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Analysis of local structures around Mn and Fe atoms doped in ZnO by fluorescence EXAFS

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Introduction

Diluted magnetic semiconductors (DMS) have attracted much interest as materials with both optical and magnetic properties. Recently, the ZnO-based DMS with high Curie temperature above room temperature has been predicted by a mean field theory [1]. High Tc is beneficial in utilizing ZnO-based DMS for novel magneto-electronic devices.

In the present work, Fe- and Mn-doped ZnO thin films grown by combinatorial laser molecular beam epitaxy (CLMBE) were investigated by fluorescence x-ray absorption fine structure (XAFS) measurements using synchrotron radiation. We have successfully fabricated 3d transition-metal-doped ZnO films by CLMBE [2]. However, the geometric structures for the heavily transition-metal-doped ZnO are not clear.

Experimental

The Mn- and Fe-doped ZnO films were grown on sapphire (0001) substrate by CLMBE. Concentration of the Fe and Mn ions were determined by electron probe microanalysis (EPMA). The EXAFS measurements were performed at the beam line BL12C at KEK-PF.

Results and discussion

Figure 1 represents the Fourier transformed transition-metal (TM) ion K-edge $k^3\chi(k)$ extended X-ray absorption fine structure (EXAFS) spectra for Mn- and Fe-doped ZnO thin films and the theoretical EXAFS spectra for substitutional TM ion on the Zn site in the ZnO lattice are compared. The theoretical EXAFS spectra were generated by FEFF6 program [3]. Despite the high level of TM ions doped in the ZnO, several peaks are clearly observed at a longer radial distance, indicating that the local structures around TM ions are well-ordered with respect to short-range ordering. In addition, the experimental spectra correspond well to the theoretical ones. Thus, it is expected that TM ions in heavily doped ZnO substitute the Zn-site in the ZnO lattice.

References

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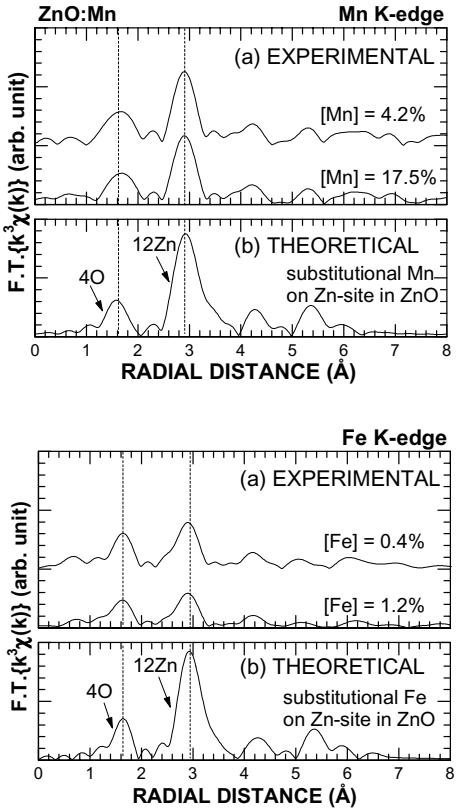

Fig. 1: (Top) Fourier transform of Mn K-edge EXAFS oscillation function $k^3\chi(k)$ spectra of (a) Mn-doped ZnO film and (b) theoretical EXAFS spectrum for the substitutional Mn ion on the Zn site in the ZnO lattice. (Bottom) Fourier transform of Fe K-edge EXAFS oscillation function $k^3\chi(k)$ spectra of (a) Fe-doped ZnO film and (b) theoretical EXAFS spectrum for the substitutional Mn ion on the Zn-site in the ZnO lattice.

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