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Electron attenuation anisotropy at crystal surfaces from LEED

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ABSTRACT

Dynamical theory of electron scattering is used to describe the electron transport in the surface regions of crystals. The angle resolved attenuation length of electrons is derived from the transmitted LEED electron current decay. Electron attenuation length energy dependence and anisotropy in polar angle are found for crystalline Cu(1 1 1) for two high symmetry azimuths. Pronounced anisotropy in polar angle distributions of attenuation lengths is found to be in qualitative agreement with the results obtained from the photoelectron diffraction. Comparison with the attenuation lengths obtained from semiclassical simulations for amorphous copper is given. This comparison demonstrates that simple transfers of the smoothly behaving surface sensitivity from amorphous materials oversimplifies the electron attenuation process and can lead to incorrect results in quantitative analyses of crystalline surfaces.

1. Introduction

Surface sensitivity of the low energy electron diffraction (LEED) and of electron spectroscopies of solids results from strong interactions of low energy electrons with atoms. The degree of the surface sensitivity as a function of electron energy can be roughly inferred from the shape of the well known 'universal curve' expressing electron mean free path as a function of electron energy. In angle resolved investigations, surface sensitivity can also be increased by detecting electrons emitted or diffracted closer to the grazing exit direction from the surface. Apart from these smooth trends, much less is known about the anisotropy due to crystalline structure, however. Experimental determination of the electron escape depth from crystals are not easy and reliable. Theoretical calculations based on semiclassical simulations [1–3] are restricted to deal with disordered solids in order to avoid undesired electron interferences manifested by diffraction phenomena in ordered crystals.

Theoretical calculation incorporating full quantum mechanical description of electron propagation in surface regions of crystals can provide a detailed description of the energy dependence and of the angular anisotropy of the electron attenuation at crystal surfaces. Apart from a realistic evaluation of intensities of back diffracted electron beams, the dynamical theory of LEED correctly describes the attenuation of the incident electron beam towards the bulk of a crystal as well.

Electrons on their way to the surface undergo elastic and inelastic collisions with atoms and both collisions influence the overall electron decay from the elastic channel. Inelastic scattering reduces electron flux directly by removing propagating electrons from the elastic channels. Elastic collisions reduce electron flux indirectly: their role can be classically represented by a longer distance traveled along a zig-zag trajectory in a crystal than along a straight line and correspondingly greater probability of an inelastic collision there.

In crystals, elastic scattering of excited electrons is described by the real inner potential and their decay from the elastic channel is governed by the imaginary optical potential. Here the imaginary part of the optical potential is incorporated into the description isotropically by means of the energy dependent imaginary component.

LEED dynamical theory has been used for determination of low-energy electron (30–400 eV) attenuation from the electron flux decay [4]. Purely exponential decay of the electron beams has been observed deeper below the surface region only and the investigation has been concentrated to the bulk of the crystal. The results have been compared with those obtained by Monte Carlo simulations for amorphous materials after angular averaging [4]. The flux reversal theorem presented in Ref. [4] shows that the electron flux decay is the same in the bulk for the directions of electron propagation into and out of the crystal when crystal structure exhibits a center of inversion. Transmitted electron intensities can be used to derive electron attenuation length for crystalline surfaces as well.

Photoelectron diffraction (PED) has been recently used to determine the electron attenuation in the surface region, important for surface sensitive photoelectron spectroscopies [5]. For large enough cluster representing the crystal surface region pronounced anisotropies of the emitted electron beams have been calculated and interpreted.

Here, we utilize the LEED evaluations to get the information about the electron flux attenuation anisotropy, both, in the surface

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and in the bulk region of a crystal. Results for the former region are compared with those of PED.

Copper crystal with the (1 1 1) surface is investigated. Polar angle dependence of the electron attenuation in two high symmetry azimuthal directions (Fig. 1) is calculated. The results of 320 eV energy electrons are compared with the analogous results of Mg Kα excitation from the Cu $3p_{3/2}$ core level in PED.

2. Calculation

In LEED, the incident electron plane wave scatters from periodically placed atoms. The theoretical description starts from scattering properties of individual atoms to get scattering properties of atomic layers parallel to the crystalline surface and finally evaluates scattering from a stack of atomic layers. It gives possibility to follow the electron beam intensity changes at every step of calculation. Scattering processes take into account elastic as well as inelastic electron collisions with atoms. Description of processes with strong interactions of low energy electrons with atoms requires dynamical theory of electron scattering, taking into account multiple scattering processes. The finally established electron current gets gradually smaller when penetrating deeper under the crystal surface. The electron beam intensities within a crystal (obtained during evaluation of back diffracted LEED intensities) are used to determine the electron flux decay between two subsequent atomic layers. Evaluation of the electron attenuation length, λ, is similar to the procedure described in Ref. [4]. Plane wave amplitude, $B_{g'}^{(i+1)}$, of the beam g' in the $(i+1)$th layer is obtained from the preceding ith layer plane wave amplitude as [6]:

$$B_{g'}^{(i+1)} = T_{gg'}^{+(i)} B_{g'}^{(i)}, \qquad (1)$$

where ' + ' denotes direction to the bulk and $T^{+(i)}$ is the transmission matrix, which describes the propagation of plane wave amplitudes incident on layer i from above into the space between layers i and $i+1$. The intensity transmitted through the ith layer, $I_g^{(i)}$, is proportional to $|B_g^{(i)}|^2$. The total intensity of all beams passing through the ith layer is:

$$I_{tot}^{(i)} = \sum_g I_g^{(i)}. \qquad (2)$$

The attenuation length, $\lambda^{(i)}$, of the region consisting from i atomic planes can be expressed as [4]:

$$\lambda^{(i)} = -\frac{d^{(i)}}{\ln\left(I_{tot}^{(i)}\right)}, \qquad (3)$$

where $d^{(i)}$ is the distance of the ith layer from the surface.

We used TensErLEED code [7] to evaluate the transmitted LEED intensities. The Cu(1 1 1) surface was represented by layer stacking method [6]. Sixteen atomic planes of Cu atoms deposited on top of a semiinfinite bulk crystal (treated by layer doubling method). This procedure differs only slightly from that described in Ref. [4], where layer doubling method has been used to compute LEED intensities and thus intensities only between surface with $i = 2$, 4, 8 and 16 stacks of atomic planes are available. The relativistic phase shifts [8] with $l_{max} = 8$ were used to treat scattering properties of Cu atoms represented by muffin-tin type potentials. Energy dependent real and imaginary parts of the inner potential were adopted from Ref. [4], where excellent agreement with experimental LEED I–V curves has been achieved.

3. Results

Our calculated LEED I–V curves and the logarithmic transmission gradients are in agreement with those of Ref. [4]. In order to deal with the electron attenuation anisotropy we investigate propagation of electron currents under the crystal surface when incident beam polar angle is varied in two higher symmetry azimuths, Φ, in a direction to next-nearest neighbor atoms along the surface (Fig. 1). Polar angle of the current propagating towards the surface, Θ, is counted with respect to the surface normal (direction [1 1 1]).

The truly exponential decay of the electron intensity has been found [4] and explained to be limited to incident angles restricted to the off-normal incidence angle less than about 45°. The gradual decrease of electron current intensity, $I_{tot}^{(i)}$, in subsurface atomic

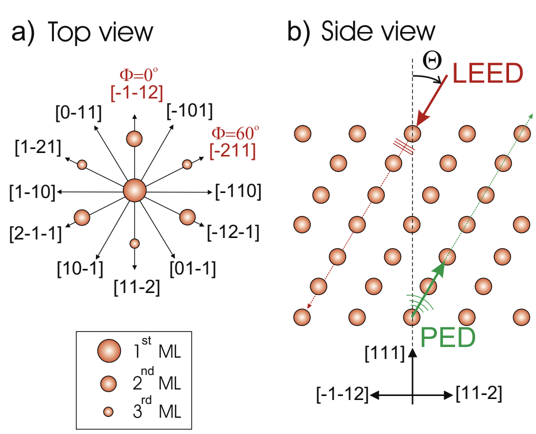

Fig. 1. Top (a) and side (b) view of the high symmetry directions in the (1 1 1) surface plane of the face centered cubic crystal. In (a) atoms from the first three layers are indicated by circles. Side view shows highly packed atomic rows in a plane perpendicular to the (1 1 1) surface for the azimuthal direction $\Phi = 0°$.

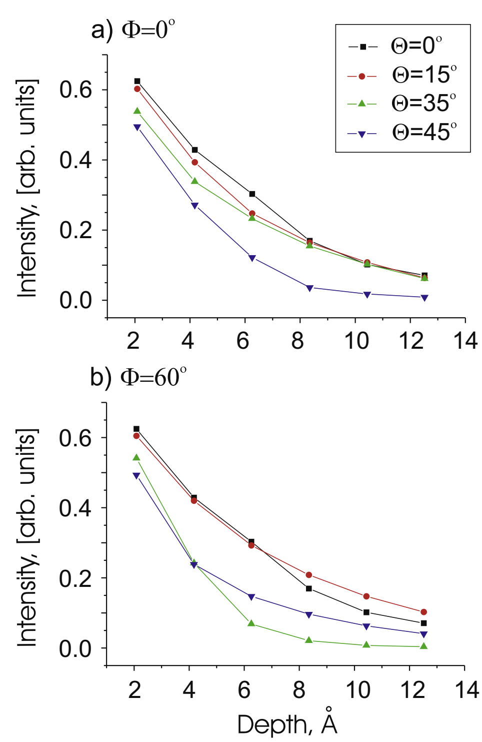

Fig. 2. Layer resolved electron current intensities, $I_{tot}^{(i)}$, in the elastic channel under the Cu(1 1 1) crystal surface for LEED with electron beams (energy 320 eV) incident at several polar angles, Θ, and two azimuths (a) $\Phi = 0°$ and (b) $\Phi = 60°$. Values for the ith layer are taken as intensities in the middle between the ith and $(i+1)$th layer.