Local atomic structure of 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 effects on electronic, optical and mechanical properties. Knowing the accurate local structure is important to clarify the origin, relevant to the local strain relaxation. Here we report results of the detailed analysis for XAFS measurements of bulk crystalline GeSi alloys in the whole composition, preliminarily reported [1].

Experimental

Ge K-edge XAFS spectra of $Ge_{1-x}Si_x$ samples ($0<x<1$) at 20K were measured in transmission mode at BL-10B of KEK-PF. Channel cut Si (111) was used for monochromator. EXAFS parameters for quantitative analysis are calculated by FEFF6 program.

Results and Discussion

Figure 1 shows the first-shell Ge and Si coordination numbers around Ge 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 dimer across the whole composition range. As seen in Fig. 2, the Ge-Ge and Ge-Si bond lengths in GeSi alloys vary linearly and are parallel to each other as a function of Si content. At x=0.5 the Ge-Si bond length is 0.24 nm, the sum of the Si and Ge covalent radii. The results confirm that the bonding feature in bulk GeSi alloys is close, but not completely, to the Pauling limit [2]. The topological rigidity parameter a^{**} [3] is estimated to be around 0.6, which implies that most of the strain originating into the alloying in GeSi crystals may be accommodated by changes of both the bond length and bond angle.

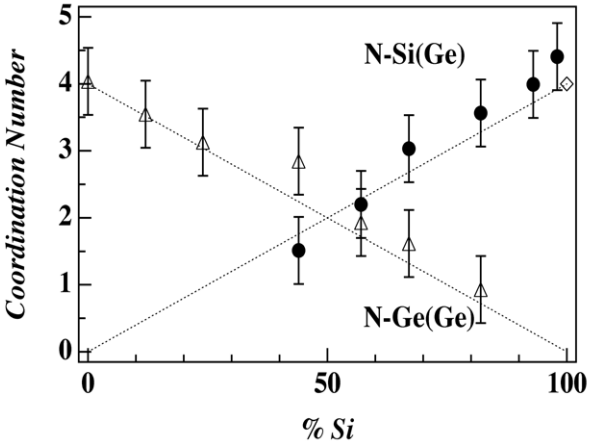

Fig. 1. Ge and Si coordination numbers around Ge atoms derived from XAFS data as a function of Si content. The symbol ◇ is for pure Si. The dashed lines show the coordination numbers predicted from a random mixture of Si and Ge atoms.

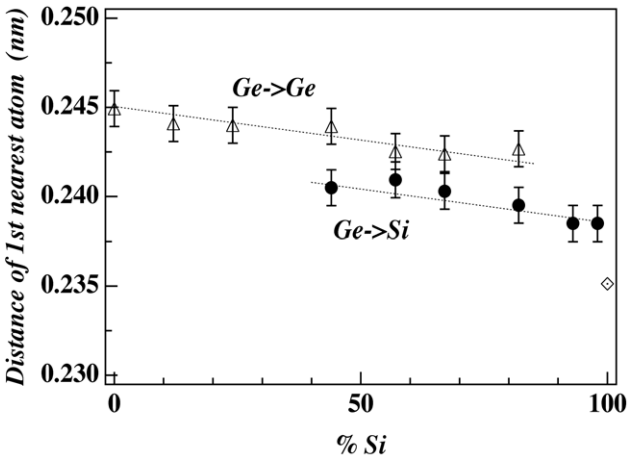

Fig. 2. Ge-Ge bond length (Ge->Ge) and the Ge-Si bond length (Ge->Si) in GeSi alloys as a function of Si content. The symbol ◇ shows Si-Si bond length of in pure Si. The dashed lines are the predicted compositional dependence of the bond lengths within the topological rigidity model (a^{**}=0.60).

References

[1] I. Yonenaga and M. Sakurai, Photon Factory Activity Report 1999 (No. 17), p. 186.
[2] L. Pauling, *The Nature of the Chemical Bond* (Cornell University Press, NY, 1967).
[3] N. Mousseau and M. F. Thorpe, Phys. Rev. **B**46, 16872 (1992).

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