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Hyperfine local probe study of alkaline-earth manganites BaMnO3 and SrMnO3

text + figure + references

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Summary

We report perturbed angular correlations (PAC) and first-principles calculations with 111mCd/111Cd and 111In/111mCd probes, implanted at the ISOLDE-CERN laboratory, in the compounds/polymorphs BaMnO3-6H and BaMnO3-15R and SrMnO3-4H. Magnetic and structural studies were also performed. The experiments are complemented with calculations of the electric field gradient (EFG), with density functional theory, by the LAPW method (Wien2k code [1]). Calculations consider different magnetic states, and for the case of BaMnO3 the results from different polymorphs are analyzed. Comparison with the experimental results requires considering supercells with diluted Cd impurities, to account for the presence of the radioactive probe in the host material (ppm). The results of the calculations are checked for convergence with increasing dilution of Cd probes, corresponding to increasing size of the supercell. Based on the calculations, the assignment of the sites for the 111mCd and 111In probes at the Ba (for BaMnO3-6H) and Sr (SrMnO3-4H) sites gives good agreement for most cases. The EFG shows no visible changes with temperature in BaMnO3-6H and SrMnO3-4H, in the range 20-700 C, as shown in the figure). The PAC spectra of BaMnO3 in the two polymorphs reveal different frequencies. The results on BaMnO3 using 111In/111mCd, show an additional interaction frequency in comparison with Cd.

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