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Determination of a correction factor for the interaction potential of He^+ ions backscattered from a Cu(100) surface

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Abstract

We have used coaxial impact collision ion scattering spectroscopy (CAICISS) data collected from 3 keV He^+ ions backscattered from a Cu(100) surface in different azimuthal orientations to investigate the influence of the screening length on CAICISS polar angle scans. We have compared the experimental data to computer simulations generated with the FAN code and found that for our experimental conditions an exceptionally low value of 0.53 was required for the correction factor to the Firsov screening length used with the Thomas–Fermi–Moliere potential. In addition we found that the Ziegler–Biersack–Littmark potential is not applicable, resulting in incorrect peak positions in the CAICISS polar angle plots.

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Keywords: Interaction potential; ISS; Computer simulations; Surface structure analysis; Cu(100)

1. Introduction

In the low energy ion scattering regime, the commonly used interaction potentials, such as the Thomas–Fermi–Moliere (TFM) [1] or the Ziegler–Biersack–Littmark (ZBL) potential [2] play a vital role when performing high precision quantitative measurements of surface and near-surface structures. It is also well known that these potentials have to be adjusted in order to reproduce the experimental data, particularly in grazing ion-surface scattering [3,4]. A simple way to correct the interaction potential is to adjust the screening length by a multiplicative factor. In the case of surface structural analysis by coaxial impact collision ion scattering spectroscopy (CAICISS) [5,6] variation of the screening length leads to changes in the shadowing of target atoms and therefore to shifts in peak positions in the resulting polar angle spectra. To demonstrate the effect of small changes in the multiplication factor and its influences on these spectra, we have performed 3D computer simulations with the FAN code ([7] and references therein) and compared the results to experimental data. The experiments were done using our modular CAICISS experimental setup, which is described in detail elsewhere [8,9]. The experimental spectra were collected using a 3 keV He^+ ion beam, incident on the Cu(100) surface in different azimuthal orientations, e.g. ⟨100⟩ and ⟨110⟩. Polar angle scans from 0° to 180° (measured with respect to the surface plane) were taken in 1.8° intervals.

The Cu(100) surface was chosen for two reasons. Firstly, it is easily prepared by cycles of sputtering and annealing [10], and secondly the termination of the Cu(100) surface is well known [11,12].

The trial structure consisted of an interlayer spacing between first and second layer of $d_{12} = 1.74$ Å (a contraction of 3.9%) and an interlayer spacing between second and third layer of $d_{23} = 1.83$ Å (an expansion of 1.3%) as shown in Fig. 1. From the third layer on the bulk value of $d = 1.807$ Å has been chosen to model the Cu(100) crystal. The enhanced surface vibrations have a negligible effect on the resulting CAICISS spectra and have been neglected here.

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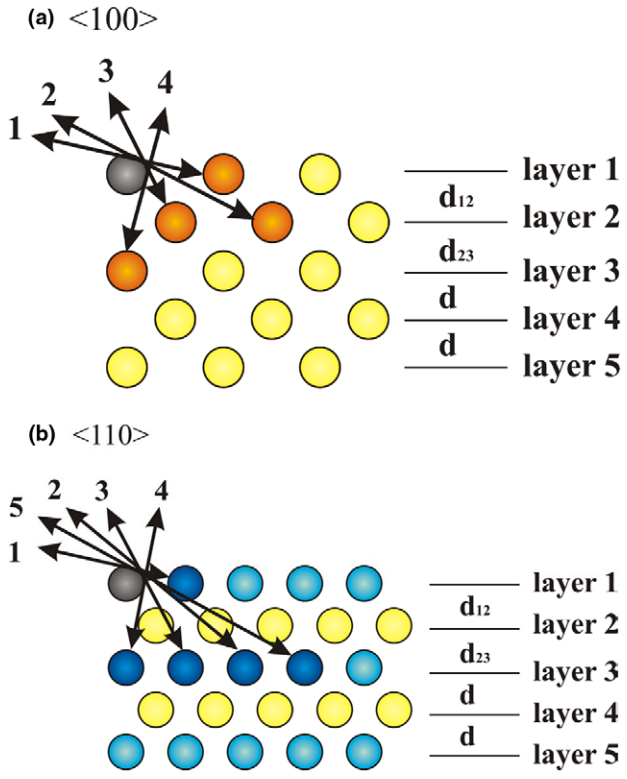

Fig. 1. Schematics of the origin of the peak intensities in CAICISS polar angle scans in the (a) ⟨100⟩ and (b) ⟨110⟩ directions. The numbers correspond to specific peak intensities as shown in Fig. 3. Note that in ⟨110⟩ all even numbered layers are not in the same plane as the odd numbered layers.

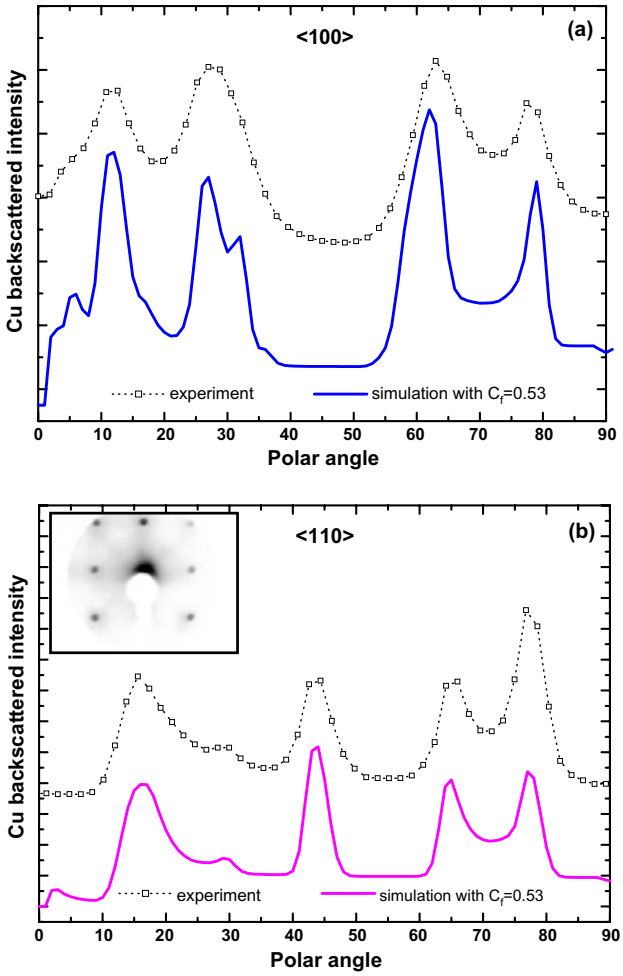

Fig. 2. Comparison of the experimental spectra and best fit simulation (for details see text) in the (a) ⟨100⟩ and (b) ⟨110⟩ directions. The inset shows a LEED pattern of the crystal taken at 65 eV. Note that ⟨100⟩ and ⟨110⟩ are symmetric directions with respect to the surface normal, therefore we just show 0–90° and not the full 0–180° range.

2. Results

In Fig. 2 CAICISS polar angle scans of Cu(100) in the (a) ⟨100⟩ and (b) ⟨110⟩ azimuths are shown together with the low energy electron diffraction (LEED) pattern taken after crystal preparation. A clear (1×1) pattern is obtained, indicating a well ordered surface. X-ray photoelectron spectroscopy (XPS) also revealed that the surface was free of contaminants. The CAICISS polar angle scan spectra exhibit peaked intensities resulting from shadowing of first layer atoms onto second and third layer atoms, as schematically shown in Fig. 1.

Simulations with different correction factors, C_f, to the Firsov screening length [13] used in conjunction with the TFM potential have been generated and are shown in Fig. 3 together with a simulation using the ZBL screening length [2] in conjunction with the ZBL potential, again in two different azimuthal directions, e.g. (a) ⟨100⟩, (b) ⟨110⟩. For these FAN simulations, the bulk Debye temperature of Cu (343 K) and a substrate temperature of 300 K have been used, as the experiments were carried out at room temperature. Not surprisingly, there is an influence on the peak positions in the resulting CAICISS polar angle spectra when changing the screening length, although the magnitudes of the angular shifts were found to be rather large, i.e. up to several degrees. Note that a peak (numbered 5 in Fig. 3(b) – see also Fig. 1) emerges as the correction factor for the screening length gets smaller and smaller, thus making the corresponding shadow cone radius smaller and smaller. This means that additional atoms can be "seen" by incoming projectiles yielding an additional peak in the CAICISS polar angle spectra. Comparison is made between the experimental CAICISS polar angle plots and the simulated FAN spectra, again for both azimuthal directions, e.g. ⟨100⟩, ⟨110⟩. The best fit value of the correction factor to the screening length was found to be 0.53. This value is obtained from the best match of the position of the simulated surface peak compared to the experimentally observed peak positions.

3. Discussion

Good agreement between the experimental and simulated spectra indicates that the trial structure is in good agreement with the "real" structure of the crystal. Nevertheless, the very low value of the correction factor (0.53)

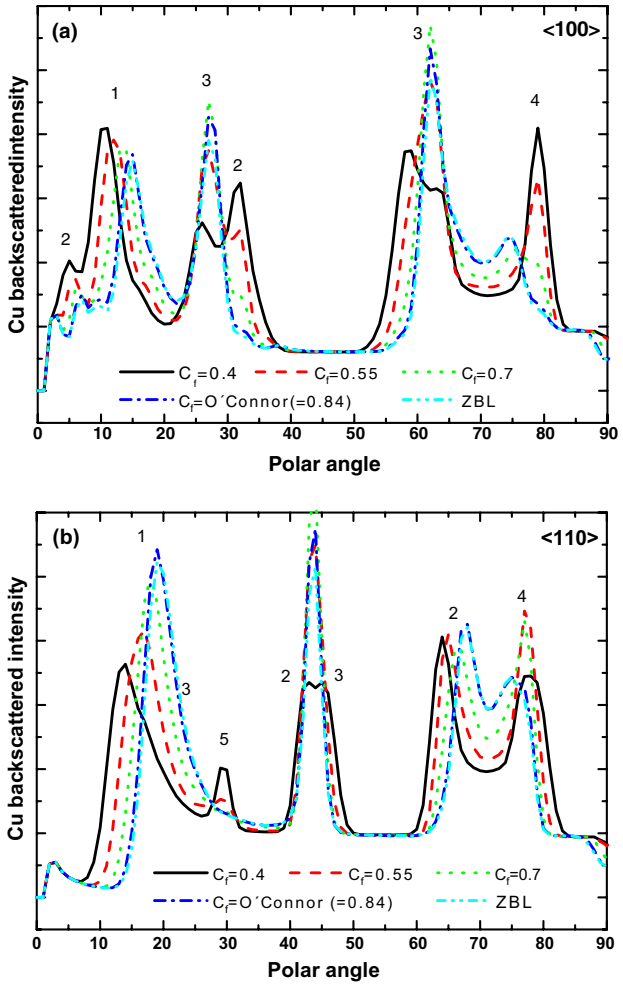

Fig. 3. Cu(100) FAN simulations of our trial structure with different correction factors, C_f, for the Firsov screening length. (a) ⟨100⟩, (b) ⟨110⟩. The "O'Connor" correction factor is a factor depending on Z_1 and Z_2 (see also [24]).

for the Firsov screening length is a surprising result. In addition, the fact that the use of the ZBL screening length together with the ZBL potential yields completely wrong peak positions is an even more surprising result, although the ZBL screening is known to be in general too repulsive for larger distances [14]. In the published literature there are several reports of different correction factors to choose from for the TFM potential, depending on energy and ion-atom combination, but these values are always in the range of 0.65–1.25 [15–19], the most commonly used correction factor being between 0.8 and 0.9 [20]. For primary energies between 1 and 3 keV suggested values for the correction factor for the Firsov screening length range from 0.6 to 0.8 [21]. It has also been reported that the ZBL potential is essentially "parameter free" and usually no correction to the screening length is necessary [22], with some exceptions. Kato et al. suggested a correction factor of 0.9 for the ZBL screening when using a combination of low Z_1 projectiles and high Z_2 substrate atoms [23]. Nevertheless the comparison of the simulated to the experimental spectrum suggests that under our experimental conditions the ZBL screening and potential is not an appropriate choice at all.

4. Conclusions

We have compared coaxial impact collision ion scattering spectroscopy data from 3 keV He^+ ions backscattered from Cu(100) in different azimuthal orientations to computer simulations generated with the FAN code. We have found that the Firsov screening length used in conjunction with the Thomas–Fermi–Moliere interaction potential needs to be adjusted in order to have a reasonable well comparison between experiment and simulation. A value of 0.53 was found to be the best correction factor, which is an exceptionally low value. FAN computer simulations using the Ziegler–Biersack–Littmark screening length in conjunction with the Ziegler–Biersack–Littmark interaction potential have shown that this combination is not a useful choice because it underestimates the actual electron screening at large distances.

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