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Geometric mean-field models for ilmenite-hematite solid solutions

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The ilmenite-hematite solid-solution series Ilm$X$ (X $FeTiO_3(1-X)$ Fe_2O_3) is an important system for homogenous or exsolved natural minerals with unusual magnetic properties. Statistical mean-field models are successful in predicting the ferromagnetic (FM) Curie temperatures T_C and $M_S(T)$ curves of the Ilm$X$ solid solutions. The results depend on the choice of interaction coefficients, which either have been determined by neutron diffraction measurements (Samuelson and Shirane, 1979), by Monte Carlo model fits (Harrison, 2006), or by density-functional theoretic calculations (Nabi *et al.*, 2010). To implement the varying Fe and Ti concentrations, and the random distribution of Fe ions in the solid solutions, the models either use statistical interactions between sites, whereby they effectively average over all possible configurations, or they describe specific random configurations. Both types of models will be discussed. A special class of mean-field modelling has been suggested by Ishikawa (1957), to estimate the size of interacting clusters in Ilm$X$ beyond the FM percolation threshold ($X > 87$), where global ferrimagnetic order breaks down, and only finite ferrimagnetically ordered clusters generate a pseudo-Langevin magnetization curve at temperatures between the FM Curie temperature and the antiferromagnetic Néel temperature T_N. Using a numerical inversion method, it is possible to fit measured hysteresis loops of synthetic Ilm$X$samples ($X = 92, 97$) by improved theoretical pseudo-Langevin curves which depend on cluster-size- and exchange-interaction- distributions. Apart from statistical mean-field models, it is also possible to investigate specific atomic configurations, each corresponding to some fixed Ilm$X$. These models contain several tens to hundreds of ilmenite unit cells (e.g. $3 \times 3 \times 3$ or $5 \times 5 \times 5$) with periodic boundary conditions. Their main advantage is that they permit visual inspection of the geometric configuration in relation to the magnetic behaviour.