

The Fit of the Partial Pair Distribution Functions of BaMnFeF7 Fluoride Glass Using the Buckingham Potential by the Hybrid RMC Simulation

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Abstract : The BaMnMF7 (M=Fe,V, transition metal fluoride glass, assuming isomorphous replacement) have been structurally studied through the simultaneous simulation of their neutron diffraction patterns by reverse Monte Carlo (RMC) and by the Hybrid Reverse Monte Carlo (HRMC) analysis. This last is applied to remedy the problem of the artificial satellite peaks that appear in the partial pair distribution functions (PDFs) by the RMC simulation. The HRMC simulation is an extension of the RMC algorithm, which introduces an energy penalty term (potential) in acceptance criteria. The idea of this work is to apply the Buckingham potential at the title glass by ignoring the van der Waals terms, in order to make a fit of the partial pair distribution functions and give the most possible realistic features. When displaying the partial PDFs, we suggest that the Buckingham potential is useful to describe average correlations especially in similar interactions.

Keywords : fluoride glasses, RMC simulation, hybrid RMC simulation, Buckingham potential, partial pair distribution functions

Conference Title : ICPS 2015 : International Conference on Physical Sciences

Conference Location : Istanbul, Türkiye

Conference Dates : December 21-22, 2015