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Anisotropy of the angle resolved electron attenuation at crystal surfaces

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ABSTRACT

Photoemission multiple scattering theory is used to describe the electron transport in the surface region of a crystal. Intensities of photoemission from core levels of atoms situated in subsurface atomic layers are calculated as a function of the emitter distance from the surface. The electron angle resolved attenuation length (ARAL) is extracted from the exponential fitting of the intensity decays of photoemission into different directions. Substantial anisotropy of the electron ARAL is found for the Cu(1 1 1) surface in Mg Kα photoexcitation of Cu $2p_{3/2}$ levels and correlated with the orientation of highly packed atomic rows. Enhanced photoemission contributions from specific subsurface layers, caused by electron forward focusing effects, are reported.

1. Introduction

Surface sensitivity of electron spectroscopies is governed by the attenuation length of excited electrons propagating toward the crystal surface. It results from a short mean-free-path of electrons with energies in the range 10–1000 eV with the energy dependence described by the well-known 'universal curve' with a minimum at around 50 eV. Experimental determinations of the electron escape depth from solids (overlayer method) are not very easy and reliable. Theoretical simulations based on semiclassical Monte Carlo simulations [1,2] are directed to disordered systems in order to avoid undesired diffractions. Crystalline effects consisting in coherent quantum interferences are thus ignored and such simulations cannot describe electron attenuation in crystals in general and, in particular, at low electron energies (in the so called band structure regime).

Electrons excited within a solid have to propagate a certain distance before they escape through the surface to the vacuum. On their way to the surface they undergo elastic and inelastic collisions, which influence the intensity of the emitted electron current. In photoemission, the photoemitted current is directly reduced by inelastic electron scatterings (removal of propagating electrons from the elastic channel) and influenced by elastic scatterings: directly in crystals in those directions where the band structure of excited electron states exhibits band gaps (attenuated waves instead of propagating waves) and indirectly in general by prolonging the path traveled within a solid (classically longer distance along a zig-zag trajectory than along the straight line).

Electron propagation and attenuation from different depths can be obtained from calculations of intensities of photoemission from core levels of atoms placed as emitters into subsurface atomic planes. Here, we use a realistic theoretical description of intensities in the photoelectron diffraction to get the anisotropy of attenuation of photoelectrons in a crystal. Related studies have been reported earlier (e.g. mean emitter depth determination for the whole surface region in [3]) and in our investigation the details of the electron attenuation in the surface region are obtained. This enables to deduce the surface sensitivity changes of the photoelectron diffraction in special directions: a general decrease of the overall surface sensitivity accompanied by relative enhancements of contributions from specific subsurface layers.

In crystals, the elastic scatterings of the excited electrons are described by the real part of the effective optical potential Σ and the electron decay from the elastic channel is governed by the imaginary part of Σ. Here, the anisotropy of the electron propagation is investigated at a fixed energy and the role of the electron band structure is taken into account by considering multiple electron-atom scatterings. The imaginary part of Σ is incorporated into the description isotropically by means of a proper magnitude of the electron inelastic mean-free-path λ.

In Section 2 calculations providing the electron photoemission intensity decay as a function of the distance of the emitter from the surface are described. The input data for cluster description and for photoelectron diffraction from the Cu $2p_{3/2}$ core level emitters are given. Section 3 brings the layer by layer decomposed intensities of photoelectron diffraction from emitters under the

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Cu(1 1 1) surface. Extracted mean-emitter-distances and electron attenuation lengths display pronounced enhancements in some directions which are correlated with the directions of highly packed atomic rows in the face centered cubic system. Conclusion stresses the role of forward focusing effects in crystals in enhancing the photoemission from specific subsurface planes in angle-scanned photoelectron diffraction.

2. Electron attenuation from photoemission

The experimental overlayer technique, where electron flux photoemitted from a substrate source is attenuated during electron propagation through overlayers of varying thicknesses requires preparation of perfect overlayers. In the theoretical modelling perfect atomic layers are deposited on top of the plane of emitters and the decrease of photoemission intensity is recorded as a function of a distance of the emitter plane from the surface. The adequate theoretical description of core level photoemission from these emitters is utilized to determine the ARAL. Multiple elastic and inelastic scatterings are taken into account properly. The polar plots of total photoelectron intensities are decomposed into contributions from individual subsurface atomic layers and provide the information about the attenuation of the electron flux during electron propagation to the surface.

Photoelectron diffraction from a large enough atomic cluster representing the clean Cu(1 1 1) surface parabolically shaped cluster with 800 atoms in six atomic layers parallel to the surface) is investigated. The angle resolved intensities of electrons photo emitted by Mg Kα radiation from the Cu $2p_{3/2}$ core level have been calculated by the code EDAC [4]. Their kinetic energy (320.8 eV in the vacuum) ensures that the emitted electrons originate from the surface region due to a short inelastic mean-free-path at this energy (around 7 Å). For a realistic description of photoemitted intensities the parameters entering the computations have been adopted from [5] where excellent agreement of EDAC calculations with experimental data collected over the full hemisphere has been achieved (l_{max} = 8, λ = 7 Å, T = 300 K).

3. Results for Cu(1 1 1)

Polar plots of photoelectron intensities were calculated for two high symmetry azimuths $\Phi = 0°$ and 60° (non-equivalent directions to the next-nearest neighbors along the surface). Contributions to the total photoemission intensity from individual subsurface atomic layers were obtained by placing single emitter atoms into deeper and deeper lying layers till their contributions became negligible. For general angles of photoelectron emission, the contributions from deeper lying atomic layers decay monotonously as is to be expected intuitively. But strong deviations from a simple decay can be encountered with strong enhancements from some subsurface atomic layer at some angles. These amplifications can be understood by electron focusing effect along the highly packed atomic rows. This effect, well-known for higher-energy electrons [6], due to strongly forward-peaked scattering amplitude of electron-atom scattering, is encountered here at a lower energy where forward scattering is less dominant. Similar deviations from a monotonous decay have been found recently in normal photoemission calculation from the core level Fe 2s [7]. A proper choice of the photoelectron exit direction can thus be utilized to focus the investigation to the desired subsurface atomic plane.

Table 1
Polar angles (in degrees from the surface normal) and distances of the neighboring atoms along closely packed atomic rows (in crystal lattice units) for the two atomic planes perpendicular to the (1 1 1) surface of the fcc crystal structure. Letter notation of atomic rows is from Fig. 1.

	A[1 1 1]	B	C	D[0 1 1]	E	F	G
Azimuth 0°							
Polar angle	0	10	15.8	35.3	56.8	60.5	70.5
Distance [a]	1.74	2.35	2.99	0.71	2.99	2.33	1.73
	A[1 1 1]	B	C[1 1 2]	D	E	F	G[0 0 1]
Azimuth 60°							
Polar angle	0	7.3	19.5	29.5	35.3	41.5	54.7
Distance [a]	1.74	2.92	1.22	3.32	2.13	3.08	1

Directions where enhanced photoelectron intensities for the geometrical focusing reasons are to be expected can be seen from side views of the face centered cubic structure with the (1 1 1) surface in Fig. 1. Planes, cutting the structure normally to the surface and containing higher symmetry azimuthal directions connecting next-nearest neighbors along the surface, are shown in Fig. 1a ($\Phi = 0°$) and Fig. 1b ($\Phi = 60°$). Capital letters in Fig. 1 denote individual highly packed atomic rows: their orientations (polar angles with respect to the surface normal [1 1 1]) and distances between the neighbors within the atomic chain are listed in the related Table 1.

Polar angle resolved contributions from the surface and from five subsurface atomic layers to the total photo emitted intensity are shown in Fig. 2 together with the total intensity. Apart from the gradual decrease of the contributions from deeper lying layers the qualitative difference between the photoemission from the surface (topmost) layer and the others can be observed: the much weaker anisotropy of the contribution from the topmost layer can be understood by the absence of any focusing atoms above this

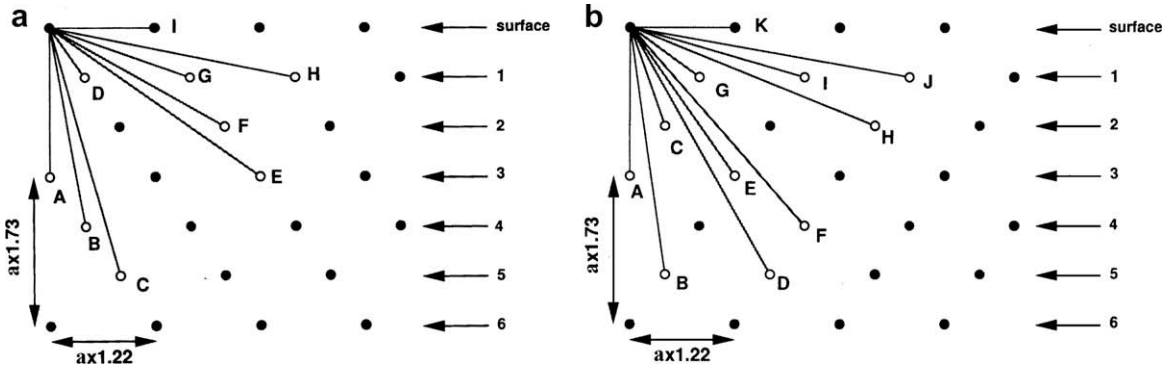

Fig. 1. Side view of the fcc crystal structure with the (1 1 1) surface at the top in two higher symmetry azimuthal directions in the surface plane (corresponding to next-nearest neighbor directions along the surface): (a) $\Phi = 0°$ and (b) $\Phi = 60°$. Capital letters denote individual atomic rows (see Table 1): D denotes the most highly packed atomic row for $\Phi = 0°$, C and G such rows for $\Phi = 60°$.