

Local structure around Si atoms in GeSi alloy semiconductors

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Introduction

Germanium-silicon is a complete solid solution system, having the diamond cubic structure. The 4% difference in the lattice constants of constituent Ge and Si atoms leads various unique alloying phenomena on electronic, optical and mechanical properties. Knowing the accurate local structure is important and crucial in order to clarify the physical origin of such alloying phenomena, relevant to the local strain relaxation. We performed an XAFS study of the local structure of $\text{Ge}_{1-x}\text{Si}_x$ alloys grown by the Czochralski method in the whole composition range $0 < x < 1$ [1]. From Ge-K-edge spectra measured at 20K, the followings are revealed: GeSi alloy possess random substitutional site occupancy of Si and Ge atoms but no preferential ordering across the whole composition range. Ge-Ge and Ge-Si bond lengths maintain distinctly different lengths and vary linearly with alloy composition and to be close, but not completely, to the Pauling limit [2] rather than Vegard limit [3], similar to other semiconductor alloys as GaInAs [4]. The estimated topological rigidity parameter 0.6 suggests that the bond lengths and bond angles are distorted with alloy composition [5]. Thus, it is a task to clarify the local atomic structure and the compositional dependence of Si-Si bond length in GeSi alloys. Here we report preliminary results of XAFS investigations on the local structure around Si atoms in bulk crystalline GeSi alloys in the whole composition.

Experimental

High quality $\text{Ge}_{1-x}\text{Si}_x$ samples ($0 < x < 1$) were prepared from bulk alloy crystals grown by the Czochralski technique [6]. Si K-edge XAFS spectra of $\text{Ge}_{1-x}\text{Si}_x$ samples were measured using the total electron yield (TEY) detection at the soft X-ray XAFS station (BL-11B) of KEK-PF at room temperature. Channel cut InSb (111) was used for monochromator.

Results and Discussion

Figure 1 shows absolute values of Fourier transform $|F(r)|$ of Si K-edge $\kappa^3\chi(\kappa)$ of GeSi of various Si content x at room temperature. The intensity of the main peak around $r = 2 - 2.2 \text{ \AA}$, which is due to the nearest-neighbour atoms around Si atoms, decreases and the distance is shortened with an increase in Si content. Though detailed analysis of the above-shown results is now being conducted by FEFF6 program, the obtained XAFS signals at room temperature seem to be too poor to obtain quantitative information. Thus, we are conducting XAFS measurements at low temperature 20K.

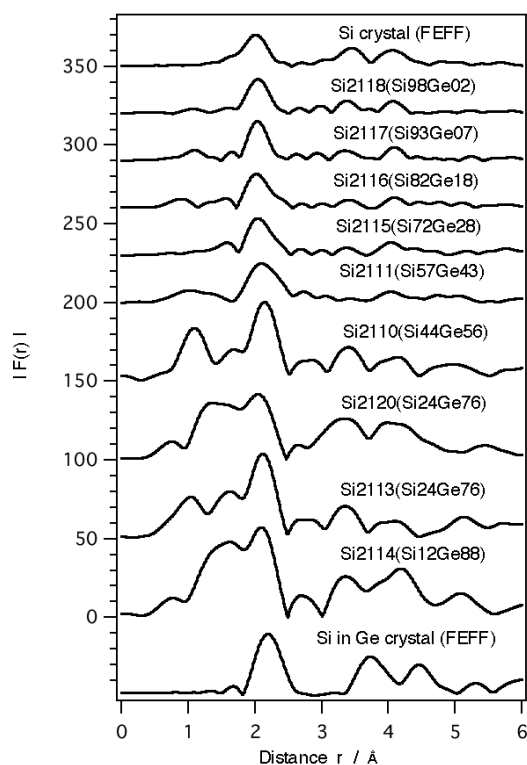


Fig. 1. The Absolute values of Fourier transform $|F(r)|$ of Si K-edge $\kappa^3\chi(\kappa)$ of GeSi of various composition x at room temperature.

In addition, it should be mentioned for future works that some absorption edges originating into unexpected impurities as S, P, Cl, etc. from the used beam-line were recorded on the XAFS spectrum.

References

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