

Quadratic crystal field tensors and spin Hamiltonian tensors of Fe³⁺ in Li₂Ge₇O₁₅ above and below the phase transition temperature

Galeev A., Khasanova N., Bykov A., Bulka G., Vinokurov V., Nizamutdinov N.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Dopant Fe³⁺ ions in tetrahedral and octahedral positions of Ge⁴⁺ in the crystal Li₂Ge₇O₁₅ were studied using EPR. Fe³⁺ substitutes for Ge⁴⁺ with a local charge compensation. The octahedral site and the tetrahedral sites significantly differ by the value of the invariant sum $S(B_4)$ of the B_4 tensor of the spin Hamiltonian of Fe³⁺. The irreducible tensor products $\{V_4 \otimes V_4\}_4$ and $\{V_4 \otimes V_4\}_2$ the V_4 tensor of the crystal field calculated using the point-charge model for octahedral and tetrahedral complexes provide the predominant contribution of the crystal field to the B_4 and B_2 tensors of the spin Hamiltonian of Fe³⁺, respectively. A comparison of the fourth-rank tensors B_4 of the spin Hamiltonian and $\{V_4 \otimes V_4\}_4$ of the crystal field determined at 300 K with those determined at 77 K supports the conclusion that the phase transition is accompanied by combined rotation of the [GeO₄] tetrahedra with the [Ge(1)O₆] octahedron almost unaltered. The spectrum lines are narrow and the variety of point defects in the vicinity of the paramagnetic impurity ions Fe³⁺, Cr³⁺ and Cu²⁺ is not detected. These facts are inconsistent with the statistically distributed model for the Li(2) atom. In specific cases at 300 K, when the wings of the two spectrum lines of the $M \rightarrow M+1$ and the $M+2 \rightarrow M+3$ transitions of Fe³⁺ ions belonging to one system of translationally equivalent positions overlap an extra line appears in the center between these lines. It is suggested that this effect is due to the soft phonon mode above the phase transition temperature. © 1996 Springer.

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