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Magnetic Phase Diagram of Ferrites with Selective Sublattice Dilution

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Abstract: The magnetic phase diagram has been calculated for two-sublattice ferrite type magnets $\text{AB}_2\text{O}_4$, with A and B sublattices partially filled by nonmagnetic ions. The fraction of magnetic ions was controlled separately for each sublattice and it has been denoted as $X_A$ and $X_B$ respectively. The system has been represented as a set of classical spins interacting with their nearest neighbours by Heisenberg hamiltonian. The numerical procedure used to calculate the magnetic ground state for each $(X_A, X_B)$ pair was global energy minimisation by corrections of local spin directions. The resulting magnetic state has been analyzed by calculating the spin-spin correlation functions, Fourier transforms of magnetic order and some local variables like site and bond energy distributions. The final results is the magnetic phase diagram in the $(X_A, X_B)$ plane i.e. the determination of the types of magnetic order, the magnetic phase borders and the collinearity region for the dominant ferrimagnetic phase.

1. FERRITES WITH SELECTIVE SUBLATTICE DILUTION

The well-known ferrite-type magnetic compounds with full occupation of magnetic ions in both sublattices are usually regarded as classical examples of ferrimagnetic compounds. In fact most of them actually fulfill the necessary conditions required for the formation of such a magnetic order. The antiferromagnetic A-B interactions are usually dominant, while the sign and strength of the A-A and B-B interactions are not so obvious. It is usually assumed that the A-A and B-B interactions are much weaker than A-B and in most cases also antiferromagnetic. In such a situation the ferrimagnetic ordering is a unique magnetic ground state, although it has to be noticed that for negative values of A-A and B-B interactions there is an interaction conflict and for higher values of $J_{AB}/J_{AA}$ or $J_{BB}/J_{AB}$ ratio this usually results in noncollinear magnetic ground states.

Another case leading to noncollinear magnetic states is the substitution of nonmagnetic ions into A or B sublattices. For small fractions of nonmagnetic ions it usually results in so called locally canted states (LCS). The situation seems to be more complicated for strong dilutions i.e. when the fraction of nonmagnetic ions is higher than half. In the last two decades it has been found that in many strongly diluted ferrites various types of spin glas phases are encountered [1]. This has put forward a problem of determination of the ground state type for a given degree of dilution.

The theoretical analysis by Scholl and Binder [2] has introduced the concept of selective dilution (the $X_A$ and $X_B$ fractions are treated as independent parameters). The numerical treatment of the percolation problem has lead to the determination of the phase borders for the ferrimagnetic ordering, but unfortunately the analysis included only the case with zero A-A and B-B interactions. There were also other papers which tried to determine the actual topology of the magnetic phase diagram in the $(X_A, X_B)$ plane with nonzero A-A and B-B interactions [3][4][5], but they mostly contained model propositions based on some selected facts without any well-based numerical estimates. The only known exact results are the percolation thresholds for pure A and B sublattices. The problem is additionally complicated by the fact that the exact magnetic ground state is not known for the pure B sublattice with negative n-n interactions, because the system is internally frustrated [3].

2. THE MODEL AND SELECTED RESULTS

The system has been represented by a set of classical spins, distributed on a spinel-type lattice, interacting by n-n interactions of the Heisenberg type. The orientation of each spin has been stored as spherical $(\theta, \phi)$ angles with 1 deg quantisation. The initial state of the system was a random distribution of magnetic ions in A and B sublattices with specified $X_A$ and $X_B$ parameters and random orientations of spins. The energy minimization procedure consisted of random selection of magnetic sites and correction of the local spin direction. The new orientation has been chosen along the local effective field direction, obtained by summing the effect of the nearest neighbours and the external magnetic field. During the relaxation the total energy and magnetizations of both sublattices have been monitored. After such a relaxation (usually 1000-2000 steps per spin) the system was found in the state of minimum energy (global or local). The problems with local minima (metastable states) can...
be in general attributed to creation of magnetic domains in the system. The final state was analysed by calculations of both local averages (site energy, bond energy, orientation distribution) and some global variables like amplitude of Fourier peaks, radial correlation functions and total magnetization for each sublattice. In general the Fourier transforms and correlation functions have been used to determine the type of magnetic ordering. The magnetizations were more useful in determination of the phase borders.

Two selected results of the described calculations are presented below. One is the percolation threshold along the $X_A=X_B$ cut presented in Fig.1 a,b. The value determined by Scholl&Binder [2] for the $J_{AA}=J_{BB}=0$ case is equal to 0.227. The curves presented in Fig.1 suggest that for nonzero values of interaction constants there is an intermediate region between the paramagnetic and ferromagnetic phase, (the magnetization decrease) in which the spins freeze into a noncollinear random structure, possibly a spin glass like phase. The second example presented in Fig.2 is the competition of order parameters near the $(X_A=1, X_B=0)$ corner. In Fig.2 below the asymptotic values of radial correlation functions are presented for A-A (two curves for the same and opposite sublattices in the antiferro phase) and A-B (ferromagnetic ordering). It can be clearly seen that a mixed phase region is encountered between the antiferro and ferromagnetic phase ($X_B^P=0.15-0.2$) for the $J_{AA}=J_{BB}=0.5J_{AB}$ case. This fact is also reflected in Fig.3, where the final magnetic phase diagram is presented.

References:
3. Soubeyroux J.L et al., J de Physique, 49 (1988), Coll.C8, 1117
5. J.Villain, Z.Physik B 33 (1979), 31-42

Fig.1 On the left magnetization for $H=0.1J_{AB}$ (full symbols) and $H=0$ (open symbols) calculated along the $X_A=X_B$ cut. On the right the respective magnetization step $M(H)-M(0)$.

Fig.2 The asymptotic values of the radial correlation functions for $X_A=1$. The full symbols denote $J_{AA}=J_{BB}=0.5J_{AB}$ case, the open symbols $J_{AA}=J_{BB}=0.25J_{AB}$.

Fig.3 The complete magnetic phase diagram for selectively diluted ferrite-type magnets calculated for $J_{AA}=J_{BB}=0.5J_{AB}$.