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IT-5-P-1944 Planer defect structure analysis based on electron channeling phenomena

Ichikawa T.[1], Ohtsuka M.[1], Muto S.[2]

[1]Nagoya University, Nagoya, Japan, [2]EcoTopia Science Institute, Nagoya, Japan

Email of the presenting author: ichikawa.takahiro@a.mbox.nagoya-u.ac.jp

High-angular resolution electron channeled X-ray spectroscopy (HARECXS) is based on the principle that the electron wavefunctions (Bloch waves) in a crystalline sample change their symmetry with the incident beam direction. HARECXS has been applied to the analysis of point defects, partly because ICSC [1] has been only the theoretical simulation code available to date for predicting the inelastic scattering cross sections depending on the diffraction condition, which does not allow us to include 2D/3D defects. In this study an attempt is made to apply HARECXS to a planner defect lying on the {111} plane in heavily Si-doped GaAs [2] to extend its applicability.

Thin films were prepared by dimpling the sliced single crystalline wafers followed by Ar ion milling. HARECXS was carried out using a JEM-2100 S/TEM equipped with an EDX spectrometer, operated at the beam-rocking mode at 200kV. The illuminated area was about 1μm in diameter and the incident beam angle was rocked by ±1.5 degrees with a step of 0.05 degrees under the systematic row excitation condition.

A bright-field TEM image of the planer defect nearly viewed end-on is shown Fig. 1(a) and the corresponding HARECXS profiles in (b), as functions of the incident beam direction in units of $g_{1\text{-}11}$, tilted in the direction perpendicular to the projected defect plane. The HARECXS profiles of the Ga- and As-K lines have a different symmetry due to the polarity of the GaAs. The slight asymmetric profile of Si-K similar to that of As-K suggests that Si mainly occupies the As sites. The theoretical simulations based on the model where a Si atom substitutes for the As and Ga sites are shown in Fig. 2(a), using the Bloch wave [1] method with the dynamical inelastic scattering process incorporated. For comparison, more realistic models where Si occupies the single (111) Ga or As layer are also simulated, as shown in Fig. 2(b), in which a multislice method [3] is developed for including a planar defect in the simulation. The simulation result with Si occupying the As single layer seems to be relatively more consistent with the experimental Si-K HARECXS profile.

References

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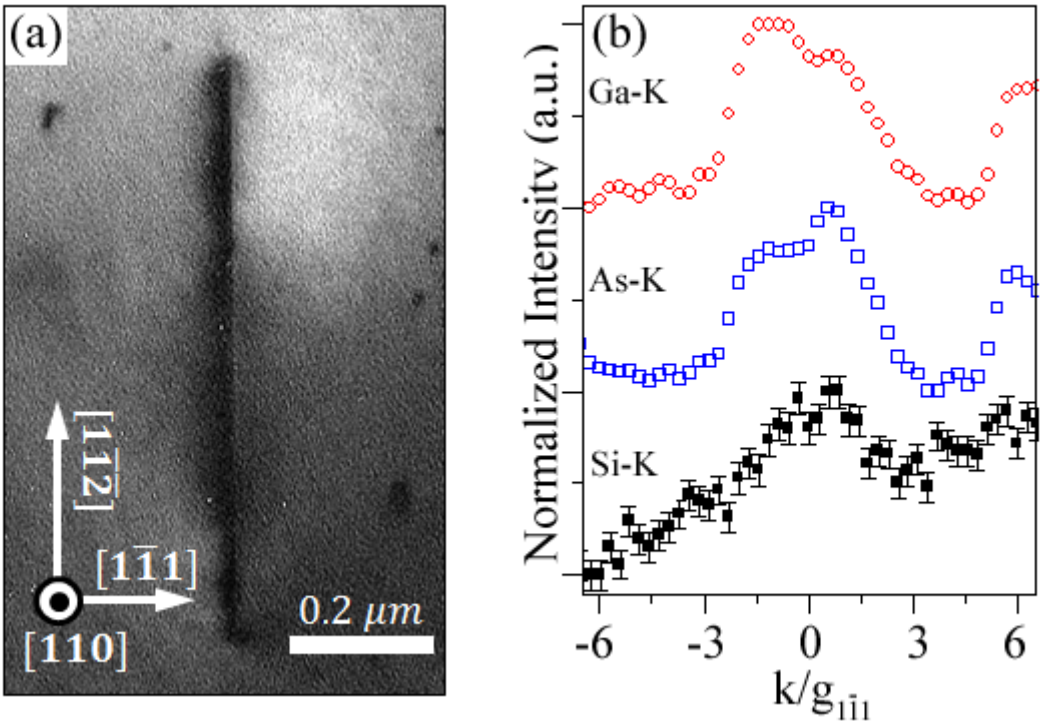

Fig. 1: (a)Bright-field TEM image of planer defect in Si-doped GaAs nearly viewed end-on. (b)HARECXS profiles of Ga-K, As-K, and Si-K characteristic X-ray peaks as functions of incident beam direction in units of $g_{1\text{-}11}$.

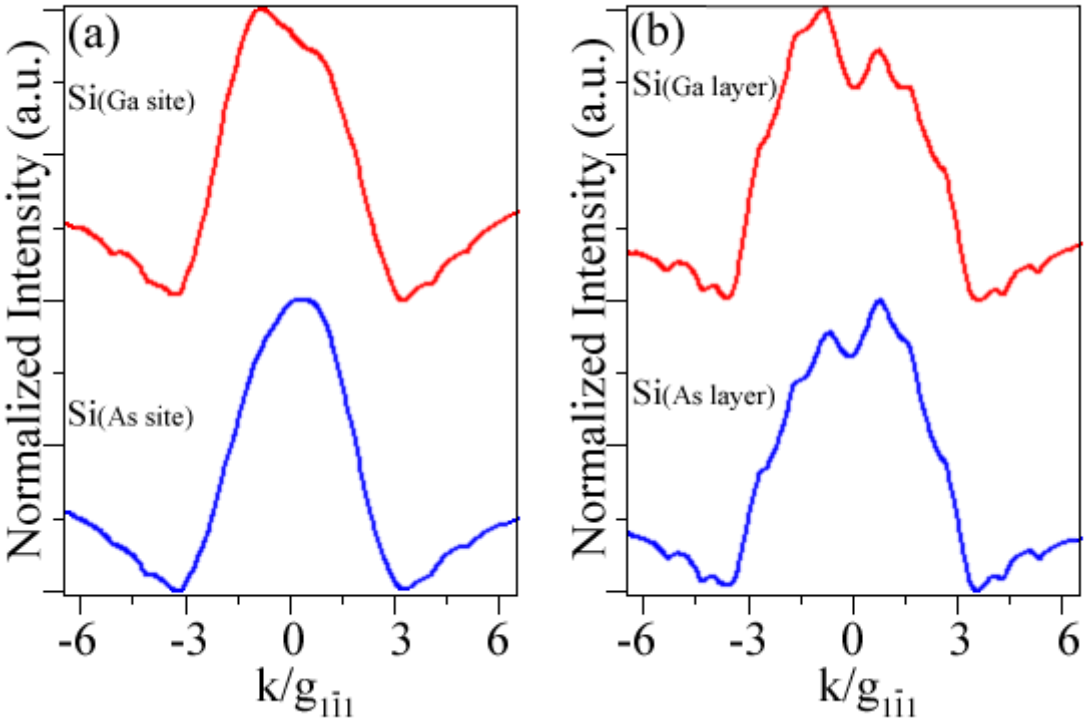

Fig. 2: Theoretically simulated HARECXS profiles for models where Si atom substitute for Ga (red) and As (blue) sites (a) and Si occupies single (111) Ga (red) and As (blue) atom layers (b).