

X-ray Characterization of Quadruple-period Ordering in a GaAs_{0.87}Sb_{0.13} Alloy on GaAs (001)

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Introduction: Atomic ordering in semiconductor alloy films is a surface induced phenomenon. Such ordering can modify the electronic and optical properties of the materials significantly, and thus require thorough understanding. Here we present a quantitative synchrotron x-ray diffraction analysis of quadruple-period atomic ordering in [110] direction in a GaAs_{0.87}Sb_{0.13} alloy film.

Methods and Materials: The GaAs_{0.87}Sb_{0.13} alloy film was grown by MBE at ~ 625°C. X-ray diffraction was carried out on a standard four-circle diffractometer with an x-ray energy of 8.048keV.

Results: The upper panel of Fig. 1 shows an x-ray transverse scan along [110] direction (from reciprocal lattice point 111 to 331). Sharp ordering peaks at one quarter, three quarters, five quarters and seven quarters of the scanning range are observed. However, the peaks of two, four and six quarters were not seen. This indicates that a superstructure has been formed in the film that causes the extinction of the even order peaks.

To explain this data, a model of atom arrangement, including displacements is proposed, as shown in the lower panel of Fig. 1. The unit cell of the superstructure is composed of 8 Ga atoms (labeled 1-8), 4 As atoms (labeled A,B,a,b), and 4 atoms (labeled C,D,c,d) which can be either Sb or As with a corresponding probability of P_s and P_a . Considering our particular sample, we assume $P_s=0.26$ and $P_a=0.74$. As seen in the model, atoms are displaced from the ideal zincblende lattice sites. These displacements were obtained by a valence force field model calculation via minimizing the total energy of the system.¹ The model structure in Fig. 1 shows schematic displacement of the atoms. The structure factor of a superstructure unit cell can be written as:

$$F(\mathbf{q}) = \sum_{j=1}^8 \left(\sum_{k=1}^m P_{jk} e^{2\pi i \mathbf{q} \cdot (\mathbf{r}_j + \Delta \mathbf{r}_{jk})} \right) \cdot f_{Ga}(\mathbf{q}) + \sum_{j=1}^4 e^{2\pi i \mathbf{q} \cdot (\mathbf{r}_j + \Delta \mathbf{r}_j)} \cdot f_{As}(\mathbf{q}) \\ + \sum_{j=1}^4 e^{2\pi i \mathbf{q} \cdot (\mathbf{r}_j + \Delta \mathbf{r}_j)} \cdot f_{As}(\mathbf{q}) \cdot P_a + \sum_{j=1}^4 e^{2\pi i \mathbf{q} \cdot (\mathbf{r}_j + \Delta \mathbf{r}_j)} \cdot f_{Sb}(\mathbf{q}) \cdot P_s$$

A simulation without atom displacements is shown in the inset of Fig. 1. Clearly, the simulation does not fit the measured intensity profile. To obtain a satisfactory fit, atomic displacements must be taken into account. By doing so, we obtain the fit in Fig. 1 (solid line). A good agreement was then achieved for the intensity profile. The poor fit of the peak width at the one quarter and the seventh quarter position is due to the anti-phase structure in the film, which is not considered here.

Based on the structural model in Fig. 1, we propose that the quadruple-period ordering is caused by a 2×4 surface reconstruction together with the atomic displacements.

Conclusions: Quadruple-period ordering along [110] in a GaAs_{0.87}Sb_{0.13} alloy film is observed by XRD. A superstructure model was proposed which considers the atomic displacements due to the disparate property of the two group V atoms. Both of them are essential in order to fit the experimental curve. Our results suggest a possible mechanism for the formation of the quadruple-period ordering.

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References: 1. P.N. Keating, Phys. Rev. **145**, 637 (1966).

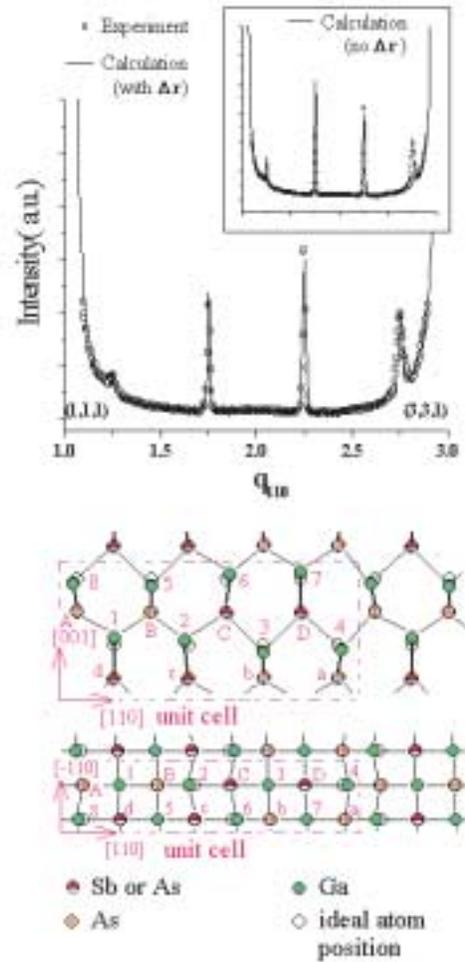


Figure 1. The upper panel is an x-ray transverse line scan along the [110] direction in between of the two reciprocal lattice points 111 and 331. Solid line is the theoretical fit to the measured data (solid dots). The inset shows the fit without taking into account the atomic displacements. The lower panel is the proposed atomic structural model containing a super unit cell.