Probing Magnetic Interactions in Gd^{3+}-Doped Y_2O_3 via EPR and Monte-Carlo Simulations

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Electron Paramagnetic Resonance spectroscopy (EPR) serves as a powerful technique for investigating magnetic interactions in systems containing unpaired electrons, particularly Gd^{3+} ions with their $4f^7$ electronic configuration. While Gd^{3+} EPR signals are typically intense, their spectral features are known to be sensitive to the local crystal field and dipolar interactions between neighboring ions [1,2]. Previous studies have examined Gd^{3+} in various matrices [3], but systematic studies in crystalline Y_2O_3 remain limited.

In this study, Y_2O_3 samples doped with varying concentrations of Gd^{3+} were synthesized using a solid-state reaction in a Carbolite RHF 1500 furnace at 1100°C for 5 hours. Phase purity and structural properties were confirmed by powder X-ray diffraction (XRD). Room-temperature X-band EPR measurements revealed concentration-dependent spectral variations, including linewidth broadening and g-factor shifts, suggesting the onset of magnetic interactions at higher doping levels.

To understand these effects, Monte-Carlo simulations were performed to model the distribution of the smallest Gd^{3+}-Gd^{3+} distances for different concentrations, up to 10%. The experimental EPR spectra shows clear correlation with the simulated distance distributions, demonstrating how spectral features evolve with decreasing interionic separation. This combined experimental and computational approach provides valuable insights into the magnetic coupling behavior of Gd^{3+} ions in the Y_2O_3 matrix.

This approach bridges experimental EPR data with theoretical distance modeling, advancing the understanding of Gd^{3+} magnetic behavior in solid-state systems.

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References

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