpretation of the data is beyond the scope of the present paper.

In conclusion, we have performed studies on electron emission during grazing scattering of fast Ne atoms from an Al(111) surface. The coincident detection of energy loss of scattered projectiles via a TOF method with the number of emitted electrons provides detailed information on the electronic interaction mechanisms. We observed a transition of electron emission from binary encounter excitation at small angles of incidence to a promotion mechanism for impact under larger angles. Our work is in accord with previous studies on this subject showing the relevance of electron promotion for electronic excitations and electron emission during atom/ion impact on metal surfaces. Furthermore, we have demonstrated the considerable potential of our technique with respect to a detailed analysis of the relevant electronic excitation and interaction mechanisms.

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