Relationship among the Curie-Weiss temperature, the anisotropic electrical conductivities, and spin exchange constants valid for a magnetic system of nonequivalent magnetic ions

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For a magnetic system containing nonequivalent magnetic ions, we derived a relationship among the Curie-Weiss temperature, the anisotropic electrical conductivities, and spin exchange constants within the mean field theory by introducing the average-moment approximation and taking each spin site as a spin sublattice, and tested its validity.

Magnetic properties of a system containing magnetic ions are related to its electronic structure,1-4 and are commonly probed by measuring the temperature-dependence of its magnetic susceptibility (T) at a given magnetic field, the field-dependence of its magnetization M(H) at a very low temperature, or the magnetic specific heat as a function of temperature. When fitted with a Curie-Weiss law, the paramagnetic region of the (T) vs. T plot leads to the Curie-Weiss temperature  and the effective magnetic moment eff. For a given magnetic system, the  provides information about the nature of its dominant spin exchange (i.e., ferromagnetic when  > 0, and antiferromagnetic when  < 0), and the eff about the spin S of its magnetic ion. For a magnetic system consisting of equivalent magnetic ions, the mean field theory (MFT)2-4 provides a simple expression that enables one to estimate its θ once its spin exchange constants are known.

In recent years the spin exchange constants of any magnetic system, regardless of whether or not it has nonequivalent magnetic ions, can be readily determined by performing energy-mapping analysis5 based on first principles density functional theory (DFT) calculations. Thus it is highly desirable to derive a MFT relationship valid for a magnetic system composed of nonequivalent magnetic ions. In this work we develop such a MFT relationship and test its validity by evaluating the  values of Bi4Cu3V2O14, whose magnetic structures were previously investigated in terms of their calculated spin exchange constants.6 Also the anisotropic electrical conductivities of a magnetic insulator for Co2SiO4 can be predicted on the basis of its spin exchange parameters and Ohm's law, which was applied for Fe2SiO4 system.7

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