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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 system. 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 to clarify the origin with the local strain relaxation. From the XAFS Ge-K-edge spectra study on the Czochralski grown $Ge_{1-x}Si_x$ alloys ($0 < x < 1$) [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, we studied the local atomic structure and compositional dependence of Si-Si bond length in GeSi alloys [3]. Here we report the results of the detailed analysis for 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 the first-shell Ge and Si coordination numbers around Ge and Si atoms derived from the XAFS data as a function of Si content. The results show the random substitutional site occupancy of Si and Ge atoms but no preferential ordering of the Ge-Ge and Si-Si across the entire composition range. 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.

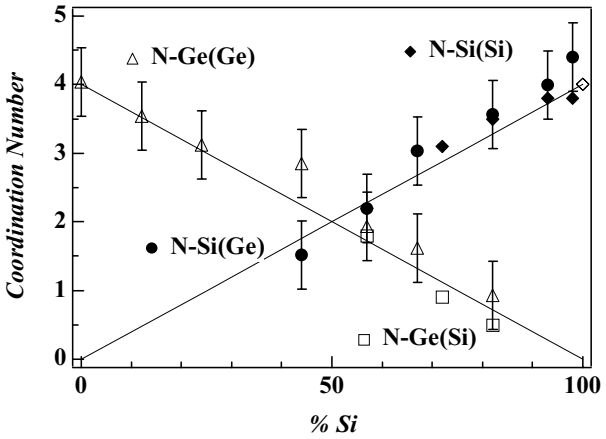

Fig. 1. Ge and Si coordination numbers around Si and Ge atoms derived from XAFS data as a function of Si content.

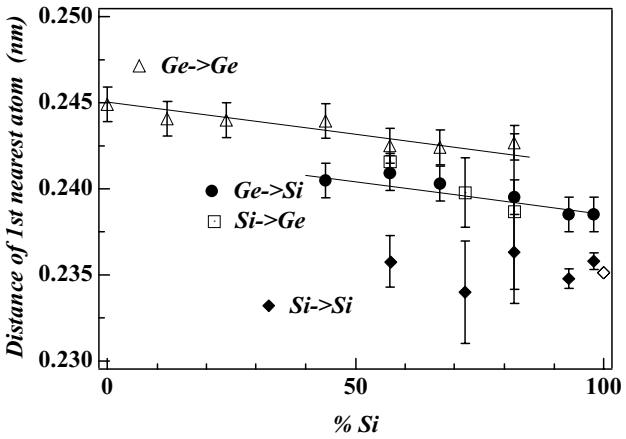

Fig. 2. Ge-Ge, Ge-Si and Si-Si bond lengths as a function of Si content. The symbol shows Si-Si bond length in pure Si.

References

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