

Atomic structures of As/Si(111)-(1 x 1) by normal and anomalous crystal truncation rods

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Introduction

Surface x-ray diffraction is a powerful tool in the study of thin-film surface growth and structure. Crystal truncation rod (CTR) analysis is uniquely sensitive to surface atomic arrangement. Moreover, CTR analysis can be used in combination with anomalous scattering techniques to isolate the contribution of surface adatoms of different atomic species. We present our effort to study atomic structures of As adatoms adsorbed on the Si(111) surface by collecting normal and anomalous CTRs through deposition. The resultant (1 x 1) surface has a very simple structure that has been studied by various methods such as medium-energy ion scattering, x-ray standing wave, and photoelectron holography [1].

Methods and Materials

Our experiment was performed at the UNI-CAT surface/interface experimental station on the undulator beamline of sector 33. The experimental station provides an ultrahigh vacuum surface diffractometer with molecular beam epitaxy capabilities. A Si(111) wafer was cleaned by direct current heating up to 1250°C and verified by observing a (7 x 7) diffraction pattern. Arsenic vapor was generated by heating well-outgassed GaAs chips in an effusion cell; 1.4 to 1.8 x 10⁻⁷ torr of As ambient maintained for 10 minutes. The sample was held at room temperature during adsorption.

We then annealed the sample at progressively higher temperatures from 470°C to 690°C. At each step, the annealing time was one to three minutes. We observed reflection high-energy electron diffraction (RHEED)-like RSXD (reflection surface x-ray diffraction) patterns using a cooled CCD during annealing. We continued the annealing steps until 7 x 7 spots dimmed and completely disappeared at 600°C. The spot intensities disappeared at different heating steps. The sample was annealed at 690°C for 10 more minutes. No more improvement on the spot width was observed.

Results and Discussion

First, crystal truncation rods were measured at different x-ray energies near the As K-edge (11.867 keV). The measured CTRs are (10L) and (00L) rods in the conventional (111) diamond surfaces. At various fixed momentum transfers, intensity changes were measured to observe anomalous x-ray scattering in CTRs. The well-

accepted model for the As/Si(111)-(1 x 1) is an ideally truncated (111) surface with the top layer of the bilayer occupied by As atoms.

Analysis is under way. The preliminary results show that the As layer is relaxed outward from the normal Si position by 0.27 Å. The various published values are from 0.17 to 0.24 [2]. These results are from fitting the model to (10L) CTR shown in Figure 1. The same set of parameters were used to fit (00L) CTR and anomalous x-ray scattering at (1 0 1.9) shown in Figures 2 and 3.

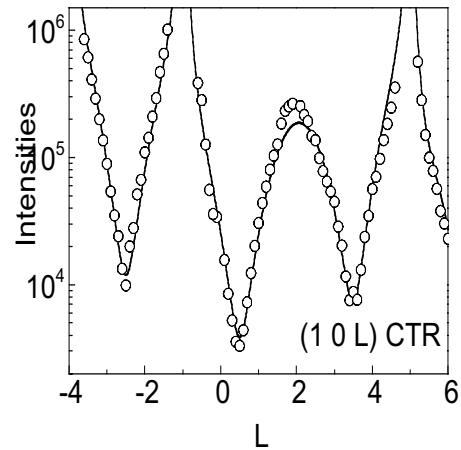


Figure 1: Results from fitting the model to (10L) CTR.

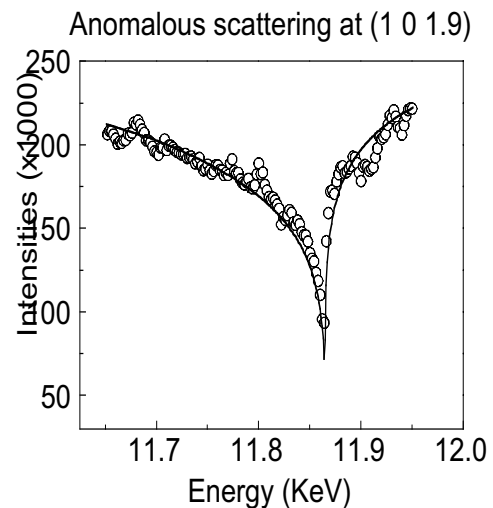


Figure 2: Anomalous scattering at (1 0 1.9).

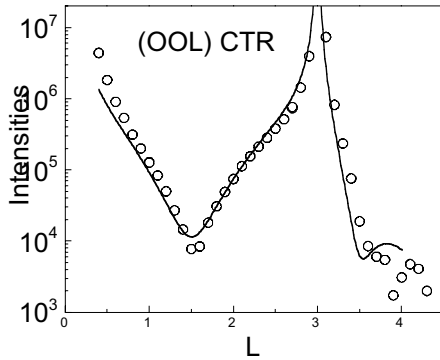


Figure 3: Fit (00L) CTR.

Only the overall scaling factor was varied to make them fit. Figure 4 shows other anomalous scattering data at (0 0 3.5) where the interference between the As layer and the underlying Si crystal is destructive. Further analysis should produce reliable structural values.

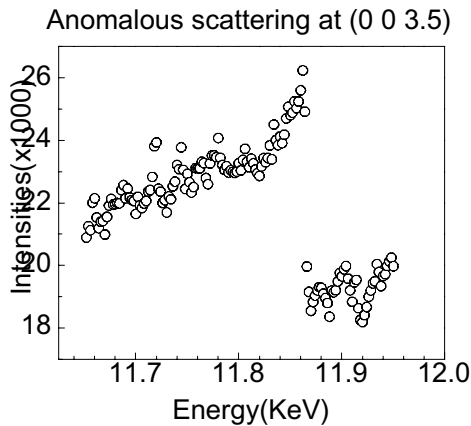


Figure 4: Anomalous scattering at (0 0 3.5).

References

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Acknowledgments

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