ATOMIC SCALE ANALYSIS OF DEFECT STRUCTURES IN SINGLE CRYSTALS BY ION SCATTERING AND CHANNELLING

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The defect structures such as surface atomic steps and point defects have been studied by computer simulation of ion scattering and channelling processes. The energy and angular distributions of ions scattered and dechannelled from semi-infinite and isolated steps on the Cu(100) and GaP(100) surface as well as the characteristics of particles channelled through Cu(100) with point defect structures have been calculated. It was shown that the low energy ion scattering and channelling can be use successfully for analysis of defect structures in single crystals.

Key words : *surface atomic steps, point defects, ion scattering, channeling, computer simulation*

1. Introduction

Ion bombardment of a solid surface leads to radiation-induced vacancy defects, atomic steps and their clusters, as well as the atomic scale relief ($< 100\,\text{Å}$) formation. There is a correlation between the defect type, the blocking angles of the reflected beam and the energy distributions of the scattered particles [1–4]. The detection of scattered ions which is known as ion scattering spectroscopy or low-energy ion scattering provides a powerful tool for surface analysis that is exclusively sensitive to the outermost atomic layers.

In [5] the number of step-atoms formed on the Cu(100) surface at $T = 300\,\text{K}$, predamaged by 10 keV Ar^+ ion bombardment with the current density on the target within the range of 10^{-16}–$10^{-8}\,\text{Å}\,\text{cm}^{-2}$, has been estimated. Fig. 1 shows both the energy distributions of the total number (ions plus neutrals) and the ion component of the argon particles scattered by the Cu(100) surface in the direction ⟨100⟩ for two incidence angles of $\psi = 7°$ (a) and 23° (b) and a constant scattering angle of $\theta = 30°$. A possibility of scattering at the angle $\theta = 30°$ under small ($\psi < 10°$) and large ($\psi > 20°$) angles of incidence is conditioned by the fact that the bombardment introduces irregularities into the perfect infinite atomic chain, i.e. it becomes finite and is followed with the step-'up' or 'down' (See, the top of Fig. 1a, b). The particles having undergone the quasi-single scattering on the edge of step contribute to the peaks 1 and 1' of the spectrum, and the particles reflected by the edge of step with the previous or subsequent specular scattering on the ordered atomic chain contribute to the peaks 2 and 2' [5]. The number of the step-atoms formed under ion bombardment, and

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