EXAFS study on the diffusion of Zinc dopant in GaAs crystal lattice

Kiyoshi SUGIYAMA*[1], Toshio AKAI[2], Masaharu NOMURA[3]
[1]CACs Inc., Yokkaichi Laboratory, 1 Toho-cho, Yokkaichi, Mie, 510-8530, Japan
[2]CACs Inc., Tsukuba Laboratory, 8-3-1 Ami, Inashiki, Ibaraki, 300-0332, Japan
[3]KEK-PF, 1-1 Oho, Tsukuba, Ibaraki, 305-0801, Japan

Introduction

Zn dopant in GaAs has a high diffusion coefficient [1] and is easy to diffuse by anneal treatment. This character is not suitable for forming abrupt doping profile. On the other hand, zinc diffusion is used as a processing technique for construction of electronic and opto-electronic device [2]. Knowledge and control of Zn doping is necessary for development of device performance. In this study, we measured Zn K-edge EXAFS of Zn dopant in GaAs crystal with/without anneal treatment and investigated the insertion site of dopant in GaAs lattice.

Experimental

Zn doped GaAs layer (Zn:GaAs, Zn concentration is ~1×10^{20} cm^{-3}) was grown on (100) surface of undoped GaAs wafer by metal-organic chemical vapor deposition. Annealing treatment for Zn diffusion was carried out at 700 ºC.

The EXAFS measurements were performed at Photon Factory, BL12C. The x-ray beam was monochromatized with Si(111) double crystal. The incident angle of monochromatized x-ray was 3~5º from the sample plane in order to reduce the background from scattering. Zn kα fluorescence was collected with Ge 19-elements solid state detectors. The Ga K-edge EXAFS of undoped GaAs was also measured as a reference data.

Results and discussion

Figure 1 shows the Fourier transforms FT(*R*) of Zn K-edge EXAFS oscillation $k^3\chi(k)$ for Zn:GaAs with/without anneal treatment and Ga K-edge EXAFS for undoped GaAs. FT(*R*) for annealed Zn:GaAs is similar to that of undoped GaAs. The first, second, and third neighbor peaks are observed at 2.1, 3.7, and 4.5 Å, respectively. This suggests that Zn dopant in GaAs after anneal treatment locates at the Ga-substituted (*S*) site. FT(*R*) for non-annealed Zn:GaAs is different from those for annealed one and undoped GaAs at the second and the third peaks. Single peak A is observed at 3.2 Å for non-annealed sample while no peak exists in other samples at the corresponding region. The peaks around 4 Å for non-anneal sample are also different from the corresponding peaks for annealed one and undoped GaAs. This suggests that some of Zn atoms in GaAs do not occupy the *S* sites, but interstitial sites. The SIMS (secondary ion mass spectroscopy) profile showed that Zn diffusion up to 200 nm depth from the epitaxial layer/substrate interface by anneal treatment at 700 ºC. Zn atoms located at interstitial sites are considered to diffuse easier than those at *S* sites. It is considered that the interstitial Zn atoms at the doped layer diffuse to GaAs substrate by anneal treatment and occupy *S* sites after the diffusion.

In diamond lattice, there are two symmetric interstitial sites, tetrahedral (*T*) and hexagonal (*H*) [3]. However, the position of peak A calculated with the consideration of phase shift (3.5 Å) does not fit to any interatom distances for *T* and *H* sites. In non-annealed Zn:GaAs, Zn dopant might occupy the asymmetric interstitial site, or the local structure around Zn atom might distort.

Conclusion

The sites of Zn dopant in GaAs with/without anneal treatment were investigated by EXAFS. Fourier transform of the Zn K-edge EXAFS for annealed Zn:GaAs is similar to that of Ga K-edge EXAFS of undoped GaAs, suggesting that the Zn dopant occupy the *S* site of the GaAs lattice. On the other hand, the local structure of the Zn dopant in GaAs without anneal treatment is different from annealed one. The possibility that Zn dopant without anneal occupy the interstitial site of the GaA s lattice.

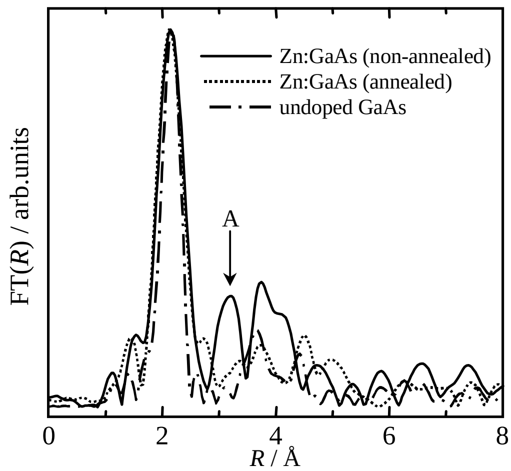

Figure 1. Fourier transforms FT(*R*) of EXAFS vibrations $k^3\chi(k)$ for Zn:GaAs with(———)/without(··············) anneal treatment and undoped GaAs (— · — ·).

References

[1] P. Enquist, et al., J. Appl. Phys., 63, 4485 (1988).
[2] H. Kumabe et al., Appl. Phys. Lett., 33, 38 (1978).
[3] K. Weiser, Phys. Rev. 126, 1427 (1962).
* 4307409@cc.m-kagaku.co.jp