분과초청 1

Investigation of the thermal vibration correlation of [110] silicon lattice atoms by ion scattering

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In former experiments [1], diffraction rings of 3.7 MeV α-particles passing through thin silicon crystals were observed around the [110] axis direction. The angular radii of the rings are in good agreement with theoretical calculations of Lindhard [2, 3] and Kagan [4]. 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 [5].

It indicates that the vibrational correlation of the normal displacement of two neighboring atoms along [110] is unusually strong ($C \approx 1$) and greater than theoretical calculations [6, 7] estimate: according to Steif et al. [7], the correlation coefficient between nearest-neighbor lattice atoms was found to be $C_{||}=0.815$ along the bond and $C\perp=0.303$ in the directions normal to the bond.

In the present work, the thermal vibration correlation of [110] silicon lattice atoms was investigated by ion scattering. It has been shown that energetic light ions ($^4He^+$, H^+) which are incident along the [110] direction can be used as a sensitive probe for studying the vibrational correlation of the normal displacement of nearest-neighbor lattice atoms along [110]. When a parallel beam of fast ions hits an atom, a shadow cone is formed behind the atom. By varing the ion energy, the radius of the shadow cone can be changed and also the interaction probability between ions and lattice atoms. 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 for ionization of the K shell is comparable to the shadow cone radius. 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.

The low-index [110] crystal axis of silicon was determined by Rutherford backscattering. The yield of the Si-$KL_{23}L_{23}$ Auger electrons was measured as a function of the incidence angle Φ about the [110] axis thereafter. The correlation coefficient C was determined by comparison of the minimum Auger electron yield Y_{min} (= Y_{cha} / Y_{ran}) with the results of computer simulations. In computer program, the trajectories of incident particles and their reactions (Auger electron emission) with lattice atoms are simulated. The degree of correlation in the lattice motion is modulated by the correlation coefficient C which is inserted in computer program as parameter. Within the region between C=0.0 and C=0.6, the minimum yield is a nonsensitive measure for the correlation. However, the dependence becomes strong for C>0.6.

Auger electron yield profiles were measured at room temperature and at high temperatures (T = 670K and 870K). At room temperature, 2.14 MeV $^4He^+$, 1.14 MeV $^4He^+$ and 0.64 MeV H^+ projectiles were used. The value of the vibrational correlation coefficient of 0.5 MeV H^+ measurements at room temperature agrees well with those of high energetic projectiles as expected. Within the temperature region studied, no significant dependence between the vibrational correlation coefficient and the crystal temperature can be found.

Consequently, the correlation coefficient of the normal displacement of nearest-neighbor silicon atoms along [110] at room temperature is determined to be C=0.90±0.02. It is obviously greater than the expected value in theoretical calculations.

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