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EXAFS of typical n-type semiconductor Si:As for clarifying real local structure around As

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Introduction

Si:As is the typical n-type semiconductor (although the Si:P is more common now.). In most of texts of solid state physics, the electronic property of the n-type semiconductor and its origin are explained using atomic model of local structure around As. On the other hand, EXAFS analysis by other researchers showed anomalously long interatomic distance between As and 1st neighbor Si, which was 2.44 Å, which was around 0.1 Å longer than Si-Si distance. This distance is about 0.06 Å longer than those of Ga-Si and Ge-Si, implying that strong local distortion forms around As. To clear this atomic distortion, we have performed the X-ray fluorescence holography study of Si:As, where As concentration was 4×10^{-19} cm^{-3}. The obtained 3D atomic image showed 6-coodinated local structure, but did not show 4-coordinated diamond structure unlike to that of Si:Ge. This experimental result is quite different from atomic model in classical idea. Part of this result was described in Ref. 3. However, one problem of our holography experiments was that the Si:As sample measured in holography experiment was very high-doped, and we doubted that its local structure was different from that of the actual Si:As semiconductor. Therefore, we measured EXAFS of both high doped and low-doped Si:As samples, and compare their spectra.

Experimental

Two Si:As samples, whose concentration were 4×10^{-19} and 2×10^{-17} cm^{-3}, were obtained by Czochralski method. Then, they were powdered. As K EXAFS measurements were carried out in fluorescence mode using multi-elements solid state detector. The sample temperatures were 100 K and room temperature, respectively.

Results and Discussion

Figures 1 shows the EXAFS spectra for the Si:As sample of 4×10^{-19} and 2×10^{-17} cm^{-3}. The displayed both spectra are quite similar, revealing that local structures of both samples were same. Therefore, it is known that the six-coordinated local structure verified by the X-ray fluorescence holography normally exists in the semiconductor Si:As.

For 1st shell, we tried to compare experimental EXAFS oscillation χ and theoretical one using the parameters obtained by the X-ray fluorescence holography, as shown in table 1. (lower parameters in table 1) These two χ oscillations fit very well. Then, using the parameters of four coordinated local structure (upper parameter in table 1), we also compare experimental EXAFS oscillation χ and theoretical one. This fitting showed good result. This fact revealed that only the EXAFS measurement cannot clear true local structure. The combination of EXAFS and X-ray fluorescence holography will open a new way of exploring the atomic structures around specified element.

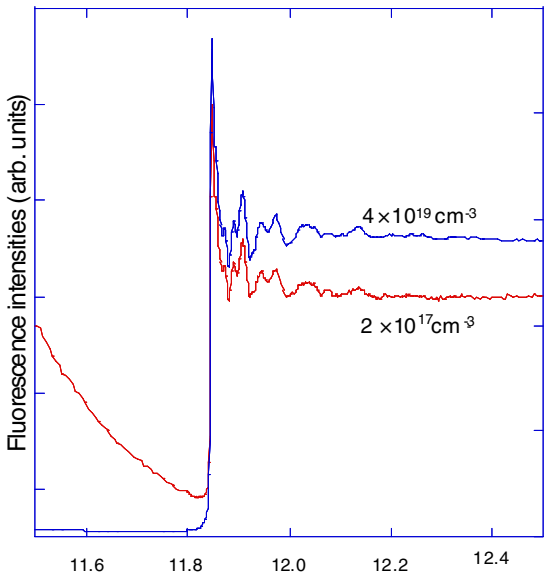

Fig. 1. As K EXAFS spectra of Si:As.

Table 1 Parameters for 1st shell in Si:As. Lower parameters are obtained by X-ray fluorescence holography.

	distance	Cood. num.
4 coordinate	2.44 Å	4
6 coordinate	2.44 Å	4
	2.95 Å	2

References

[1] A. Erbil, et al. Phys. Rev. B 34, 1392 (1986).
[2] S. Wei, et al. J. Appl. Phys. 82, 4810 (1997).
[3] K. Hayashi and I. Yonenaga, Materia Japan 46 (2007) 829.

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