Journal of Low Temperature Physics 2016 vol.185 N5-6, pages 627-632

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

Biktagirov T., Gafurov M., Iskhakova K., Mamin G., Orlinskii S.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

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 Ca10(PO4)6(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 NO32- 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 T1e at T> 20 K can be fitted via two-phonon Raman type processes with the Debye temperature ΘD≈280K evaluated from the phonon spectrum.

http://dx.doi.org/10.1007/s10909-015-1419-2

Keywords

Debye model, DFT, Phonons, Spin-lattice relaxation