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Monte Carlo Simulations of Magnetic Ordering in Spinel High Entropy Oxides

High-entropy oxides are materials of significant technological interest due to their tunable magnetic properties, which strongly depend on the cation distribution within their crystal structure. In this work, we present a Metropolis Monte Carlo simulation of ferrimagnetic ordering in a high-entropy spinel oxide (space group Fd3m), specifically of the form $(Co_{0.33}Ni_{0.33}Cu_{0.33})(Mn_{1-x}Fe_x)_2O_4$. Magnetic interactions are described using the classical Heisenberg model, which considers nearest-neighbor spin exchange between cations. The elemental distribution within the unit cell is determined statistically, taking into account thermal effects associated with synthesis conditions and exchange interactions characteristic of this space group. This approach enables modeling of the intrinsic cation disorder of spinel structures under realistic synthesis conditions. From these simulations, the total magnetization and sublattice magnetizations are calculated as a function of temperature. The Curie temperature is estimated for each studied composition by varying the Fe concentration. Magnetic hysteresis loops were also simulated to characterize the material's response to external magnetic fields. The results show that the Fe content controls the Curie temperature in a manner consistent with experimental observations, with the inter-sublattice exchange interaction emerging as the dominant contribution. The model enables systematic exploration of the compositional space and predicts high Curie temperatures for various compositions, providing relevant insights for the design of new magnetic materials.

Key Words: high entropy oxides, spinel, monte Carlo, magnetic hysteresis, curie temperature

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