# AUGER NEUTRALIZATION OF $HE^+$ ON CU SURFACES: SIMULATION OF AZIMUTHAL SCANS

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## 1. INTRODUCTION

Charge exchange between ions and surfaces is a topic of great interest in many research fields, e.g. catalysis, plasma-wall interactions or surface analysis. When an ion approaches a surface, charge exchange can occur due to two-electron Auger-processes or due to resonant processes. This investigation is focused on Auger-Neutralization (AN). In an AN-process an electron from the conduction band tunnels to an unoccupied level of higher binding energy of the approaching ion. The gain in potential energy is dissipated by excitation of another electron (Auger-electron) or by excitation of a plasmon.

Since the pioneering work of Hagstrum [1], many theoretical investigations were devoted to the understanding of AN. Recently, a study of AN in Low-energy ion scattering (LEIS) revealed that the AN probability strongly depends on the binding energy of the He 1s level [2]. This is insofar of importance, as interactions between projectile and target do modify the binding energy as a function of the ion-atom distance. The aim of the present investigation is to verify whether the obtained results for Cu(111) are also valid for other Cu surface orientations and if this model correctly predicts second layer contributions.

## 2. RESULTS AND DISCUSSION

We present simulations of LEIS experiments for He ions scattered from Cu(110) and Cu(100) surfaces in the energy regime $E_0 < 2$keV, where neutralization is exclusively due to AN. In this regime, the fraction of ions amongst the backscattered particles, $P^+$, depends on the AN-rate, $\Gamma$, and the projectile trajectory, $\vec{r}(t)$, in the following way:

$$P^+ = \exp(-\int \Gamma(\vec{r}(t))dt) \qquad (1)$$

$\Gamma$ was calculated using the above mentioned model and projectile trajectories were obtained employing the MD-simulation package KALYPSO [3].

We performed two different kinds of calculations: Calculations of $P^+$ as a function of energy for fixed geometries and calculations of ion yields for a fixed energy as a function of the azimuthal exit angle of the backscattered projectiles. For the energy dependent calculations, geometries are selected where He trajectories comprise a single-scattering event from a first or second layer atom. Results for Cu(110) are shown in Fig.1 for exit in $[1\bar{1}2]$ direction (1st layer visible) and in $[1\bar{1}0]$ direction (1st and 2nd layer visible). Scattering from the 2nd layer contributes more to the neutral yield than to the ion yield. Therefore, $P^+$ is reduced by 2nd layer contributions.

From the exit angle dependent calculation, we can extract the specific influence of scattering geometry and neutralization rates on the resulting ion yield.

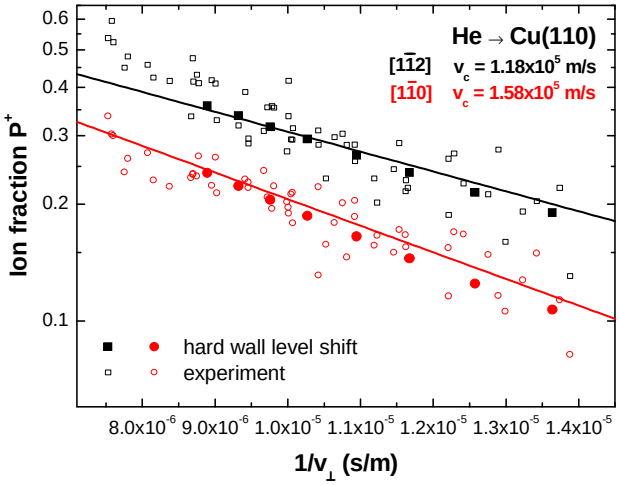


Figure 1: Ion fraction of $He^+$ scattered from Cu(110) in $[1\bar{1}2]$ and $[1\bar{1}0]$ azimuth directions (squares and circles, respectively). Calculations were performed with the hard wall level shift model to approximate the distance dependent He 1s level shift (for details, see [2]).

## 3. REFERENCES

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