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Neutron diffraction and atomistic simulation of magnetic and cation ordering in titanohematite: new insight into the mechanism of self-reversed thermoremanent magnetization

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Here we review recent experimental investigations of cation and magnetic ordering in ilmenite-hematite solid solutions using in-situ neutron diffraction. The results are analysed using an atomistic model of magnetic and cation ordering via Monte Carlo simulations. The result is significant new insight into the origin of self-reversed thermoremanent magnetiztion.

Synthetic samples of the solid solution containing 60% and 65% FeTiO3 (ilm60 and ilm65) were heated under vacuum to a maximum of 1350 ˚C. Powder diffraction patterns were collected at several temperatures on heating and cooling and the nuclear and magnetic scattering components separated. Quenched samples displayed diffuse superlattice reflections, indicative of short-range cation order. The short-range ordered structure is interpreted with the aid of statistical simulations to be a fine-scale alternation of ordered and antiordered ilmenite-like twin domains, separated by hematite-like twin domain boundaries (TDB's). Peak width analysis demonstrates that the twin domains have a pronounced shape anisotropy, with average lengths of 20 $\pm$ 1 Å and 60 $\pm$ 2 Å along the c-axis, and 100 $\pm$ 9 Å and 100 $\pm$ 4 Å along [0-11]* in ilm60 and ilm65, respectively.

Analysis of the magnetic scattering and spontaneous strain demonstrates that short-range magnetic order remains at temperatures well above the bulk Curie temperatures in quenched ilm60 and ilm65. This indicates significant magnetic heterogeneity in the samples, which may be related to the presence of a high density of Fe-enriched TDB's in the quenched material. Monte Carlo simulations of magnetic ordering in quenched samples show no self reversal occurring in systems containing two equally well-ordered ferrimagnetic domains separated by an Fe-enriched antiferromagnetic boundary. Systems displaying partial long-range order, however, do display self-reversed magnetization. Partial long-range order is characterised by a mixture of well-ordered Ti-rich ferrimagnetic domains and less-well ordered Fe-rich domains with a weak net ferrimagnetic moment. The two ferrimagnetic domains are negatively coupled via exchange interactions, leading to self reversal.