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Local structure around Si atoms in GeSi alloy semiconductors

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Introduction

Germanium-silicon is a complete solid solution. The 4% difference in the lattice constants of constituent Ge and Si atoms leads various unique alloying effects on electronic, optical and mechanical properties. Knowing the accurate local structure is important and essential to clarify the origin with the local strain relaxation. From the Ge-K-edge spectra study on the Czochralski grown $Ge_{1-x}Si_x$ alloys ($0 < x < 1$) at the hard X-ray XAFS station (BL-10B) of KEK-PF [1] we found that GeSi alloy possess random substitutional site occupancy of Si and Ge atoms but no preferential ordering across the whole composition range and that 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]. These results suggest that the bond lengths and bond angles are distorted with alloy composition. Under these results, it is quite interesting to clarify the local atomic structure and compositional dependence of Si-Si bond length in GeSi alloys [3]. Here we report the results of the XAFS measurements of bulk crystal GeSi alloys in the whole composition.

Experimental

High quality $Ge_{1-x}Si_x$ samples ($0<x<1$) were prepared from bulk alloy crystals grown by the Czochralski technique [4]. Si K-edge XAFS spectra of $Ge_{1-x}Si_x$ 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 with channel cut InSb (111) 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. A main peak around r = 2Å, which is due to the nearest-neighbour atoms around Si atoms, is observed and the distance is shortened with increasing Si content. As seen in Fig. 2, the length of Si-Si bond in GeSi alloys vary linearly, similar to those of Ge-Ge and Ge-Si bonds and are parallel to each other as a function of Si content. The results confirm that the bonding feature in GeSi alloys is close to the imperfect Pauling model [1,5] and that the strain due to the alloying in GeSi crystals is accommodated by changes of both the bond length and bond angle.

References

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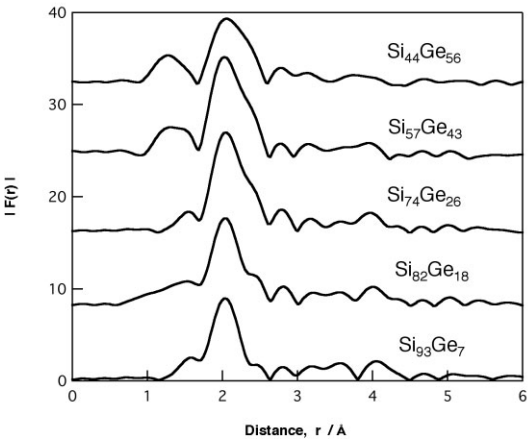

Fig. 1. The absolute values of Fourier transform $|F(r)|$ of Si K-edge $\kappa^3\chi(\kappa)$ of GeSi of various Si content x at room temperature.

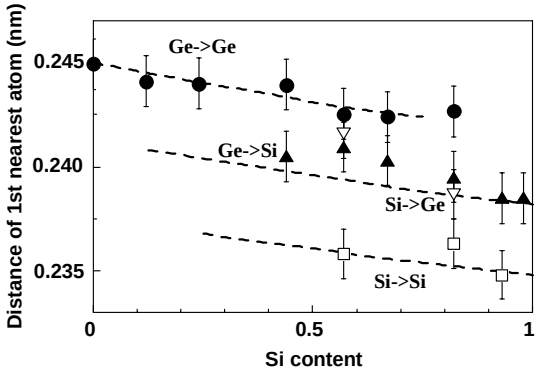

Fig. 2. Ge-Ge, Ge-Si and Si-Si bond lengths as a function of Si content.