X-ray Analysis of CuPt-ordered III-V Semiconductor Ternary Films

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Introduction: CuPt ordering in III-V semiconductor alloy films of the form of $A_xB_{1-x}C$ has been known for quite a long time.[1] However, quantitative analyses have not been done due to the complex structure of the ordered films. This work attempts to fill this need.

Methods and Materials: We have studied two kinds of samples – $Ga_{0.5}In_{0.5}P$/GaAs (001) and $Al_{0.5}In_{0.5}As$/InP (001). X-ray diffraction was done in an inclined geometry by rotating the χ-angle on a four-circle diffractometer, where the diffraction plane is not perpendicular to the film surface. In this way, many inaccessible ordering reflections in a conventional coplanar geometry can be achieved, making our x-ray analyses possible.

Results: Both x-ray reciprocal space maps and line scans were made. Results from one of our samples is shown in the left panel of Fig. 1. In addition to the fundamental reflections, inclined ordering reflections stretched along a direction ~10° away from the [001] direction were also presented, forming a characteristic wavy pattern. Appearance of the ordering reflection in the two {111} directions indicates the existence of two ordering variants along these two directions. The streak running from the upper-left corner to the lower-right corner is due to stacking faults or micro twinning.

To analyze the diffraction data, a structural model considering both the coexistence of two ordering variants along either [1-11] direction or [-111] direction and random distribution of anti-phase domain boundaries in the film was proposed. The atomic displacements due to the bond length difference between the two constitutive binary alloys AC and BC was also considered, which is found to superimpose an extra modulation on the intensity of the ordering reflections.

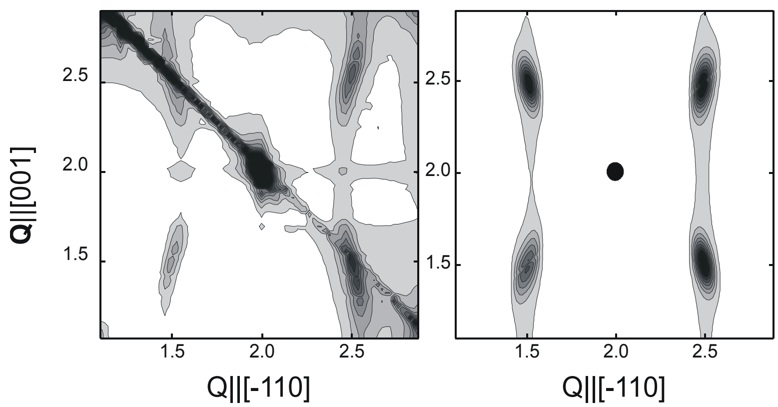

Figure 1. X-ray reciprocal space maps from a CuPt ordered III-V ternary ally film. Left and right panels show respectively the experimental and calculated results.

The right panel of Fig.1 shows a calculated reciprocal space map based on the above considerations, which basically fit quite well the features in Fig.1(a), particularly the inclination and stretching of the ordering peaks and the streaks along the [001] direction. A quantitative comparison of the measured and calculated data is given in Fig. 2, where cross-sectional line scans through the ordering peaks were displayed. The calculated curves agree with their experimental counterparts quite well on both height and width. It is important to notice that the higher order (-2.5,2.5,2.5) reflection is considerably stronger than the lower order (-1.5,1.5,1.5) reflection. This is attributed to the atomic displacements mentioned above. Our analyses also yield an order parameter of ~ 0.3 for both variants.

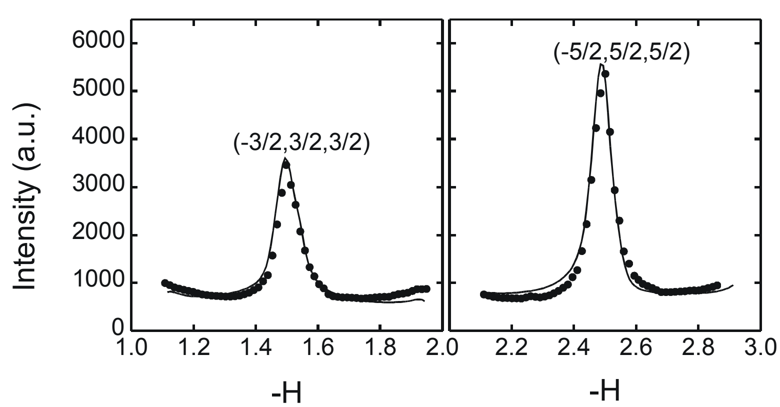

Figure 2. Cross-sectional line scans through the (-1.5,1.5,1.5) reflection (left panel) and the (-2.5,2.5,2.5) reflection (right panel). Solid dots and lines are experimental and calculated data, respectively.

Conclusions: By using a synchrotron x-ray source and a four-circle diffractometer together with a structural model considering the size distribution of the two coexisting ordering variants and anti-phase domains, we have made quantitative analyses of the CuPt ordered III-V ternary alloy films.

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References: 1. C.S. Baxter, W.M. Stobbs, and J.H. Wilkie, J. Cryst. Growth **112**, 373 (1991).