

# Neutralization of low energy $\text{He}^+$ ions by Cu in the Auger regime

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Available online 22 December 2006

## Abstract

Neutralization of light  $^4\text{He}^+$  ions in backscattering geometry is studied on a single crystalline Cu(100) and on a poly crystalline Cu-poly surfaces by means of direct comparison of the ion yields. Below 2 keV neutralization is only restricted to the Auger transition involving two electrons. Measurements in this regime revealed a  $\sim 35\%$  higher ion fraction for the single crystal Cu(100) with respect to the Cu-poly. The observed difference in the neutralization probability is ascribed to a different extension of the electron jellium edge, resulting from different atomic arrangement.

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PACS: 34.50.Dy; 68.49.Sf; 79.20.Rf

Keywords: Neutralisation; Low energy ion scattering; Single crystal; Copper; Helium

## 1. Introduction

In LEIS, a beam of primary ions is directed onto the surface of the sample at a small angle  $\alpha$  with respect to the surface normal. Projectiles scattered by a large angle  $\theta$  are detected. The intensity of detected ions expressed in the area of the ion peak  $A_+$  in the spectrum is given [1] by:

$$A_+^i = \frac{N_0}{\cos \alpha} \cdot \frac{d\sigma}{d\Omega} \cdot n_i \cdot P_i^+ \cdot \Delta\Omega \cdot \eta_+, \quad (1)$$

with the primary number of projectiles,  $N_0$ , the atomic surface density,  $n_i$ , the scattering cross section  $d\sigma/d\Omega$ , the ion fraction  $P^+$ , the detector solid angle  $\Delta\Omega$  and detection efficiency for ions  $\eta_+$ . Index  $i$  denotes a different kind of samples (Cu(100) or Cu-poly, in our case). The Thomas–Fermi–Moliere potential, which is a screened Coulomb potential [2], is a reasonable basis to calculate  $d\sigma/d\Omega$ . The theoretical basis for  $P^+$  is less safe. Since the pioneering work by Hagstrum [3], it is generally accepted that

Auger neutralization (AN) plays an important role, at least at low energies. Hagstrum derived a relation for the probability  $P_A^+$  that the ion is not neutralized by AN when approaching or leaving the surface. Because of the nonlocal character of AN,  $P_A^+$  depends on the velocity component  $v_\perp$  perpendicular to the surface:

$$P_A^+ = \exp \left[ -\frac{v_c}{v_\perp} \right]. \quad (2)$$

Here,  $v_c$  characterizes the neutralization efficiency and has the dimension of a velocity, since  $v_c = \int ds [1/\tau_A(s)]$  is obtained by integration of the Auger transition rate  $1/\tau_A$  from 0 to  $\infty$  over the distance  $s$  to the surface.

When using a single crystal, the main advantage is that in channeling/blocking geometry [2] scattering is only due to atoms in the outermost atomic layer, since scattering from the second layer is suppressed due to the large width of the shadow cone in this regime [4].

In this work, we study the survival probability of He ions scattered from Cu(100) and Cu-poly surfaces in the Auger regime ( $E \leq 2000$  eV). From yields of backscattered ions (1), the ratio of the ion fractions  $P_{100}^+/P_{\text{poly}}^+$  is deduced

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in a straight-forward manner, as described below. When keeping the number of incident ions  $N_0$  constant for both samples, and making use of the fact that  $\Omega$  and  $\eta$  are identical, the ratio of the ion fractions  $P_{100}^+/P_{\text{poly}}^+$  is obtained in a straight-forward manner:

$$\frac{P_{100}^+}{P_{\text{poly}}^+} = \frac{A_+^{100} \cdot n_{\text{poly}}}{A_+^{\text{poly}} \cdot n_{100}} \quad (3)$$

Note that this is the most direct approach to measure the ratio  $P_{100}^+/P_{\text{poly}}^+$ , since much more information is required to deduce the absolute values  $P_{100}^+$  and  $P_{\text{poly}}^+$ , e.g. for polycrystalline sample one might apply the routine described in [5] and for the single crystal, proper background subtraction to extract the neutral peak area would be demanded [4].

## 2. Experiment

The measurements were performed in the ultra-high vacuum (UHV) set-up ACOLISSA [6], which has recently been modified so that now sample preparation is performed in the UHV analysis chamber ANA which is separated from the ACOLISSA main chamber by a gate valve. This minimizes contamination of the samples in the ACOLISSA main chamber, keeping the vacuum at  $\sim 5 \cdot 10^{-11}$  mbar there. The preparation of the Cu(100) surface is performed using continuous cycles of sputtering by scanning a beam of 3 keV  $\text{Ar}^+$  ions with a current of  $\sim 250$  nA and subsequent annealing to 400 °C; the Cu-poly sample is just sputtered. The surface purity is controlled by Auger electron spectroscopy (AES) monitoring the low energy Cu peak intensity until it reaches a maximum. The AES spectra are free from peaks due to any other elements like S, C, O. TOF-LEIS experiments were performed on the clean Cu surfaces.

## 3. Results and discussion

In Fig. 1, typical TOF-LEIS spectra are shown for  $^4\text{He}^+$  1.9 keV ions and Cu-poly, and for Cu(100) in double alignment geometry ( $\alpha = 0^\circ$ ,  $\varphi = 0^\circ$ ). Note that due to post-acceleration of the ions along part of the flight path between the sample and the detector, the ions arrive earlier at the detector than the neutrals. Therefore, they appear at higher channel numbers in Fig. 1, where the abscissa is proportional to  $T_0 - \text{TOF}$ , with  $T_0$  being a well defined time delay ( $T_0 = 6.45 \mu\text{s}$ ) [6]. One channel corresponds to 1.95 ns. Note that only projectiles that have not been neutralized contribute to the ion peaks ( $E < E_{\text{th}} \approx 2 \text{ keV}$  [5,7]).

The spectrum for Cu(100) exhibits a (relatively) low background and a sharp neutral peak. For Cu-poly, the spectrum of the neutrals consists of a broad continuum and a pronounced surface peak [8] proving the purity of the surface. Integration of the ion peak gives the numerical value for  $A_+^i$ .

The structural quality of the Cu(100) surface was proved by polar and azimuth scans which showed the

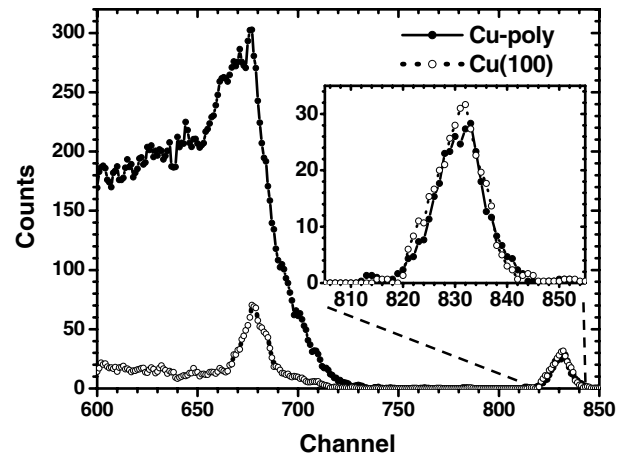


Fig. 1. TOF-LEIS spectra measured using 1.9 keV  $\text{He}^+$  projectiles are shown for Cu(100) and Cu-poly. The measured spectra are shown as a function of  $(T_0 - \text{TOF})$ . As an insert, the zoomed in ion peaks are shown.

expected symmetry with excellent precision (see Fig. 2). The spectra were measured for 3 keV  $\text{He}^+$  ions in the angular intervals  $-17^\circ$  to  $110^\circ$  and  $-16.5^\circ$  to  $68.5^\circ$  for the azimuth and the polar scans, respectively. In Fig. 2, only the areas obtained by integrating the channels containing the peak of detected neutrals are plotted versus the angle.

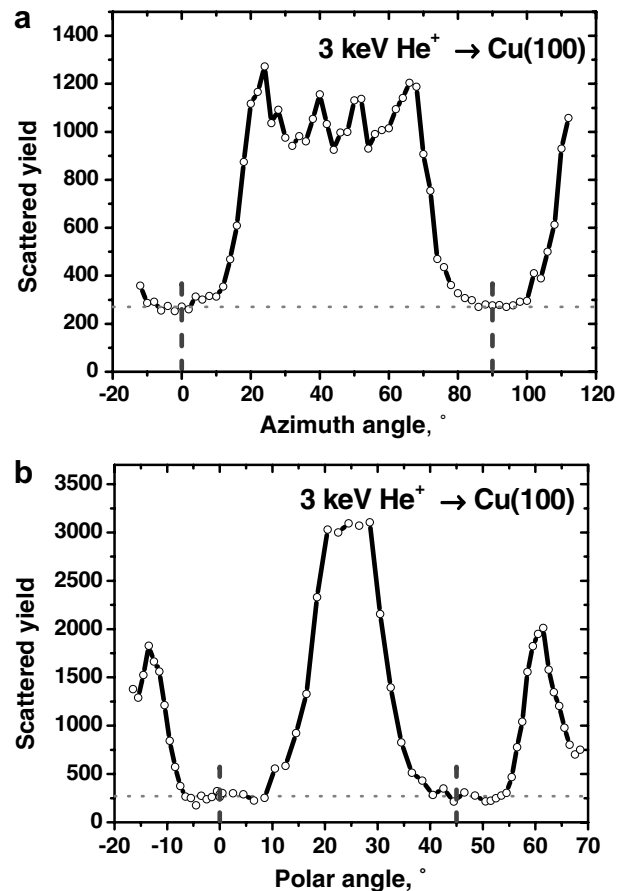


Fig. 2. Azimuth (a) and polar (b) scans performed by using of  $\text{He}^+$  3 keV ions at Cu(100).

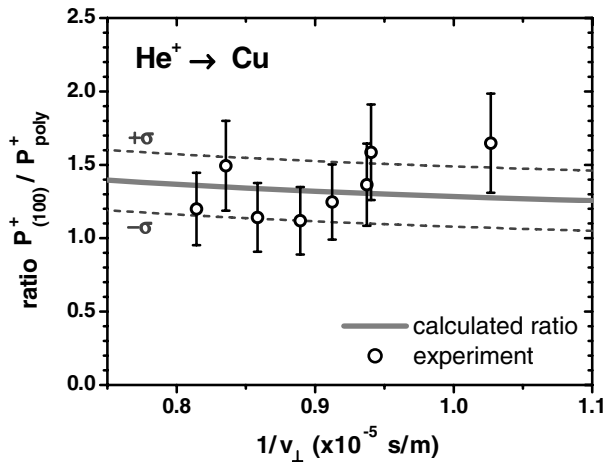


Fig. 3. The ion fraction measured in a straight-forward comparison of ion yields for Cu(100) and Cu-poly using Eq. (3). For comparison also calculated data using  $P^+$  from [5] is presented (see text for explanation).

The  $90^\circ$  periodicity of the double alignments minima in the azimuth scan (Fig. 2(a)) proves the four fold symmetry of the crystal surface. Fig. 2(b) shows a polar scan measured for  $0^\circ$  azimuth, corrected for the increase of the number of visible surface atoms for non-perpendicular incidence (cosine correction). This is the reason why identical neutral peak intensities are observed for normal incidence and for  $\alpha = 45^\circ$ , as is expected for double alignment geometries. For more details about angular resolved analysis of the Cu(100) surface using  $\text{He}^+$  ions see e.g. [4].

Let us now focus on the ion fraction results. In Fig. 3, the resulting ion fraction ratios  $P_{100}^+/P_{poly}^+$  are presented in the range of 1.5, ..., 2 keV. From the ion peak ratios  $A_{100}^+/A_{poly}^+$ , the ion fraction ratio is deduced via Eq. (3) and making use of the atomic surface densities for the two samples. For Cu(100) the atomic surface density is  $n_{100} = 1.531 \cdot 10^{15}/\text{cm}^2$ , for Cu-poly the density of Cu(111) was adopted ( $n_{111} = 1.767 \cdot 10^{15} \text{ at}/\text{cm}^2$ ), since for fcc metals at room temperature the polycrystal is assumed to consist of an array of (111) facets. Note that the alternative way to estimate the atomic surface density of a polycrystal  $n_{poly}$  from the atomic volume density  $n$ ,  $n_{poly} = n^{2/3}$ , would yield a value larger than  $n_{111}$  ( $n_{poly} = 1.93 \cdot 10^{15}/\text{cm}^2$ ), which does not seem realistic.

From the results presented in Fig. 3 it is clear that for Cu(100) the resulting ion fraction is higher than that of Cu-poly, by about 35%. Even in the raw data (see

Fig. 1), the ion peak area corresponding to Cu(100) is larger than that of Cu-poly, despite the fact that the (100) face contains less atoms per unit area than the polycrystal ( $n_{100} < n_{poly} \approx n_{111}$ ). This is in qualitative agreement with the predictions of the “jellium” model for free electron gas [9]. The position of jellium edge, which usually is set to half of the interlayer distance, is at  $0.91 \text{ \AA}$  for the Cu(100), while it is at  $1.05 \text{ \AA}$  for Cu(111). Therefore, one may expect a higher survival probability for  $\text{He}^+$  in case of Cu(100) than in Cu(111) or Cu-poly.

One may also calculate the ratio of the characteristic velocities for Cu(111) and Cu(100),  $v_c^{111}/v_c^{100}$  from the jellium model, since there it is just due to the different positions of the jellium edge, leading to  $v_c^{111}/v_c^{100} = d_{111}/d_{100} = 2.09/1.81 \approx 1.15$ . Substituting the value for the  $v_c^{111}$  from the value for Cu-poly [5], one derives  $v_c^{100} = 1.67 \cdot 10^5 \text{ m/s}$ . From this, one obtains a weak  $v_{\perp}$  dependence for the ratio  $P_{100}^+/P_{poly}^+$ , as is presented in Fig. 3 (solid line).

To conclude, we have determined the ratio of the ion fractions  $P_{100}^+/P_{poly}^+$  experimentally by just evaluating the ion peak ratios corresponding to Cu(100) and Cu-poly. As a result we obtained that the ion fraction  $P_{100}^+$  is larger than  $P_{poly}^+$  by about 35%, which is in good agreement with the expectation from the jellium model, which yields a ratio of the corresponding characteristic velocities  $v_c^{111}/v_c^{100} \approx 1.15$ . The main advantage of the chosen experimental approach is its simplicity and the fact that no information apart from the atomic surface densities is required.

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