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XANES OF Mn IN $CuIIIS_2$ (III = Al, Ga, In) CHALCOPYRITES

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In search for suitable spintronic materials, diluted magnetic semiconductors have been studied for a long time. However, there are still difficulties in obtaining room temperature ferromagnetism, which is a prerequisite of spintronic applications, in typical elemental and binary semiconductors. In recent years room temperature ferromagnetism has been found in some of Mn-doped chalcopyrites [1]. The theoretical calculations show that the ferromagnetic ordering in such systems depends critically on the site occupation of Mn in the host lattice. According to theoretical predictions, the stable ferromagnetic ordering is obtained when Mn substitutes on the III group atom site in $CuIIIS_2$ (III = Al, Ga, In) compounds. Using the X-ray absorption fine structure for determining the Mn site preference encounters some difficulties when atomic numbers of constituent cations (Cu and III) are close to each other. In such a case, similar photoelectron scattering amplitudes and phases prevent from discrimination between two possible substitution sites Mn_{Cu} and Mn_{III} in the EXAFS analysis [3, 4]. However, we expect that some specific features of electronic structure (local density of states) reflected in the X-ray absorption near edge structure (XANES) show differences for these two sites.

In this report we present an attempt to determine the site preference of Mn atoms from the XANES study of three Mn doped compounds: $CuAlS_2$, $CuGaS_2$ and $CuInS_2$. We used polycrystalline samples with varying Mn concentration within each series. A fluorescence detector was employed to record the Mn K edge XAFS spectra at A1 station at HASYLAB.

We used two methods of modeling XANES: the real-space multiple-scattering method represented by the FEFF 8.4 program and the full-potential linear augmented plane wave (FLAPW) in the Wien2k package. Special attention has been paid to reconstruction of the pre-edge structure of the spectra which is sensitive probe of the charge state and the local electronic structure of Mn atoms. We found that the Mn_{Cu} substitution gives generally much weaker pre-edge peak than the Mn_{III} site substitution. However, the intensity of the pre-edge structure shows strong dependence on the Fermi energy, which is hard to control in the studied materials. Applicability of the XANES spectra for the Mn site determination is discussed by comparison of the results of two theoretical methods with the experimental data.

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