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XAFS studies on Si_xMn_{1-x} dilute magnetic semiconductors

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Introduction

Diluted magnetic semiconductors (DMS) with the room temperature ferromagnetism have recently attracted considerable research interests for their potential applications in "spintronic" devices[1]. In particular, the Si-based DMS, Si_xMn_{1-x}, is compatible with the mature microelectronics technologies. Hence, a number of studies have been paid on this topic. Although Dalpian *et al.*[2] have theoretically predicted that the substitutional site Mn can stably exist in the Si matrix, the substitutional and the interstitial Mn sites in DMS have not been observed experimentally. In this report, XAFS is used to characterize the local structure around Mn atoms in Si_xMn_{1-x} DMS thin films grown by cosputtering deposition. We found that the substitutional site Mn atoms exist in the Si_xMn_{1-x} DMS.

Experimental

Si_xMn_{1-x} DMS thin films with the thickness of about 300 nm were prepared by the magnetron cosputtering method at 573 K. The sizes of Mn and Si targets for sputtering are 76 mm, and the growth rate of Si_xMn_{1-x} films is 0.5 nm/min.

The Mn K-edge XAFS spectra of Si_xMn_{1-x} DMS samples were measured at beamline BL-13B1 of Photon Factory, High Energy Accelerator Research Organization (PF, KEK). The monochromator is Si (111) double crystals. The XAFS signal was collected in fluorescence mode using a 100-element high purity Ge SSD.

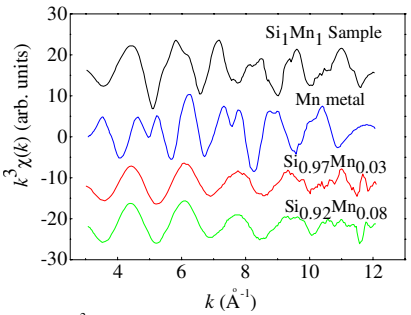

Figure 1. The $k^3x(k)$ function of Si_xMn_{1-x} thin films, Si_1Mn_1 sample and Mn metal.

Results and Discussion

Figure 1 shows the Mn K-edge EXAFS $k^3x(k)$ oscillation functions of the Si_xMn_{1-x} DMS thin films. The metallic Mn and the Si_1Mn_1 compound are used as references. Obviously, the $k^3x(k)$ functions for both of $Si_{0.97}Mn_{0.03}$ and $Si_{0.92}Mn_{0.08}$ are different from that of metallic Mn, but quite similar to that of the Si_1Mn_1 alloy which demonstrates strong EXAFS oscillation peaks in the low k region. This indicates that the first neighbour of Mn atoms in the Si_xMn_{1-x} thin films is surrounded predominantly by Si atoms. Therefore, we considered that the Mn atoms are incorporated into the Si matrix.

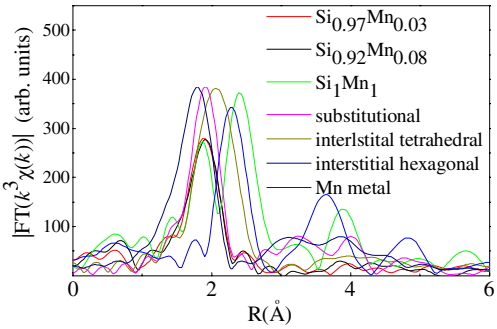

Figure 2. The radial structural functions of the Si_xMn_{1-x} thin films and references.

Figure 2 shows the Fourier transformations (FT) of the Mn K-edge $k^3x(k)$ functions for the Si_xMn_{1-x} thin films, Si_1Mn_1, Mn metal and theoretical calculations. It can be observed that there is only a strong peak at 1.90 Å in the Si_xMn_{1-x} thin films. By considering the FT features as shown in Fig. 2, one can safely exclude that the existence of Mn metal and the Si_1Mn_1 alloy in the Si_xMn_{1-x} thin films. In order to determine the real location of Mn atoms in the Si_xMn_{1-x} thin films, we performed theoretical calculations at the Mn K-edge using the Feff 8.2 code for the three typical structural models: the substitutional Mn_{Si}, the tetrahedral interstitial Mn_{It} and the hexagonal interstitial Mn_{Ih}. The theoretical calculations show that the first peak is centered at 2.06, 1.90 and 1.78 Å for the Mn_{It}, Mn_{Si}, and Mn_{Ih}, respectively. Their different peak positions favor to distinguish the Mn sites in the Si_xMn_{1-x} thin films. It can be found that the position of the first coordination peak of Mn atoms in the Si_xMn_{1-x} was exactly reproduced by that of the calculation spectrum of the substitutional Mn_{Si}. Therefore, we propose that the Mn atoms in the Si_xMn_{1-x} thin films are located at the substitutional site.

References

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