Auger electron emission from metals induced by low energy ion bombardment: Effect of the band structure and Fermi edge singularity

A. Sindona a,b,*, S.A. Rudi a,b, S. Maletta a, R.A. Baragiola c, G. Falcone a,b, P. Riccardi a,b,c

a Dipartimento di Fisica, Università della Calabria, Via P. Bucci 31C, 87036 Rende (CS), Italy
b Istituto Nazionale di Fisica Nucleare (INFN), Gruppo Collegato di Cosenza, Via P. Bucci 31C, 87036 Rende (CS), Italy
c Laboratory for Atomic and Surface Physics, University of Virginia, Engineering Physics, Charlottesville, VA 22901, USA

Received 16 September 2006; accepted for publication 11 December 2006
Available online 19 December 2006

Abstract

Calculations of the kinetic energy distributions of electrons ejected from plane metal surfaces by Auger neutralization of slow monoatomic ions are reported. A many body theory is used that includes both the band structure of the target material and the Fermi singular response of metal electrons (to the sudden neutralization of the projectile). Application is made to experiments of electron emission from polycrystalline Al by Ar+-ions, at varying incident energies and angles. Adjustment of the broadening parameters of the distribution of shake-up electrons leads to excellent agreement between the theory and the measurements.

© 2006 Elsevier B.V. All rights reserved.

Keywords: Ion beam impact and interactions with surfaces; Electron emission and Auger neutralization; Charge transfer; Theories and models of many-electron systems

1. Introduction

Ion induced electron emission from solids is a fundamental phenomenon based on the following three steps: excitation of the electron, its transport to the surface, and its escape through the surface barrier [1–3]. The energy required to eject an electron originates from the conversion of kinetic or potential energy of the incident ion in two different mechanisms, known as kinetic electron emission (KEE) and potential electron emission (PEE).

KEE contributes to the electron yield to an increasing extent with increasing impact velocities. While most of the target electrons are emitted by fast projectiles in direct binary collisions, other processes concur to KEE at lower impact velocities. This is confirmed by recent studies observing KEE below the classical threshold for transferring enough kinetic energy in a single binary collision with the ion to eject a valence electron of the target [4–6].

PEE clearly dominates for low impact velocities [7] and is generally understood as the result of two-electron Auger type processes, i.e., Auger neutralization (AN) and resonant neutralization (RN) followed by inter-atomic Auger de-excitation (AD). In particular, projectiles with large ionization energies mostly neutralize via AN, where the screened repulsion between two target electrons leads to one of the electrons tunnelling to neutralize the incoming ion and the other being excited [8,9].

Simple metals, as Aluminum or Magnesium, can also convert a part or the whole of the potential energy, released by projectile neutralization, into many body excitations. One of these is the excitation of a surface plasmon whose decay mostly occurs by energy transfer to a single valence electron (plasmon-assisted neutralization [11–13]).
process requires the neutralization energy to exceed the plasmon energy, thus, slow He$^+$ and Ne$^+$ projectiles can excite the surface plasmon of Al and Mg, while Ar$^+$ ions cannot. Another form of collective response of the metal target is the singular behavior of electrons at the Fermi level, due to the abrupt change of charge of the projectile, which causes permanent deformations in the conduction band [14,15]. Such a final-state effect parallels the sudden creation of a core hole, by absorption of a soft X-ray photon, as described by the Mahan–Nozieres–De dominicis (MND) theory [16]. So called shake-up electrons originate both from the electronic structure of the conduction band and the Pauli principle. Their signature, observed in experiments of Ar$^+$ impact on Al surfaces [14,15], is the exponential tailing of the kinetic energy distributions of ejected electrons. Indeed, since the seminal work of Hagstrum [1,8], the study of the broadening of the Auger peaks, with the projectile velocity, has been used to identify or propose new processes occurring in AN [9–15].

Another issue of PEE from metal targets is related to the low impact velocities of the projectile: neutralization occurs outside the solid, before the ion can penetrate, thus, electron excitations are confined just to the surface region, making the process sensitive to the surface band structure. This is confirmed by recent studies exploring the dynamics slow ion neutralization from metals with a projected band gap [10,17]. In particular, experiments on Al(100) and Ag(1 1 1) surfaces have measured significant differences in both resonant and Auger transfer rates [10,18].

For this reason, we present a theory of ion-induced shake-up in metal surfaces with a projected band gap specifically examining the Ar$^+$/Al(1 1 1) system at varying projectile perpendicular velocity [14,15], $k_F$ labels the Fermi wave vector, and

$$V^a_{kk'}(t) = \left\{ \begin{array}{ll} V^a_{kk'}(t), & \text{if } |\epsilon_k - \epsilon_{k'}| \leq \epsilon_0(v_L), \\ 0, & \text{otherwise} \end{array} \right.$$  

where $\epsilon_0(v_L)$ is a cut-off parameter, that depends on the projectile perpendicular velocity [14,15], $k_F$ labels the Fermi wave vector, and

$$V^a_{kk'}(t) = \int \frac{d^2\Omega_k}{4\pi} \int \frac{d^2\Omega_{k'}}{4\pi} \langle k_F|\Omega_k|v^a_{FE}(r,t)|\Omega_{k'}\rangle \langle \Omega_{k'}|v^a_{EE}(r,t)|\Omega_k\rangle$$  

denotes the average coupling of two metal states at the Fermi surface.

We focus on the calculation of $N(E,v)$, the distribution of electrons ejected from the target with a kinetic energy $E$, following AN of the projectile with impact velocity $v = (v_L, v_\perp)$. To do this, we need the distribution of electrons excited by the ion to the state $|k\rangle$, here denoted by $N_k(k,v)$, and the probability $P(E, \Omega_k)$, that an excited electron with kinetic energy $E$ and wavevector $k$ – of solid angle $\Omega_k$ – escapes the metal barrier.

$N_k(k,v)$ is proportional to the differential cross-section for a transition from the unperturbed ground state of the conduction band, with the ion state empty, to all possible excited states, with the ion state occupied. As reported in Ref. [15], this can be written as the convolution integral

$$N_k(k,v) = \int_{-\infty}^{\infty} d\epsilon N_0^k(\epsilon - \epsilon, k,v) B(\epsilon, v_\perp)$$  

of a pure spectrum, $N_0^k(\epsilon, k,v)$, and a broadening function, $B(\epsilon, v_\perp)$. The pure spectrum is the number of excited electrons, per unit time, by a projectile with constant ionization energy $\epsilon_0^k = \epsilon_0(Z_0)$, in the Fermi golden rule approximation:
\[
N^0_1(\mathbf{q}, \mathbf{k}, \mathbf{v}) = N_0 \rho(\mathbf{q}) \sum_{\mathbf{k} \neq \mathbf{k}'} \int_{-\infty}^{\infty} dt |\mathbf{V}_{\mathbf{kk}'}(t)|^2 \times e^{i(\mathbf{k} + \mathbf{q} - \mathbf{k} - \mathbf{v}) \cdot \mathbf{r}}. \tag{6}
\]

In this relationship, \(\rho(\mathbf{q})\) labels the density of states available to excited electrons, \(\mathbf{q} = \mathbf{k} - \mathbf{k}' - \mathbf{k}''\) is the transferred wavevector in a single excitation process, and \(e^{-\mathbf{q} \cdot \mathbf{v}}\) accounts for the shift of the Fermi surface in the rest frame moving with the parallel velocity of the projectile. The broadening function
\[
B(\mathbf{q}, \mathbf{k}, \mathbf{v}) = \sum_{\mathbf{k}, \mathbf{k}'} \int_{-\infty}^{\infty} dt |\mathbf{V}_{\mathbf{kk}'}(t)|^2 \times e^{-|\mathbf{v}|^2 t^2/2} P_a(t, \mathbf{v}, \mathbf{k}) e^{i(\mathbf{q} \cdot \mathbf{z}(t) - \mathbf{v} \cdot \mathbf{r})} \tag{7}
\]
mainly describes many body effects that are outside the Fermi golden rule; it is shifted by the variation of the ion energy, with the change of the projectile-target distance, and contains the main broadening components identified by Hagstrum [1,8] plus the effect of many body shake-up [10,15]. In particular,
\[
P_a(t, \mathbf{v}, \mathbf{k}) = e^{-\int_{-\infty}^{\infty} d\mathbf{r} |\mathbf{v}|^2} \tag{8}
\]
defines the ion-survival probability due to both AN and RN. \(r_a(t) = |w_0(t) + 2\Delta_a(t)|\) is the total neutralization rate, including both the transition rate for Auger processes [1,8,9]
\[
w_0(t) = 2\pi \sum_{\mathbf{k}, \mathbf{k}'} |\mathbf{V}_{\mathbf{kk}'}(t)|^2 \delta[e_a(t) + \mathbf{k} - \mathbf{k}'] \tag{9}
\]
and the virtual width of the atomic level due to resonant tunnelling [20]
\[
\Delta_a(t) = \pi \sum_{\mathbf{k}} |\mathbf{V}_{\mathbf{kk}}(t)|^2 \delta[e_a(t) - \mathbf{k}]; \tag{10}
\]
e\(-\mathbf{v} \cdot \mathbf{r} / t\) is lifetime correction of the final state, with \(\Gamma_0\) the lifetime width of the band holes created by AN; \(e^{-\mathbf{q} \cdot \mathbf{v} / 2t}\) accounts for the many atom response to thermal interactions with the environment, which gives rise to electron-phonon coupling [23] of (Gaussian) broadening \(\sigma_{\text{PH}}\); finally,
\[
F_a(\mathbf{v}, \mathbf{k}, t) = \left[1 + i e_0(\mathbf{v}) \frac{t}{\mathbf{v} \cdot \mathbf{k}}\right] e^{-2} \tag{11}
\]
is a measure of non orthogonality between the initial and the final states of electrons in the metal that do not participate to AN. Its Fourier transform
\[
\mathcal{F}_a(\mathbf{v}, \mathbf{k}, \mathbf{v}) = \frac{\Theta(\mathbf{v})}{\Gamma(\mathbf{v} \cdot \mathbf{k})} \left( \frac{e}{e_0(\mathbf{v})} \right) \frac{2\pi}{\hbar} \tag{12}
\]
with \(\Theta(\mathbf{v})\) the step function and \(\Gamma(\mathbf{v} \cdot \mathbf{k})\) the Euler Gamma function, defines the distribution of shake-up electrons. Eqs. (11) and (12) depend on two parameters: \(e_0(\mathbf{v})\) is the width of the distribution, corresponding to the energy range where the sudden perturbation, activated by projectile neutralization, is non vanishing; \(\mathcal{A}(\mathbf{v} \cdot \mathbf{k})\) is a singularity index that, in the MND formulation, depends on the phase-shifts of the (static) core-hole potential, activated by the X-ray field, at the Fermi surface of the target [16]. In the present context, dealing with a time-dependent potential (3), we need the Fourier transform of the instantaneous phase shift \(\Phi(\mathbf{v} \cdot \mathbf{k}, t)\) of the average coefficient \(V_{\mathbf{kk}}(t)\) [27]. Then, we may define \(s(\mathbf{v}) = |\Phi(\mathbf{v} \cdot \mathbf{k}, t)|^2 / \pi^2\).

Eqs. (6) and (7) turn the calculation of \(N_1\) into a formidable problem that depends either on the choice of a basis for the ion/metal system or on the model used to simulate the screened electron–electron interaction.

In the simplest approximation, the AN matrix elements (2) are modelled by the exponential function \(V_{\mathbf{kk}}(t) = V_o e^{-\lambda_v \mathbf{r} \cdot \mathbf{v} / 2}\), independent on electron wavevectors, in which \(\lambda_v\) is the average decay rate of metal wavefunctions outside the solid, and the effect of the projectile parallel velocity is neglected. This gives rise to Hagstrum’s self-convolution model [1], where \(N^0_1(\mathbf{q}, \mathbf{k}, \mathbf{v})\) results from the convolution of a pure, unbrodened spectrum, and broadening function with a dominant Lorenzian trend.

In Refs. [14,15], the matrix elements (2) were evaluated using a basis of jellium states, for the metal surface, and a valence orbital for the ion, obtained from pseudopotential theory. Specifically, the (semi-infinite) Jenning’s potential [24] was used for \(v_s(\mathbf{r})\), while \(v_A(\mathbf{r})\) was given the form [25]
\[
v_A(\mathbf{r}) = \frac{1}{r} \left[ \frac{Q_i}{H(e^{-r/d} + 1)} + 1 \right], \tag{13}
\]
in which \(Q_i\) is the ion charge and \(H,d\) two adjustable parameters. It was further assumed a Yukawa potential,
\[
v_{\text{SC}}(|\mathbf{r} - \mathbf{r}'|) = e^{-\mu |\mathbf{r} - \mathbf{r}'|} / |\mathbf{r} - \mathbf{r}'|, \tag{14}
\]
with inverse screening length \(\mu\), for the electron–electron repulsion.

In the present derivation, we keep the interactions (13) and (14), while we use the semi-empirical Chulkov’s potential [19]
\[
v_s(\mathbf{r}) = A_{10} + A_1 \cos \left( \frac{2\pi}{d_s} \mathbf{r} \right), \quad z < 0
\]
\[
= A_{20} + A_2 \cos(\beta z), \quad 0 \leq z < z_1
\]
\[
= A_1 e^{-\alpha(z-z_1)}, \quad z_1 \leq z < z_{\text{IM}}
\]
\[
= e^{-\beta(z-z_{\text{IM}})} - 1, \quad z > z_{\text{IM}}, \tag{15}
\]
constructed from pseudopotential local density theory, for calculating the electron wavefunctions of the target material. Eq. (15) is completely determined by fixing \(A_{10} = -\zeta_1, A_1, A_2, \beta\) and constraining continuity and differentiability everywhere in the space; it describes plane surfaces of defined symmetry, \(d_s\) denoting the atomic plane separation and \(z_{\text{IM}}\) the position of the image plane.

Concerning the transmission of excited electrons through the surface, several models have been used for \(P(E, \mathbf{q}, \mathbf{k})\), mainly based on classical considerations [1,2].
In this approach, we refer to the quantum-mechanical derivation of Ref. [26] yielding
\[ P(E, \Omega_k) = \frac{p_k}{k_z} |T(k_z, p_z)|^2, \] (16)
which depends on the surface perpendicular wavevectors of the electron far inside, \( k = \sqrt{2(E + \xi)} \), and far outside, \( p = \sqrt{2E} \), the metal and on the transmission coefficient, \( T(k_z, p_z) \), of the metal wavefunctions \( \langle r|k \rangle \) at the image plane.

From the knowledge of \( N_1(k, v) \) and \( P(E, \Omega_k) \), we may write the kinetic energy distribution of ejected electrons as
\[ N(E, v) = \int d^2\Omega_k P(E, \Omega_k) N_1(k, v). \] (17)
In Refs. [14,15], the angular dependence of the electron escape probability was neglected. Then, \( N(E, v) \) was computed by the formula \( N(E, v) \approx T(E) N_1(E, v) \) in which
\[ N_1(E, v) = \int d^2\Omega_k N_1(E, \Omega_k, v) \] (18)
is the distribution of electrons excited to a state of kinetic energy \( E \) and \( T(E) = E/(E + \xi) \) the surface transmission function.

3. Application

We consider measurements of electron emission from polycrystalline Al surfaces, by impact of Ar\(^+\) ions at different kinetic energies and incident angles, that have been reported in Refs. [12,14,15]. Fig. 1a shows a schematic of the electron processes in the Ar\(^+\)/Al(111) system, together with the external potential (1) and its components. Energies are measured with respect to the vacuum level so that \( E = \varepsilon_k \).

The target material is specified by the surface barrier (15) with the parameters of Al(111) [19], i.e., \( A_{10} = -15.70 \) eV, \( A_1 = 0.30 \) eV, \( A_2 = 1.95 \) eV and \( \beta = 5.73 \) au. Correspondingly, the image plane takes the value \( z_{IM} = 3.49 \) au and the surface work function is \( \phi = 4.24 \) eV, in agreement with work function measurements on the polycrystalline target. This means that the (111) symmetry is possessed by the majority of grains in the sample that we approximate to a plane (111) surface. The band spectrum has a narrow projected band gap in the range \( \varepsilon_1 < \varepsilon_k < \varepsilon_2 \), with \( \varepsilon_1 = -8.89 \) eV and \( \varepsilon_2 = -8.64 \) eV. The corresponding wavefunctions read
\[ \langle r|k \rangle = \psi_{k_z}(z) e^{ik_z z}, \] (19)
in which \( L \) is the thickness of the solid, \( k = (k_{||}, k_z) \) the electron wavevectors, and \( \psi_{k_z} \) the numerical eigenfunction of the potential (15). \( L \) is fixed to \( \sim 10^3 \) Å in order to have a maximum energy spacing between two band states – at \( k_{||} = 0 \) – smaller than \( \sim 0.05 \) eV. In this way, \( \sim 500 \) perpendicular wavevectors are used to reproduce the continuum spectrum up to \( \varepsilon_k = 10 \) eV. Fig. 1b shows \( p_{k_z}(z) = |\psi_{k_z}(z)|^2 \), the spatial probability density for a metal wavefunction at the Fermi surface with \( k_{||} = 0 \), while, in Fig. 1c, we display \( p_{k_{||}}(z) = |\psi_{k_{||}}(z)|^2 \) for a metal wavefunction of the continuum spectrum above the vacuum level (with \( k_{||} = 0 \) and \( \varepsilon_k = 5 \) eV). These are compared to the corresponding quantities, \( p_{k_z}^0(z) \) and \( p_{k_z}^0(z) \), calculated for the jellium potential of Ref. [24]. We observe that the two basis are significantly different at atomic distances from the surface, thus, such a change affects the calculation of \( N_1(k, v) \). Nevertheless, unlike the Ag(100) and Ag(111) surfaces, the use of jellium wavefunctions in Al(111) is still a reasonable approximation because of the narrow band gap in the conduction band.
The projectile has the valence orbital
\[ \langle \mathbf{r} | a(\mathbf{R}) \rangle = f_a(\mathbf{r} - \mathbf{R}), \]
where \( f_a(\mathbf{r}) \) is calculated from the potential (13) with the parameters of the valence 3p state of Ar, i.e., \( Q_1 = 18 \) au, \( H = 2.18 \) au and \( d = 0.74 \) au, corresponding to the unperturbed asymptotic energy \( e_a(\infty) = -15.76 \) eV. The atomic state is, then, orthogonalized to metal states with the Graam–Schmidt method, yielding the wavefunction \( \psi(\mathbf{r}) \). In Fig. 1b, we also show the spatial probability densities \( \rho^{\text{OR}}(z, \mathbf{R}) \) and \( p_a(z, \mathbf{R}) \), associated with the orthogonalized ion wavefunction \( f_a^\text{OR}(\mathbf{r}, \mathbf{R}) \) and the valence ion wavefunction \( f_a(\mathbf{r}, \mathbf{R}) \), respectively. It turns out that the effect of orthogonalization, i.e., the oscillations of \( p_a(\mathbf{R}) \) within the solid, is non negligible only at small \( Z \), below \( \sim 5 \) au, whereas \( f_a(\mathbf{r} - \mathbf{R}) \) is approximately orthogonal to the metal wavefunctions at \( Z \gtrsim 8\)–10 au.

Then, using the inverse screening length \( \mu = 0.1k_F \) and the turning distance \( Z_0 \approx 8 \) au [15], the Auger terms (2) can be estimated by the numerical integral
\[ V^{\text{ex}}_{\mathbf{k} \mathbf{k}'}(t) \approx \frac{e^{\mathbf{q}_i \cdot \mathbf{r}_f(t)}}{L} \int d^2r f_a(z - \mathbf{R}(t)) \psi_{\mathbf{k}'}(z) \]
\[ \times \int d^2z' \frac{e^{-i|z'|\sqrt{q_i^2 + 2}}}{2\sqrt{q_i^2 + 2}} \psi_{\mathbf{k}'}(z' + z') \psi_{\mathbf{k}'}(z + z') \]
(21)
in which \( \mathbf{q}_i \) is the parallel wavevector, exchanged in a single excitation process (see also Eq. (6)), and
\[ \tilde{f}_a(z) = \int d^2r f_a(z) \]
(22)
the 2-dimensional Fourier transform of the atomic wavefunction. \( N_{\mathbf{k}'}^{\text{OR}}(\mathbf{k}, \mathbf{v}) \) is finally calculated by Monte–Carlo integration over \( \mathbf{k}' \) and \( \mathbf{k}'' \).

We introduce the distribution of electrons excited to a state of energy \( e_k \) in the Fermi golden rule approximation:
\[ N_{\mathbf{k}}^{\text{OR}}(\mathbf{k}, \mathbf{v}) = \int d^2\Omega_k N_{\mathbf{k}}^{\text{OR}}(\mathbf{k}, \mathbf{v}) \]
(23)
allows to visualize the broadening due to the long-time exponential decay of \( V^{\text{ex}}_{\mathbf{k} \mathbf{k}'}(t) \) by comparison with the pure spectrum, analytically derived from Hagstrum’s self-convolution model. The two curves, labelled I and III, are reported in Fig. 2a, where we also display \( N_{\mathbf{k}}^{\text{OR}}(\mathbf{k}, \mathbf{v}) \) obtained with a jellium description of Al [15] and referred as curve II. We see that the distribution II has a larger broadening to higher energy than the distribution I, because of the different behavior of metal wavefunctions, within the surface region, in the corresponding models (see Fig. 1b–c). This reflects in the calculation of the energy shift and the ion survival probability, which affects the shape of the broadening functions (7) as reported in Fig. 2b.

Accordingly, non negligible differences are detected in the tails of the distributions of ejected electrons, calculated form Eq. (17) by a fast Fourier transform algorithm, for the models yielding the spectra I–III of Fig. 2a. Fig. 3 shows the theoretical distributions \( \mathcal{N}(E, \mathbf{v}) \) in comparison with the distributions acquired from Al by 130–430 eV Ar\(^+\) ions [14,15]. In models I and II, the parameters of the broadening function of shake-up electrons–Eqs. (11) and (3)–were adjusted to the experiments. All other parameters were fixed, since for \( \sigma_{\text{ph}} \) we used the same value of X-ray studies on Al at room temperature, i.e., \( \sigma_{\text{ph}} \approx 0.1 \) eV [23], while \( I_0 \) was set to 0.01 eV, in agreement with previous estimations [1,8,14,15]. As for the self-convolution model (III), we used the analytical expressions
\[ e_{\text{a}}(z(t)) = e_{\text{a}}(\infty) - \frac{\delta e_{\text{a}}}{Z(t) + z_{\text{a}}} \]
(24)
for the energy shift, and
\[ r_{\text{a}}(t) = r_{\text{a}}^0 e^{\theta(t)} \Theta(-t) + r_{\text{a}}^0 (2 - e^{-\theta(t)}) \Theta(t) \]
(25)
for the total rate entering the ion survival probability (8). The parameters \( \delta e_{\text{a}}, z_{\text{a}}, r_{\text{a}}^0 \) and \( v_{\text{a}}^0 \) were adjusted to fit the corresponding numerical expressions, calculated from model I. Finally, \( z_{\text{a}} = 2 \) au was also obtained by fitting to experiments.
It is not surprising that model III is also in excellent agreement with data since the number of fitting parameters is increased, with respect to model I and II. Furthermore, the projectile parallel velocities take values in the range \( v_k = 0.01 - 0.02 \) au, while the Fermi velocity of Al(111) is \( v_F = 0.91 \) au. This means that the shift of the Fermi surface with \( v_k \) is small. In either model, the optimized values for \( a \) and \( e_0 \) increase with increasing the projectile perpendicular velocity, which clearly manifests the non-negligible effect of shake-up electrons in AN.

As a further evidence, we report in Fig. 4 the theoretical distributions calculated for an incidence energy of 1 keV, and incidence angles in the range 0–70°, in comparison with the experiments of Ref. [12]. The latter show a low energy peak due to kinetic electron emission, that is empirically fitted out with a Gaussian function. The effect of the parallel component of the impact velocity is still of second-order, since \( v_k \) takes values in the range 0–0.03 au. Even if the results are more qualitative, owing to the absence of a reliable model to reproduce the raising front of the signals, we continue to observe an increase of the parameters of \( F_a(\tau, v_\perp) \). More importantly, the tail of the distributions clearly show a non-Lorenzian behavior with a superimposed Gaussian trend due to the decreased resolution of the analyzer.

The behavior of the best fitted values of \( a \) and \( e_0 \) vs \( v_\perp \) is reported in Fig. 5, for all the experimental distributions of Refs. [12,14,15]. The singularity index takes values in the range \(-0.1 \sim 0.3\), typical of X-ray studies on metal samples [23], and increases with increasing \( v_\perp \). In fact, owing to the small perturbation, the instantaneous phase-shift of the contact potential can be approximated to \( \Phi(v_\perp, \epsilon) \), which decreases exponentially, in the long time limit, with a rate proportional to \( v_\perp \). It follows that \( \Phi(v_\perp, \epsilon) \) depends on \( \epsilon \) with a nearly Lorentzian structure. Its broadening increases with increasing \( v_\perp \), together with \( \Phi(v_\perp, \epsilon_F) \). The other parameter, \( e_0(v_\perp) \), enters the exponential part of \( F_a(v_\perp, \epsilon) \). Its increase, with increasing \( v_\perp \), is clearly observed in the increase of the exponential tailing of the experimental kinetic energy distributions. We believe that this is a consequence of the increase of the efficiency of the singular
response of the metal band to the sudden neutralization, as attested by the increase of the neutralization rates.

4. Conclusions

We have reported on the kinetic energy distributions of electrons ejected from plane metal surfaces, of well defined Miller indices, by low energy ion impact. Comparison to experiments on the Ar+/Al system, has confirmed the role of many body shake-up of metal electrons in explaining the high energy exponential tailing of the distributions. Shake-up electrons are inherent in ion neutralization of metals, as a consequence of a Fermi level, with high density of states, within the valence band of the target material: they originate from the abrupt change of the surface potential caused by electron capture by the incident ion outside the surface. Therefore, we expect the effect to be absent in materials with a Fermi energy within the band-gap. In such cases, although some form of shake-up will still occur, the effect on the electron energy distributions will be markedly different because of the absence of a Fermi edge singularity. In addition, notwithstanding the narrow projected band gap of Al(1 1 1), we have found that the surface band structure affects the kinetic energy distribution of ejected electrons. We expect this effect to be crucial in electron emission from metal targets with large projected band gap, such as Ag(100) or Ag(1 1 1).

References