IEEE Magnetics Letters 2021

Mutual orientation of electric intracrystalline and magnetic fields in iron borate single crystals

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Abstract

X-ray structural analysis, Mssbauer spectroscopy, and ab-initio calculations were used to study the structural properties and refine the orientation of intracrystalline fields in FeBO3 crystals in the region of the magnetic phase transition. It was found that in the temperature range of 293 - 403 K, the trigonal lattice parameters increase monotonically. Analysis of the electron density distribution maps did not show visible local disordering over the entire investigated temperature range. It was found that iron borate has an axially symmetric electric field gradient (EFG), whose main axis is directed along [001]. This orientation is maintained above and below the Neel point. In magnetically ordered state of the crystal, the main axis of the EFG is orthogonal to the direction of the hyperfine magnetic field at iron nuclei. The results obtained will be used to develop a theoretical model of the formation of hyperfine structure in iron borate, which is important for applications of such crystals in the synchrotron technologies of a new generation.

http://dx.doi.org/10.1109/LMAG.2021.3130853

Keywords

ab-initio calculations, Crystals, Electric fields, electric filed gradient, Iron, Iron borate single crystals, Magnetic resonance, Magnetism in Solids, Mossbauer spectroscopy, Spectroscopy, Temperature distribution, X-ray diffraction