

Study of the Phenomenon Nature of Order and Disorder in BaMn(Fe/V)F7 Fluoride Glass by the Hybrid Reverse Monte Carlo Method

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Abstract : Fluoride glasses with a nominal composition of BaMnMF₇ (M = Fe/V assuming isomorphous replacement) have been structurally modelled through the simultaneous simulation of their neutron diffraction patterns by a reverse Monte Carlo (RMC) model and by a Rietveld for disordered materials (RDM) method. Model is consistent with an expected network of interconnected [MF₆] polyhedra. The RMC results are accompanied by artificial satellite peaks. To remedy this problem, we use an extension of the RMC algorithm, which introduces an energy penalty term in acceptance criteria. This method is called the Hybrid Reverse Monte Carlo (HRMC) method. The idea of this paper is to apply the (HRMC) method to the title glasses, in order to make a study of the phenomenon nature of order and disorder by displaying and discussing the partial pair distribution functions (PDFs) $g(r)$. We suggest that this method can be used to describe average correlations between components of fluoride glass or similar system.

Keywords : fluoride glasses, RMC simulation, neutron scattering, hybrid RMC simulation, Lennard-Jones potential, partial pair distribution functions

Conference Title : ICAPM 2014 : International Conference on Applied Physics and Mathematics

Conference Location : Istanbul, Turkey

Conference Dates : April 22-23, 2014