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Investigation of thermal vibration correlation of [1 1 0] silicon lattice atoms by ion scattering

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Abstract

When a beam of fast ions hits an atom, a shadow cone is formed behind the atom. By varying the ion energy, the radius of the shadow cone can be changed and also the interaction probability between ions and lattice atoms. At strong vibration correlations, neighboring atoms are located almost inside the shadow cone and this acts to reduce the interaction probability. The Si–$KL_{23}L_{23}$ Auger electron emission was used to detect the reduction of the interaction between ions and lattice atoms, which is a measure for the vibration correlation. The yield of the Si–$KL_{23}L_{23}$ Auger electrons was measured as a function of the incidence angle around the [1 1 0] axis with ions. The correlation coefficient was determined by comparison of the minimum Auger electron yields with the results of computer simulations. It has been shown that the ion induced Auger electron emission can be used as a sensitive method for studying the thermal vibration correlation of a surface. The correlation coefficient of the normal displacement of nearest-neighbor silicon atoms along [1 1 0] at room temperature is determined to be 0.90.

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1. Introduction

In former experiments [1], diffraction rings of 3.7 MeV α-particles passing through thin silicon crystals were observed around the [1 1 0] axis direction. The angular radii of the rings are in good agreement with theoretical calculation [2]. The intensity distribution of the diffraction rings (four rings were observed), however, can be explained only if neighboring lattice atoms vibrate almost completely in phase. It indicates that the vibrational correlation of the normal displacement of two neighboring atoms along [1 1 0] is unusually

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strong (the correlation coefficient $C \approx 1$) and greater than theoretical calculation [3]. According to Steif et al., the correlation coefficient between nearest-neighbor lattice atoms was found to be $C_{\parallel} = 0.815$ along the bond and $C_{\perp} = 0.303$ in the directions normal to the bond.

In the present work, the thermal vibration correlation of [1 1 0] silicon lattice atoms was investigated by ion scattering. When a parallel beam of fast ions hits an atom, a shadow cone is formed behind the atom. By varying the ion energy, the radius of the shadow cone R_M can be changed and also the interaction probability between ions and lattice atoms [4]. At weak vibrational correlations, there is a computable probability that neighboring atoms will be outside the shadow cone. So the interaction between ions and lattice atoms will be increased. At strong vibrational correlations, however, neighboring atoms are located almost inside the shadow cone and this acts to reduce the interaction probability. The amount of this reduction is a measure for the vibrational correlation coefficient. The Si–$KL_{23}L_{23}$ Auger electron emission was used to detect the reduction of the interaction between ions and lattice atoms. In this case, the adiabatic distance $r_{ad} = \hbar v/E_K$ for the ionization of the K-shell, where v is the velocity of the ion and E_K is the binding energy 1839 eV of the K-shell [5], is comparable to the shadow cone radius R_M. The ratio r_{ad}/R_M is 0.69, 0.37, 0.60 and 0.47 for $^4He^+$ 2.14 MeV, $^4He^+$ 1.14 MeV, H^+ 0.64 MeV and H^+ 0.5 MeV, respectively. This increases the sensitivity of this method especially at strong vibrational correlations. Additionally, the small escape length of the Auger electrons enhances this sensitivity, for the Auger signal comes only from some upper layers.

2. Experimental

The experiments were carried out in an ultra-high vacuum (UHV) chamber with a base pressure of less than 2×10^{-7} Pa, connected to a 3 MeV Van-de-Graaff accelerator. Monoenergetic 2.14 MeV and 1.14 MeV $^4He^+$ ion beams and 0.64 MeV and 0.5 MeV H^+ ion beams with a current density of typically 60 nA/mm^2 and a maximum divergence of ±0.01°, entered the chamber through a 1 mm diameter collimator. The beam is incident on the Si(1 0 0) surface at an angle of 45°, along the low-index [1 1 0] direction. The chamber is equipped with a surface barrier detector for Rutherford backscattering spectrometry (RBS) at nearly 180° to the beam and a cylindrical mirror analyzer (CMA) for ion induced Auger electron spectroscopy (AES) at 90° to the beam. A step motor with an accuracy of 0.01° is attached to the goniometer of the sample holder in order to scan the channeling profile around the low-index [1 1 0] direction. The surface of the silicon sample was cleaned in situ by cyclic sputtering and annealing. After this procedure, the Auger spectrum showed an atomically clean surface, and a sharp two-domain (2×1) diffraction pattern was observed with low energy electron diffraction (LEED). The CMA was operated in an energy-differential mode with the conventional lock-in technique. The Auger electron yield was determined from the peak-to-peak height in the differentiated spectrum.

The low-index [1 1 0] crystal axis of silicon was determined by RBS measurement. The yield of the Si–$KL_{23}L_{23}$ (1619 eV) Auger electrons was measured as a function of the incidence angle Φ between the incident beam and the [1 1 0] lattice direction. Ion induced Auger electron emission has been the subject of numerous studies [5–9]. Fig. 1 shows the relative reaction yield of (a) RBS and (b) Si–$KL_{23}L_{23}$ Auger electrons induced by 2.14 MeV $^4He^+$ as a function of angle Φ. The half-angular width $\Phi_{1/2}$ and the minimum yield Y_{min} ($= Y_{cha}/Y_{ran}$), which is the ratio of the yield at channeling condition ($\Phi = 0.0°$) to the yield at random condition ($\Phi = \pm 1.0°$) of the RBS channeling profile are 0.43° and 0.057, respectively. The half-angular width $\Phi_{1/2}$ and the minimum yield Y_{min} of the AES channeling profile are 0.47° and 0.45 ± 0.04, respectively. The theoretical value of $\Phi_{1/2}$ that can be calculated by the critical angle Φ_C [2,10] is 0.47°. A great discrepancy reveals in the minimum yields of RBS and AES, which can be understood with the difference in the interaction probability between ion beams and lattice atoms. Because of the adiabatic distance r_{ad} of the K-shell, the minimum yield of AES is greater than that of RBS. Table 1 summarizes the experimental