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Spatial Occupation of Co Dopants in $Zn_{0.98}Co_{0.02}O$ Nanowire Studied by XAFS

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Introduction

Dilute magnetic semiconductors (DMSs) are envisioned as promising candidates for future spintronic technologies, which would simultaneously utilize the spin and charge of the carriers [1]. A number of experimental results on the magnetic behaviors and structures have been studied. More recently, increasing number of papers reported the RT-FM in the one-dimensional (1D) doped ZnO DMS nanowires due to their superior properties such as low dimensionality and quantum confinement effect, etc. However, the argument of the distribution of Co ions in the $Zn_{1-x}Co_xO$ nanostructures is not strong and the magnetic property in these nanomaterials is ambiguous until now. In this report, the local structure around Co in $Zn_{0.92}Co_{0.08}O$ nanowire was determined by means of XAFS to clarify the spatial occupation of the doping atoms.

Experimental

The $Zn_{0.98}Co_{0.02}O$ nanowire was synthesized by the thermal decomposition of transition metal acetate in refluxing trioctylamine at 310ºC. The Co K-edge EXAFS spectrum of $Zn_{0.98}Co_{0.02}O$ nanowire was measured in a fluorescence mode at the BL-12C beamline of Photon Factory, High Energy Accelerator Research Organization (PF, KEK), using a Si (111) double crystal monochromator.

Results and discussion

Figure 1(a) and (b) show the Co K-edge extended-XAFS (EXAFS) $k^3\chi(k)$ function of $Zn_{0.98}Co_{0.02}O$ and their Fourier transforms (FT), respectively. The Co and Zn K-edge function of PLD-grown $Zn_{0.98}Co_{0.02}O$ thin film, Co foil and wurtzite ZnO are also shown as references. It can be seen from Figure 1(a) that both of the $Zn_{0.98}Co_{0.02}O$ nanowire and thin film exhibit similar oscillation shape, which are also very close to that of the wurtzite ZnO powder. In addition, the FT of $Zn_{0.98}Co_{0.02}O$ nanowire and thin film shown in Figure 1(b) are both similar to that of the pure ZnO, presenting two strong peaks at around 1.6 and 2.8 Å, respectively. We have quantitatively fitted these two peaks assuming the Co substitution for Zn sites in $Zn_{0.98}Co_{0.02}O$ nanowire. This structure model can give a good fitting quality as shown by the empty circles in Figure 1(b). These results confirm that all the Co ions occupy the Zn sites in the ZnO lattice in the $Zn_{0.98}Co_{0.02}O$ nanowire.

To clarify whether the substitutional CoZn ions are homogeneously distributed or clustered together around oxygen atoms, Figure 2 displays the O K-edge XANES of the $Zn_{0.98}Co_{0.02}O$ nanowire with the calculated spectra for four model structures of replacing one, two, three, and four Zn nearest neighbors of the absorbing O atom by Co, respectively. The spectral shape of $Zn_{0.98}Co_{0.02}O$ nanowire exhibits quite identical features with those of pure ZnO powder and the calculated spectrum for undoped ZnO. However, the pre-edge peak A which is be mainly attributed to the substitutional Co clustering effect appears only as a shoulder in the spectrum of the $Zn_{0.98}Co_{0.02}O$ nanowire. Moreover, compared with the $Zn_{0.98}Co_{0.02}O$ nanowire, the amplitude of peak B is significantly damped for PLD-grown $Zn_{0.98}Co_{0.02}O$ thin film and the calculated spectra for the clustering model structures in which the prominent existence of CoZn clusters has been suggested previously [2]. Therefore, we consider that in the solution-prepared $Zn_{0.98}Co_{0.02}O$ nanowire the Co dopants are not in the clustering configurations Co-O-Con ($n \geqslant 0$) are likely to distribute homogenously in the host ZnO matrix.

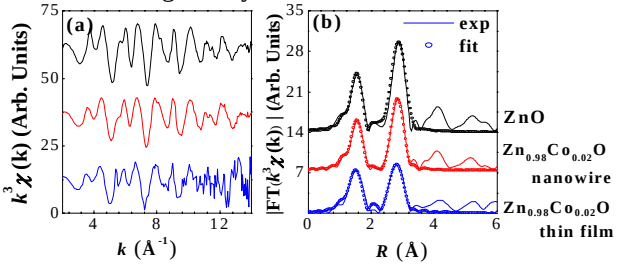

Fig.1 (a) Co K-edge EXAFS oscillation functions $k^3\chi(k)$ for the $Zn_{0.98}Co_{0.02}O$ nanowire, $Zn_{0.98}Co_{0.02}O$ thin film (PLD) and the Zn K-edge function for reference ZnO powder. (b) Their Fourier transforms spectra (solid lines).

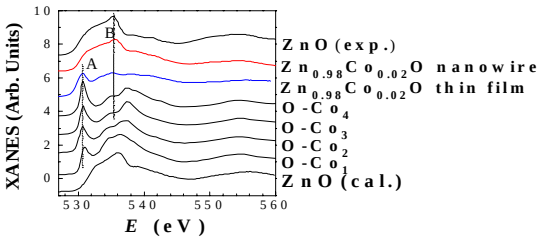

Fig. 2 O K-edge XANES spectra of the $Zn_{0.98}Co_{0.02}O$ nanowire and thin film, ZnO powder, and the calculated spectra for the model structure: $Co_{Zn}+V_{Zn}$, along with four representative model structures of replacing one, two, three, and four Zn nearest neighbors of the absorbing O atom by Co, denoted as $O\text{-}Co_1$, $O\text{-}Co_2$, $O\text{-}Co_3$, and $O\text{-}Co_4$.

References

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