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Mechanism of adatom formation on Ag(1 1 0) studied by combined quasi-elastic He atom scattering and low energy ion scattering

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Abstract

Two complementary techniques, i.e. low-energy ion scattering in the neutral impact collision ion scattering spectroscopy (NICISS) mode and energy resolved He atom scattering (HAS) are combined to study the adatom formation mechanism on Ag(1 1 0). The NICISS spectra have been collected between 300 and 900 K along the $\langle 0\,0\,1\rangle$, $\langle 1\,\bar{1}\,2\rangle$ and $\langle 1\,\bar{1}\,0\rangle$ azimuthal directions while HAS measurements of the diffuse elastic peak has been performed along the $\langle 1\,\bar{1}\,0\rangle$ directions between 190 and 800 K. Both techniques are sensitive to surface disorder and HAS data have been corrected by using the NICISS results in particular on the anharmonicity estimated through a two atoms scattering model. In fact, above 500 K surface anharmonicity is clearly detected and accompanies the proliferation of thermal induced defects. Without this anharmonic correction the adatom formation energy E_a is too low and similar to the surface diffusion barrier. Instead, including the anharmonicity the estimate, $E_a = (0.38 \pm 0.03)$ eV, is in excellent agreement with the predictions of molecular dynamics simulations.

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1. Introduction

The proliferation of thermal induced defects on surfaces has been widely investigated over the last decades both experimentally and theoretically [1]. Among surfaces, the (1 1 0) face of silver has shown a rich phenomenology on increasing the sample temperature up to the bulk melting point. Surface disordering on Ag(1 1 0) sets in above ~600 K as observed by He atom scattering (HAS) [2]. Later, an STM study suggested that the step-edges which bound the flat terraces start to fringe at 500 K [3], temperature at which both HAS and low-energy

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ion scattering (LEIS) spectroscopy results show an extra increase of the mean vibration amplitude of the topmost layer atoms [4,5]. The evolution of the Ag(1 1 0) surface morphology at the onset of surface disordering was theoretically investigated by Trayanov et al. [6]. Their results suggested that anisotropic defects of the missing row type, i.e. $\langle 1\,\bar{1}\,0\rangle$ missing rows or segments of them are thermal induced above 600 K and this prediction has been recently confirmed by LEIS results [7]. The study of adatom diffusion on the flat f.c.c. (1 1 0) terraces is demonstrated to be easy along the $\langle 1\,\bar{1}\,0\rangle$ atomic channels where jumping between first neighbor absorption sites is suggested as the main diffusion mechanism while, along the cross-channel $\langle 0\,0\,1\rangle$ direction, self-diffusion is proved to be more difficult and to occur preferably by exchange [8]. We investigated surface self-diffusion on Ag(1 1 0) by quasi-elastic HAS between 300 an 800 K [9] and the energy barrier for diffusion has been estimated as $E_d = (0.29 \pm 0.3)$ eV, in good agreement with theoretical predictions. Another fundamental value is the energy to create an adatom, E_a. A method to determine E_a has been introduced by Silvestri, Graham and Toennies (SGT) [10] through the analysis of the quasi-elastic HAS intensity as a function of the temperature. Unfortunately, the study of the Ni(1 1 0) surface gave a greater adatom formation energy than that predicted by calculations and the SGT results were further questioned by Theis [11] who suggested that the observed scattering contribution is not due to adatoms but is most likely caused by step meandering. Recently, we have carried out a new set of quasi-elastic helium scattering data obtained on the (1 1 0) surface of silver [12] and we have repeated the SGT analysis because a previous LEIS study suggests that the quasi-elastic HAS intensity diffused along the $\langle 1\,\bar{1}\,0\rangle$ surface channels has to be mainly ascribed to silver adatoms [7]. We show that the SGT analysis has to be modified by including anharmonic contribution to the atomic vibration otherwise a very low value of E_a, similar to E_d, is obtained. The parameters of anharmonicity estimated by the ion scattering data provide a reliable correction for the quasi-elastic HAS data and details on the adopted model and on the calculation are given in the present article. This shows that these techniques are truly complementary and for the first time their combination is used to get a consistent description of surface properties.

2. Experimental method

The LEIS measurements have been performed in Osnabrück with the scattering machine described in detail elsewhere [13]. Briefly, a 2 keV, Ne^+ primary beam is produced within a plasma ion source, mass selected with a magnetic filter and pulsed sweeping it over a small opening in front of the magnet. The scattered ions and neutrals are collected by a time-of-flight (TOF) detection system at fixed scattering angle, $\Theta = 165°$, measured with respect to the incoming beam direction, in the neutral impact collision ion scattering spectroscopy (NICISS) mode. The operating pressure in the main chamber is in the 10^{-10} mbar range. The Ag sample is heated radiatively and the surface temperature, T, is measured using a thermocouple and a pyrometer. The target is cleaned in situ by 2 keV, Ne^+ sputtering and the possible damage is annealed at 800 K. The surface structure is checked by LEED and by NICISS in blocking mode and the azimuthal orientation of the crystal is determined within ±1°. The scattered intensity is measured versus the polar angle (ψ, referred to the surface plane) to obtain the usual NICISS scans.

The helium scattering experiment has been performed in Genova by means of the custom-built scattering apparatus described in [14]. The supersonic He nozzle beam is produced at source temperature of 36 K and source pressure of 5 bar with most probable energy, E, of about 7.3 meV corresponding to a wave vector $k = 3.76$ Å^{-1}. Before interacting with the sample, the beam is mechanically chopped in short pulses of a few μs of duration. The scattered atoms are collected at fixed scattering angle $\Theta = 70°$ using a time-of-flight detection system. The incident angle, Θ_i and the final angle, Θ_f, are referred to the surface normal and are changed simultaneously by rotating the sample ($\Theta = 180° - (\Theta_i + \Theta_f)$). The base pressure of the scattering chamber is in the 10^{-11} mbar range. The Ag specimen is cleaned in