Fluorescence EXAFS Analysis of SiC:Mn Films Synthesized on SiC Substrates

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Abstract. The geometric structures for the Mn-Si films synthesized on a *4H*-SiC homoepitaxial wafers have been investigated by fluorescence EXAFS measurements. The EXAFS analysis revealed that the synthesized Mn-Si layer formed Mn_5Si_2, and the Mn atoms in the interlayer between the Mn-Si and the SiC layer were incorporated on the interstitial site in the 4H-SiC lattice.

Keywords: diluted magnetic semiconductor, SiC, Mn, EXAFS
PACS: 78.70.Dm, 75.50.Cc, 68.55.Jk, 75.50.Pp

INTRODUCTION

For the last decade, diluted magnetic semiconductors (DMS's), which combine semiconductors and magnetism, have been extensively studied from the perspective of using spin degrees of freedom in semiconductor devices [1]. Recently, we synthesized Mn-Si related compound by using an annealing method on *4H*-SiC homoepitaxial wafer. It has been revealed that synthesized Mn-Si films showed a Tc of 300 K, although the x-ray diffraction (XRD) and selected-area diffraction (SAD) measurements suggested that paramagnetic tetragonal Mn_5Si_2 was dominant [2]. In addition, after removing the synthesized Mn-Si layer the magnetic properties changed from ferromagnetic behavior to superparamagnetic behavior. The origin of such magnetic behavior has not been fully understood.

In this work, the synthesized SiC:Mn films on *4H*-SiC homoepitaxial wafer were investigated by fluorescence extended x-ray absorption fine structure (EXAFS) measurements in order to elucidate the relationship between the local structures around Mn atoms and the magnetic properties.

EXPERIMENTAL

The SiC:Mn films were synthesized on *4H*-SiC(0001) homoepitaxial wafer. Details of the growth process were described previously [2]. Thin Mn layer was deposited on the clean SiC wafer, and then annealing was performed to diffuse the Mn atoms into the SiC wafer. The synthesized Mn-Si layer (100 nm) has been removed by chemical etching. Superconducting quantum interference device (SQUID) measurement showed that the as-grown sample has ferromagnetic behavior with Tc ~ 300K, and the etched sample has superparamegnetic behavior.

The EXAFS measurements were performed at the beam line BL12C at the Photon Factory in Tsukuba with a Si(111) double crystal monochromator and a bent cylindrical mirror using synchrotron radiation from the 2.5 GeV storage ring [3]. The EXAFS spectra were measured in the fluorescence-detection mode. Intensity of incident X-ray beam was monitored by a nitrogen-filled ionization chamber, while the X-ray fluorescence signal was detected by an array of 19 elements of Ge solid state detectors. All the EXAFS measurements were performed at 70K in order to reduce thermal vibration.

RESULTS AND DISCUSSION

Figure 1(a) shows the Mn K-edge $k^2\chi(k)$ EXAFS oscillation for the as-grown and etched samples. It is found that the feature of each EXAFS oscillation is different in the range of higher wave number. In addition, the EXAFS oscillation for the as-grown sample does not correspond to that for the Mn_5Si_2.

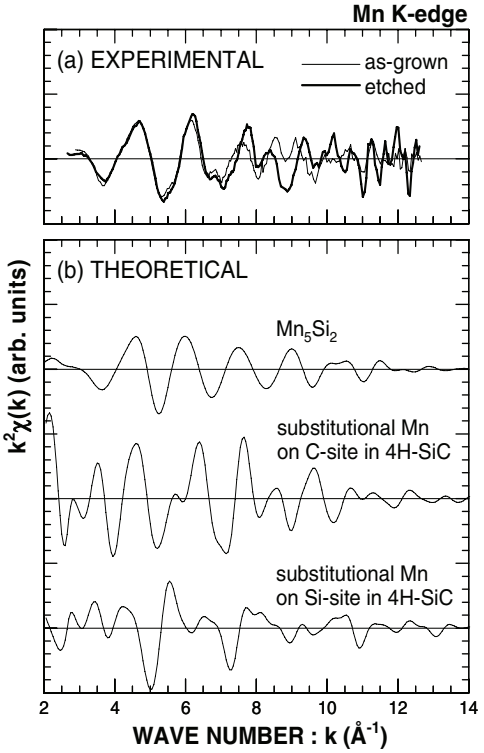

FIGURE 1. Mn K-edge EXAFS oscillation functions $k^2\chi(k)$ spectra for (a) the as-grown and polished samples, (b) theoretical EXAFS spectrum for Mn_5Si_2 and the substitutional Mn atom on the C- and Si-site in the *4H*-SiC lattice. The Debye-Waller factor was assumed as 0.075 Å for the bond length below 4.0 Å and 0.100 Å for the bond length above 4.0 Å. The theoretical EXAFS spectrum was generated by FEFF8 [4].

Figure 2(a) shows the Fourier transformed Mn K-edge EXAFS spectra for the as-grown and etched samples. For the as-grown sample, double peaks were observed at 1.6 Å and 2.2 Å, and the position of the latter peak was close to that of Mn_5Si_2 in Fig.2(b). For the etched sample, single peak was observed at 1.8 Å. From the curve-fitting, it is found that the EXAFS spectrum for the as-grown sample is fitted well by supposing the spectra of the etched sample and Mn_5Si_2. It indicates that the Mn-Si layer which was removed by etching forms Mn_5Si_2 mainly, and the Mn atoms incorporated in the interlayer form the other structure. If the Mn atoms substitute on Si- or C-site in *4H*-SiC lattice, several peaks due to second and third coordination shell have to be seen in the range of higher radial distance as shown in Fig. 2(b). However, for the etched sample no peak was observed in the range of higher radial distance. Thus, it is considered that the Mn atoms in the etched sample do not substitute on Si- or C-site in the *4H*-SiC lattice.

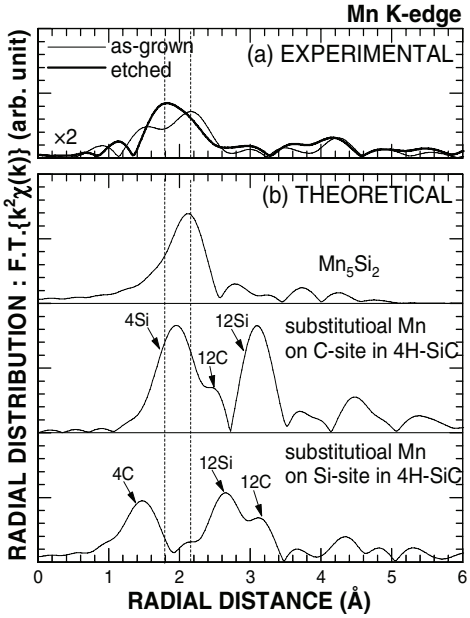

FIGURE 2. Fourier transform of Mn K-edge EXAFS oscillation functions $k^2\chi(k)$ spectra for (a) the as-grown and polished samples, (b) theoretical EXAFS spectrum for Mn_5Si_2 and the substitutional Mn atom on the C- and Si-site in the *4H*-SiC lattice. The Fourier transformation was performed in the k range of 3.0 – 12.0 $Å^{-1}$. The Debye-Waller factor was assumed as 0.075 Å for the bond length below 4.0 Å and 0.100 Å for the bond length above 4.0 Å. The theoretical EXAFS spectra were generated by FEFF8.

We also discuss the possibility that Mn atoms are interstitially incorporated in the *4H*-SiC lattice. We supposed the models that Mn atom was incorporated in the various positions z (0 ~ 1.7 Å) in the *4H*-SiC lattice as illustrated in Fig. 3(a). Figure 3(b) shows the theoretically calculated EXAFS spectra for each model in Fig. 3(a). It is found that the theoretically calculated spectrum for the position z = 0.9 Å corresponds well to that of the etched sample. Thus, it is considered that the majority of Mn atoms in the interlayer is incorporated on the interstitial site in the *4H*-SiC lattice.

The EXAFS analysis revealed that the synthesized Mn-Si layer forms Mn_5Si_2, corresponding to the XRD and SAD results. As the origin of the ferromagnetism, it is suggested that a small amount of C incorporated into the paramagnetic Mn_5Si_2 host induced the ferromagnetic order in Mn_5Si_2 [2]. On the other hand, it is found that the Mn atoms in the interlayer are incorporated on the interstitial site in the 4H-SiC lattice. To understand the magnetic behavior in the present study, further investigations such as *ab initio* calculation are needed, and are now in progress.

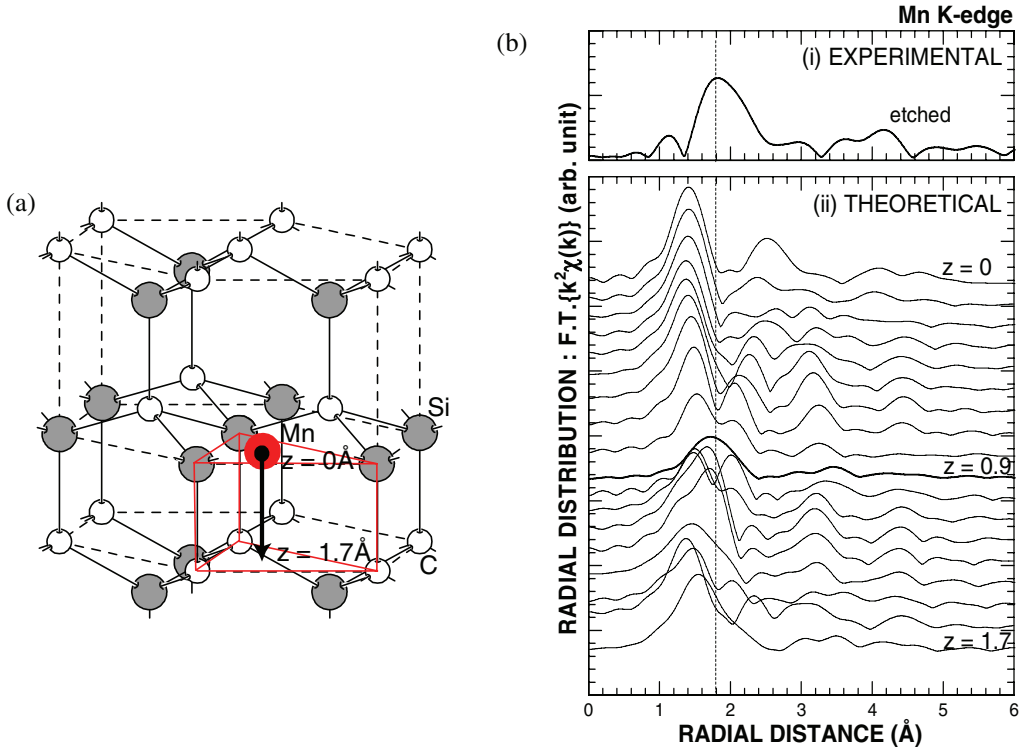

FIGURE 3. (a) Wurtzite-type crystal structure of *4H*-SiC bulk. A schematic illustration of the possible position of Mn atoms in an interstitial site in the *4H*-SiC lattice. (b) Fourier transform of Mn K-edge EXAFS oscillation functions $k^2\chi(k)$ spectra for (i) the etched sample, (ii) theoretical EXAFS spectrum for the interstitial Mn atoms in various position z (0 ~ 0.17 Å). The Fourier transformation was performed in the *k* range of 3.0 – 12.0 $Å^{-1}$. The Debye-Waller factor was assumed as 0.075 Å for the bond length below 4.0 Å and 0.100 Å for the bond length above 4.0 Å. The theoretical EXAFS spectra were generated by FEFF8.

ACKNOWLEDGMENTS

EXAFS studies were performed as part of a project (Project No. 2006G069) accepted by the Photon Factory Program Advisory Committee. These works were partly supported by NEDO under the Nanotechnology Program. The authors would like to thank Dr. K. Kojima (Power Electronics Research Center, AIST) for supplying us with *4H*-SiC homoepitaxial wafers. One of the authors (W. H. Wang) would like to acknowledge Japan Society for the Promotion of Science (JSPS) for fellowship grant (JSPS Id: P05611).

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