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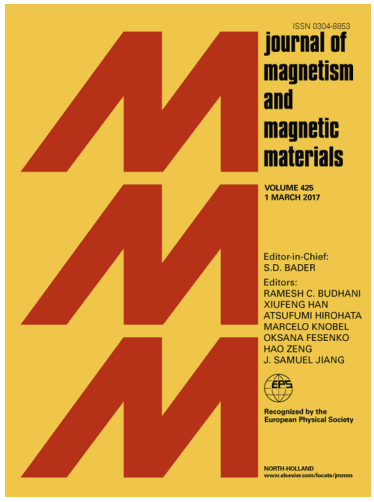

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ACCEPTED MANUSCRIPT

Electronic state and concentration of Fe^{3+} in $CuAl_{1-x}Fe_xO_2$ determined by magnetic measurements

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ABSTRACT

$CuAlO_2$ is among several ternary delafossites in which the electronic bandgap is less than the optical bandgap due to Laporte selection rules. Because alloying is expected to provide band engineering in delafossites, we are investigating Fe-doped $CuAlO_2$. Here, results from the detailed magnetic characterization of the $CuAl_{1-x}Fe_xO_2$ (x= 0.0, 0.01, 0.05, and 0.1) samples, prepared by a solid-state reaction of Cu_2O, Al_2O_3, and Fe_2O_3, at 1,100 ˚C, are reported. X-ray diffraction (XRD) of the powder samples showed an expansion of the rhombohedral unit cell with increasing x showing that the larger Fe^{3+} (r= 0.645 Å) is replacing the smaller Al^{3+}ion (r= 0.535 Å). The analysis of magnetization (M) *vs.* temperature (T, from 2 to 300 K) data in terms of the Curie-Weiss law: $M= CH/(T-\theta)$ confirms Fe^{3+} as the electronic state of Fe with spin S= 5/2 (magnetic moment $\mu= 5.9\mu_B$) as determined from the Curie constant, C; this analysis also yields a negative θ characteristic of an antiferromagnetic Fe^{3+}-Fe^{3+} exchange coupling and magnitudes of x in good agreement with the nominal values. The isothermal M *vs.* H (up to H= 90 kOe) data analyzed in terms of modified Brillouin function involving $H/(T-\theta)$ support the results obtained from the M *vs.* T analysis. The small paramagnetism observed in undoped $CuAlO_2$ is related to the presence of a few percent of $CuAl_2O_4$ impurity observed in XRD of the sample.

Key Words: Delafossites; Fe-doping; Magnetization; Antiferromagnetic exchange coupling;

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