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Charge exchange processes in He^+/Cu scattering at low energy

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ABSTRACT

In this paper we present results on charge exchange of He^+ ions at a polycrystalline Cu surface. Monte Carlo simulations were used to calculate the trajectories of projectiles scattered by an angle $\Theta = 136°$. By including Auger neutralization and charge exchange in close collisions, energy spectra of the scattered ions as well as ion fraction values were calculated for primary energies in the range 0.5–5 keV and compared to experimental results. In the simulations, the Auger neutralization rate Γ and the probabilities of resonant neutralization (P_{RN}) and reionization (P_{RI}) are treated as free parameters. Using well accepted values from literature for these quantities very good agreement between simulations and experimental data was achieved.

1. Introduction

Low energy ion scattering (LEIS) is a widely used sensitive technique for quantitative surface composition and structure analysis [1–3]. A solid surface is bombarded with noble gas ions (typically He^+) with incident energy E_0 in the range of several hundred eV to 10 keV. When moving in matter, ions interact with electrons and nuclei, leading to scattering, energy loss and charge exchange. Ions scattered by a large scattering angle Θ can be detected using an electrostatic analyser (ESA), as in the present study. From the energy spectra obtained for reference samples, e.g., polycrystalline copper, information on charge exchange processes can be deduced. This provides the basis for quantitative interpretation of LEIS data.

It is well established that for most materials charge exchange of He^+ projectiles is dominated by Auger neutralization (AN) and resonant processes in a violent projectile-target collision (resonant neutralization, RN, and reionization, RI, respectively) [4–6].

A detailed description of AN is given by Hagstrum [7]. Initially, this model was developed for very low energies (eV range) and has been extended later to the LEIS regime [8]. AN depends on the local density of the conduction electrons. It is a non-local process and is possible for all energies. Since in LEIS the projectile velocity v is smaller than the Fermi velocity v_F of the target, effects of the shifted Fermi sphere [9] are negligible [10] and can safely be neglected here.

In a one-dimensional model, the survival probability (i.e., that no AN occurs) along an in- or outgoing trajectory is given by $P^+ \approx \exp\left(-\int \Gamma(z)\,dt\right) = \exp\left(-\int \Gamma(z)\,\frac{dt}{dz}\,dz\right)$, where $\Gamma(z)$ is the Auger neutralization rate at a distance z from the surface [7]. If the perpendicular velocity, dz/dt, is assumed to be constant, the survival probabilities, P^+_{in} and P^+_{out}, for the incoming and outgoing parts of the trajectory, respectively, read:

$$P^+_{in} = \exp\left(-v_c/v_{\perp in}\right)$$
$$P^+_{out} = \exp\left(-v_c/v_{\perp out}\right) \quad (1)$$

where the characteristic velocity $v_c = \int \Gamma(z)\,dz$ reflects the neutralization efficiency for a given projectile-target combination. The projectile perpendicular velocities along the incoming and outgoing trajectories are denoted by $v_{\perp in}$ and $v_{\perp out}$, respectively.

Resonant processes may occur in collisions, in which the minimum distance between the collision partners is lower than a critical value R_0. For a given scattering angle, this is possible for projectile energies above a threshold value E_{th}. The specific value of E_{th} depends on the atomic species of the collision partners and on the scattering angle. In the scattering of He^+ ions from a Cu surface, this value is $E_{th} = 2.1$ keV for a scattering angle $\Theta = 129°$ [1]. In a resonant charge exchange process, the projectile level is promoted due to interaction with the target electrons [11]. Depending

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on the charge state of the projectile before the collision, its charge state will be changed due to RN or RI, respectively.

In the regime $E < E_{th}$, Auger neutralization is the only possible charge exchange process and P^+ represents the probability that the projectile did not undergo any charge exchange ("survival probability"). In the regime $E > E_{th}$, two types of histories contribute to P^+, namely, survivals and reionized projectiles, which have been neutralized on the way in and reionized close to the surface on the way out [12]:

$$P^+ = P^+_{in}(1 - P_{RN})P^+_{out} + (1 - P^+_{in})P_{RI}P^+_{out}. \quad (2)$$

P_{RN} and P_{RI} are the probabilities for neutralization and reionization in a close collision, respectively. In the AN regime, $E < E_{th}$, P_{RN} and P_{RI} vanish and the survival probability reads:

$$P^+ = P^+_{in}P^+_{out} \equiv \exp(-v_c/v_\perp), \quad (3)$$

where $1/v_\perp = 1/v_{\perp in} + 1/v_{\perp out}$. From this equation it is clear that AN scales with $1/v_\perp$.

From measurements of the He^+ ion yield backscattered from single crystalline and polycrystalline Cu surfaces for different primary energies, values of the ion fraction P^+ can be deduced [5,6]. P^+ values deduced from the surface peak of experimental energy spectra of backscattered He^+ ions are well described by Eq. (2) (see, e.g., [5,6]). For projectiles that are backscattered from deeper layers, however, multiple scattering becomes important and any single scattering model will necessarily break down.

In this paper, we present a method based on a Monte Carlo simulation to calculate trajectories of low energy He^+ projectiles in a polycrystalline Cu surface. The above charge exchange mechanisms are included in the model to calculate energy spectra of the scattered ions and ion fraction P^+ values. Experimental P^+ data are well reproduced in the energy range considered in the present study (0.5–5 keV). Furthermore, for primary energy higher than E_{th} where RI and RN contribute to charge exchange, the tail observed in the experimental energy spectra is well reproduced by simulation.

2. Experiment

The experiments were performed using an electrostatic analyser (ESA). A detailed description of the set-up is given in [13,14]. The typical base pressure in the main chamber in this ESA-LEIS set-up is in the low 5×10^{-10} mbar range. The ion gun produces He^+ ions with a primary energy in the range 0.3–5 keV. The polycrystalline Cu sample was cleaned with repetitive sputter-annealing cycles using 3 keV Ar^+ ions. The He^+ beam is directed perpendicularly to the sample surface. The scattered ions are detected by use of a set of micro-channel-plates (MCPs) at a scattering angle $\Theta = 136°$.

In Fig. 1 we show an experimental energy spectrum of the ion yield obtained for 4 keV He^+ and polycrystalline Cu. Since for Cu the reionization threshold is at ~2.1 keV, the energy spectrum exhibits a tail at lower energies ("reionization background") in addition to the surface peak Y^+, which can be expressed as [5,15]:

$$Y^+ = nN_0\left(\frac{d\sigma}{d\Omega}\right)\eta^+ P^+ d\Omega. \quad (4)$$

Here, n corresponds to the atomic surface concentration, N_0 is the number of incoming projectiles and $(\frac{d\sigma}{d\Omega})$ the differential scattering cross section. η^+ corresponds to the detection and transmission efficiency of the set-up and $d\Omega$ is the detector solid angle. From the measured spectrum, Y^+ may be obtained by fitting the surface peak with a Gaussian. From this, P^+ is deduced using Eq. (4).

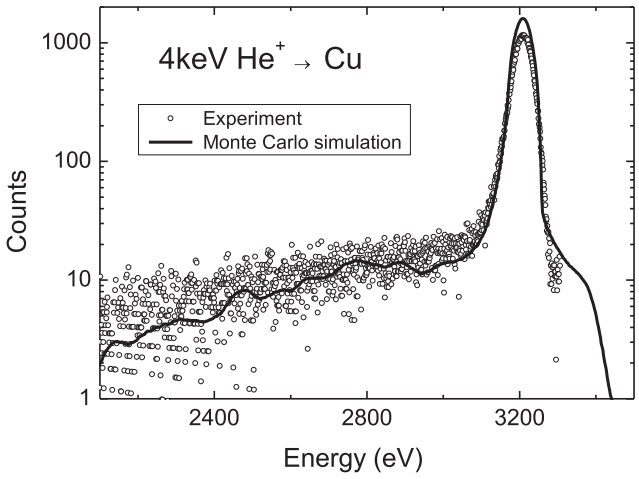

Fig. 1. Experimental ion spectrum for 4 keV He^+ ions scattered from a polycrystalline Cu surface (open circles). The calculated spectrum using a Monte Carlo simulation is also shown (line).

3. Numerical procedure

At low energies, the interaction between the projectile and the target atom is described using a screened Coulomb potential. The corresponding scattering cross section increases with decreasing energy giving rise to multiple scattering of projectiles in subsurface layers. There, single scattering models are inappropriate to describe trajectories of projectiles that penetrate into deeper layers. For this purpose, we use a Monte Carlo simulation [16] based on the TRIM (TRansport of Ions in Matter) code [17] which is valid for amorphous and polycrystalline targets. The trajectory of each incident ion is determined allowing for multiple collisions. This calculation is based on the binary collision approximation (BCA) and the trajectories are asymptotic. The Thomas–Fermi–Moliere (TFM) potential [18] is used with a correction factor $C_a = 0.75$ to the screening length [19]. For each collision, the scattering angle θ is calculated using the so-called magic formulae [17]. Electronic energy loss between two consecutive binary collisions is calculated according to the experimental values determined by Markin et al. [20].

We have adopted the following method to include charge exchange processes in the model: first, from the threshold energy for reionization, E_{th}, the minimum distance between the collision partners, R_0, was calculated for the scattering angle $\theta = 129°$, using the mentioned scattering potential. Then, the scattering angles, θ_0, corresponding to the minimum distance R_0, were calculated for different values of the projectile energy E (Fig. 2).

In the simulation of the trajectories, the scattering angle θ and the value of θ_0 are calculated for each collision. If $\theta \geqslant \theta_0$, the collision is considered as a 'close collision' where resonant neutralization and reionization are possible. The corresponding data as the projectile energy E before the collision and the scattering angle θ are stored. In this manner, we obtain a set of data for each scattered particle: the final energy, the number of close collisions, the distance between each two consecutive close collisions and the total path length.

To account for charge exchange, in a first step AN is included along the trajectory. The target electrons are described with a jellium of effective density [21], which is assumed to extend into vacuum up to the jellium edge at a distance $d/2$ (where d = 2.35 Å is the interlayer distance). Corresponding to the effective jellium density, we consider a constant Auger neutralization rate Γ.

If the trajectory includes close collisions, charge exchange due to RN and RI is taken into account with probabilities P_{RN} and P_{RI} respectively. When RI occurs in proximity to the surface, the