SIMBO and ENERMAG: TWO COMPUTING PROGRAMS FOR ANALYSING THE TOPOLOGY OF EXCHANGE INTERACTIONS AND THE CLASSICAL MAGNETIC ENERGY

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We have developed two computing programs, SIMBO and ENERMAG, which provide an invaluable help to interpret experimental magnetic structures occurring in real systems. The study of the crystal structure, and the related topology of the magnetic exchange interactions of old or new materials, by using these programs facilitates the detection of new frustrating topologies of interest in magnetism. They allow the possibility of *a priori* predictions about the magnetic ordering in new materials when approximate values of the exchange interactions are available.

The program SIMBO analyses the crystal structure of an insulator in terms of super-exchange M_1-X-M_2 and super-super-exchange M_1-X_1-X_2-M_2 paths. In case of intermetallic compounds, or if the user asks for, direct exchange paths are also considered. SIMBO needs as input the list of atom co-ordinates in the asymmetric unit, as well as their ionic charge and the saturation magnetic moment, the space group symbol and the cell parameters. The program uses this information to calculate distance, angles and exchange paths. The user may introduce some constraints concerning the geometry of the required exchange paths in order to limit and eliminate loops of involved shapes.

SIMBO produces, as output, a list of exchange paths and attributes symbols for the different exchange interactions that are also classified as a function of the inter-atomic distances. SIMBO provides also a formal description of the Fourier transform of the isotropic exchange interactions in form of an $n \times n$ matrix, where n is the number of magnetic ions in a primitive unit cell (see below). This information is summarised in a file that serves as input for the program ENERMAG.

The program ENERMAG tries to solve the problem of the first ordered state for a particular magnetic topology and a set of exchange interactions. The first ordered state is obtained in the mean-field approximation, as a function of $\mathbf{k}$, on the surface or at the interior of the Brillouin Zone (BZ), and the exchange integrals, as the eigenvector corresponding to the highest eigenvalue of the Fourier transform of exchange integral matrix [1-4]:

$$\xi_{ij}(\mathbf{k}) = \sum_m J_{ij}(\mathbf{R}_m).\exp\{-2\pi i\, \mathbf{k}\, \mathbf{R}_m\}$$

The indices i,j refer to the magnetic atoms in a primitive cell, $J_{ij}(\mathbf{R}_m)$ is the isotropic exchange interaction between the spins of atoms i and j in unit cells separated by the lattice vector $\mathbf{R}_m$ and $J_{ij}(\mathbf{R}_m)$ includes the spin modules. Our convention for magnetic energy is to take negative J's for anti-ferromagnetic coupling.

The program ENERMAG handles the diagonalisation of the above matrix that is provided by the output file coming from SIMBO. It solves the parametric equation:

$$x(\mathbf{k}, \mathbf{J})\, \mathbf{v}(\mathbf{k}, \mathbf{J}) = \lambda(\mathbf{k}, \mathbf{J})\, \mathbf{v}(\mathbf{k}, \mathbf{J})$$

where $\mathbf{J}$ stands for the given set of exchange interactions $\mathbf{J}=\{J_{ij}(\mathbf{R}_m)\}$, and $\mathbf{k}$ is a vector in the asymmetric unit of the BZ. For a given set $\mathbf{J}$, and no degeneracy, the highest eigenvalue $\lambda_{max}(\mathbf{k}_0, \mathbf{J})$ occurs for a particular $\mathbf{k}_0$, for which the ordering temperature is maximal: $3k_BT_{max}=\lambda_{max}(\mathbf{k}_0,\mathbf{J})$. The corresponding eigenvector $\mathbf{v}_{max}(\mathbf{k}_0,\mathbf{J})$, that may be complex for incommensurate structures, describes the spin configuration of the first ordered state.

The user can give the value of the exchange interaction and study the magnetic energy as a function of $\mathbf{k}$ in the BZ using lines, planes or the whole BZ including special points. Another way of working with ENERMAG is the generation of "magnetic phase diagrams" as a function of the exchange parameters. The program explore, for each point in the J-space, the asymmetric unit of the BZ and detects the value of $\mathbf{k}=\mathbf{k}_0$ for which the ordering temperature is maximal and equal to $\lambda_{max}(\mathbf{k}_0,\mathbf{J})/3k_B$. The eigenvector $\mathbf{v}_{max}(\mathbf{k}_0,\mathbf{J})$ gives the Fourier coefficients of the magnetic structure as a function of the exchange parameters $\mathbf{J}$.

Examples of the use of both programs may be found in references [5-9]. In Figure 1 it is shown the case of the $MFePO_5$ family [5], for which we have studied in detail the topology of the exchange interactions. In figure 2 a part of the phase diagram is shown. The observed magnetic structure is in the area labelled G_M+G_{Fe} (+ - + - ; + - +-).

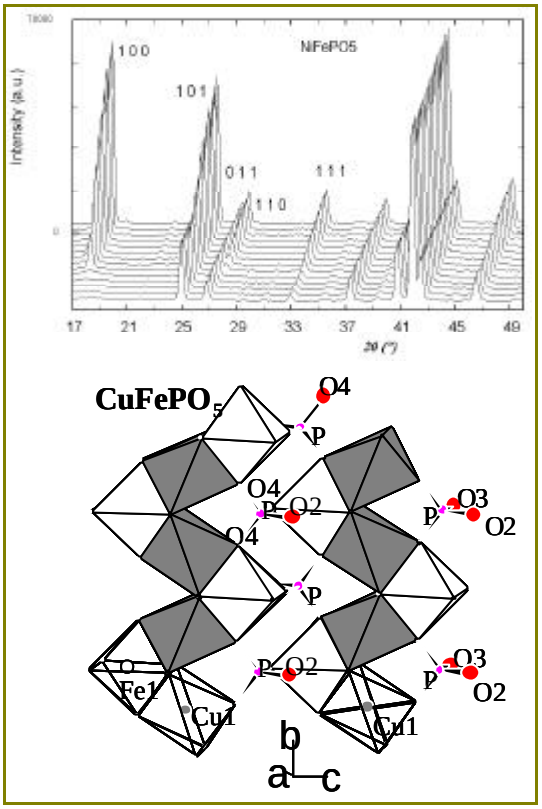

Figure 1. Neutron powder diffraction as a function of temperature for one of the members of the family $MFePO_5$ (M=Fe, Co, Ni, Cu) and schematic view of the crystal structure of the compound M=Cu [5].

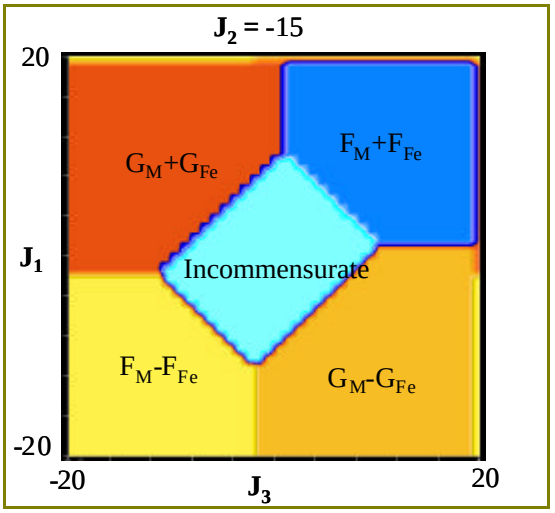

Figure 2. Part of the magnetic phase diagram generated by ENERMAG for the family of compounds $MFePO_5$

At present the most important limitation of the program ENERMAG is that only isotropic exchange interactions are allowed. For the forthcoming development we have devised the implementation of a general tensor for describing the exchange (pseudo-dipolar and Dzyalozinskii-Moriya interactions). This will extend the capabilities of the program to handle explicit spatial components (general $3n \times 3n$ exchange matrix) of the eigenvectors representing the Fourier coefficients of the magnetic structure.

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