Molecular Dynamics Modelling of Speromagnetism in Fe4(P2O7)3 Iron Phosphate Glass

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Abstract

The study uses molecular dynamics to generate multiple models of Fe4(P2O7)3 iron phosphate glass before assigning spin moments to each iron atom (fig. 1) to generate magnetic parameters for each structure. The study is based around the findings discussed in Al-Hasni et al (1), which describe the spin structure of Fe4(P2O7)3 iron phosphate glass as being "interpreted in terms of speromagnetic order". Interatomic potentials and Fe4(P2O7)3 crystal structure coordinates are input into DL_POLY molecular dynamics software to simulate the melt and quench steps needed to generate a glass model. Spin moments are then added to each iron atom, with these details input into Spinvert, a software designed to optimise paramagnetic spin distributions. Spinvert outputs diffuse neutron scattering curves, as well as data related to spin correlation. These can then be used to compare the modelled structures to experimental data to validate the legitimacy of each model. (1) B Al-Hasni, G Mountjoy. Structural investigation of iron phosphate glasses using molecular dynamics simulation, Journal of Non-Crystalline Solids, Volume 357, Issue 15, 2011

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