Hyperfine fields in Ba and Sr hexaferrites changed by lattice deformations

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M-type hexagonal ferrites are well established magnetic materials providing a broad range of applications and displaying many interesting phenomena. Recently our 57 Fe nuclear magnetic resonance (NMR) experiments on thin films of barium and strontium hexaferrites revealed a slight anomaly in spectral line shifts. NMR spectroscopy is capable of distinguishing the effect of global fields, e.g., due to demagnetization field, from the effect of local fields corresponding to particular crystal sites. Our measurements indicate that an additional mechanism other than macroscopic field contributes to the resulting spectrum. In order to investigate whether the deformation of structure is connected with the changes to the local fields, we perform a structural study by means of electronic structure calculations. Barium and strontium hexaferrites with various volumes and c/a ratios are calculated, and subsequently the hyperfine fields on iron nuclei are extracted using our semi-empirical method based on the calculated magnetic moments.