

Phonon Spectrum in Hydroxyapatite: Calculations and EPR Study at Low Temperatures

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Abstract

© 2015, Springer Science+Business Media New York. Density functional theory-based calculations within the framework of the plane-wave pseudopotential approach are carried out to define the phonon spectrum of hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ (HAp). It allows to describe the temperature dependence of the electronic spin-lattice relaxation time T_{1e} of the radiation-induced stable radical NO_3^{2-} in HAp, which was measured in X-band (9 GHz, magnetic field strength of 0.34 T) in the temperature range $T = (10-300)$ K. It is shown that the temperature behavior of T_{1e} at $T > 20$ K can be fitted via two-phonon Raman type processes with the Debye temperature $\Theta_D \approx 280$ K evaluated from the phonon spectrum.

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Keywords

Debye model, DFT, Phonons, Spin-lattice relaxation