

Analysis of the Structure of Tetragonal Oxygen Centers Associated with Yb³⁺ ions in the KMgF₃ Crystal

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Abstract

The parameters of the crystal field of the tetragonal oxygen center associated with a Yb³⁺ ion in the KMgF₃ crystal found previously in a study of optical and ESR spectra are applied to analyze lattice distortions in the vicinity of the impurity ion and the O²⁻ ion compensating for the excess positive charge. Within the super-position model, it was ascertained that the Yb³⁺ ion and the neighboring ions of fluorine and oxygen on the axis of the center shift significantly along the direction from the O²⁻ ion to the Yb³⁺ ion during the formation of the tetragonal oxygen center. As this takes place, the distances of both (fluorine and oxygen) ions from the impurity ion increase. The four F⁻ ions of the nearest octahedral neighborhood of Yb³⁺ that are arranged symmetrically in the plane perpendicular to the axis of the center slightly recede from the axis. © 2003 MAIK "Nauka/Interperiodica".

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