**Materials Science** 

# **XAFS** studies on In<sub>1-x</sub>Ga<sub>x</sub>Sb mixed crystal

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## **Introduction**

 $In_{1,x}Ga_xSb$  mixed crystals are widely used for infrared (IR) telecommunication as raw materials of detecting and emitting IR devices, because the narrow band gap of this system can be controlled simply by the change of the concentration of cations. Due to the large difference of lattice constants of InSb and GaSb crystals, however, it is hard to make a single crystal except in the very low In or Ga concentration ranges of some %.

In a similar mixed crystal Ga<sub>1-x</sub>In<sub>x</sub>As, a conflict on its structural studies were reported between X-ray diffraction (XD) and X-ray absorption fine-structure (XAFS) experiments [1]. The former indicates Vegard's law, i.e., the lattice constant linearly changes with varying the concentration x, while the latter reveals a Pauling's bond length, i.e., an almost constant Ga-As or In-As interatomic distance is preserved all over the concentration range. From a detailed XAFS analysis, they proposed a model that the anion (As) sublattice is more distorted with two distributions of As-As distances, while the cation (Ga,In) sublattice approximates a rigid fcc lattice. On the other hand, our recent study of X-ray fluorescence holography (XFH) on Zn<sub>1-x</sub>Mn<sub>x</sub>Te diluted magnetic semiconductor with the same zinc-blende structure indicates the completely opposite conclusion on the lattice distortion [2].

Before measuring XFH for the  $In_{1-x}Ga_xSb$  mixed crystal, we have measured XAFS and XD in advance to find if such a conflict between the XD and XAFS results is also observed in this mixed crystal [3].

### **Experimental procedure**

The  $In_{1,x}Ga_xSb$  polycrystals (x = 0, 0.2, 0.6, 0.8, and 1.0) were prepared as follows. After sealing the proper amount of InSb and GaSb mixtures into quartz ampoules, the molten samples were mixed at the temperature of 800 °C, and then annealed in the solid phase of 500 °C for more than one week. The XD experiment was performed by using a powder diffractometer (RIGAKU RINT2000) with Cu K<sub>\alpha</sub> radiation. The In and Sb K XAFS measurements were carried out at NW10A of the PF-AR/KEK, and the Ga K XAFS at BL9A of PF/KEK. All the XAFS measurements were analyzed by using FEFF8 code to calculate the bond lengths, the coordination number, and the mean-square displacement.

## **Results and discussion**

Figure 1 shows the concentration dependence of the nearest-neighbor distance obtained from XD and XAFS experiments for the In<sub>1x</sub>Ga<sub>x</sub>Sb mixed crystals. The triangle are the calculated values of the bond length from the lattice constant of the XD results for the zinc-blende structure. As clearly seen in the figure, the nearestneighbor distance obtained from this method shows the Vegard's law behavior, i.e., it linearly changes with varying x. On the contrary, results from the XAFS experiments show that the nearest-neighbor distance changes very little; it looks largely keeping the Pauling's bond lengths of In-Sb and Ga-Sb, being different by almost 0.02 nm. Thus, these structural results revealed a serious inconsistency between the periodicity over a wide distance range, and the local structure as previously reported for the similar mixed crystal of Ga<sub>1,x</sub>In<sub>x</sub>As [1]. The XFH experiment becomes very important to solve such a structural inconsistency [3].



Fig. 1 The concentration dependence of the nearestneighbor distance obtained from XD (triangles) and XAFS (circles) results for  $In_{Lx}Ga_xSb$  mixed crystals.

### **References**

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