Energy Levels of Erbium Centers in $KTaO_3$:Er Crystals

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Potassium tantalate ($KTaO_3$) is promising material for wide range of applications due to exceptional properties that can be tailored by adding suitable impurities. However, proper understanding of the impurity-induced phenomena is largely limited by the lack of information on the microstructure and properties of impurity centers. Therefore, a study of optical absorption and photoluminescence of $KTaO_3$ crystals doped by erbium, one of the most used rare-earth laser active impurities, appears very attractive because of deepening knowledge of optically active impurity centers in highly polarizable ABO_3 perovskite-type crystals. $KTaO_3$ crystals possess a cubic inversion symmetric structure down to the lowest temperatures but they tend to impurity induced structural and ferroelectric phase transitions. In $KTaO_3$, Er^{3+} ions can be substituted in the dodecahedral K^+ sites and/or in the octahedral Ta^{5+} sites in the crystal fields of the cubic O_h symmetry. Necessary charge compensation can occur either locally lowering the symmetry of Er^{3+} center or non-locally preserving its O_h symmetry.
The absorption spectra of the blue tinted $KTaO_3$:Er (500 ppm) crystals recorded at 2, 77, and 300 K within the 350 - 650 nm spectral region revealed the structured absorption bands corresponding to f-f optical transitions from the $^4I_{15/2}$ ground state to the excited states of $Er^{3+}(4f^{11})$ ions. An analysis of the spectra proved in the studied crystals an existence of the "major" and less concentrated "minor" Er^{3+} centers that give rise to the observed intense and weak zero-phonon absorption lines, respectively. Moreover it allowed us to determine structure of energy levels for the $^4F_{9/2}$, $^4S_{3/2}$, $^2H_{11/2}$, $^4F_{7/2}$, $^4F_{5/2}$, $^2H_{9/2}$, and $^4G_{11/2}$ excited states of the "major" Er^{3+} center. The number of zero-phonon absorption lines of the "major" Er^{3+} center observed at 2 K exactly corresponds to that theoretically possible for f-f optical transitions of Er^{3+} ions in the crystal field of non-cubic symmetry. Comparison of the ionic radii of Er^{3+}, K^+, and Ta^{5+} ion indicates together with the n-type conductivity of $KTaO_3$:Er crystals that the "major" Er^{3+} centers are formed by Er^{3+} ions substituted for K^+ ions. The emission bands corresponding to the $^4S_{3/2}$ —¿ $^4I_{15/2}$, $^4F_{9/2}$ —¿ $^4I_{15/2}$, and $^4S_{3/2}$ —¿ $^4I_{13/2}$ transitions of Er^{3+} ions were found in the photoluminescence emission spectra taken on $KTaO_3$:Er crystals within the 350 - 860 nm spectral region at temperatures between 4.2 and 300 K. The number of zero-phonon lines detected at low temperatures within the emission bands of Er^{3+} ion photoluminescence exceeded that theoretically allowed for one type of Er^{3+} center. Besides, their relative intensities were dependent on excitation wavelength. Thus a study of low-temperature excitation spectra of Er^{3+} ion photoluminescence allowed us to separate zero-phonon emission lines corresponding to the "major" and "minor" Er^{3+} centers and to determine crystal field splitting of the ground state $^4I_{15/2}$ and of the first excited state $^4I_{13/2}$ for the "major" Er^{3+} centre at 4.2 K. The possible origin, symmetry and energy level structure of the "minor" Er^{3+} centers in $KTaO_3$:Er crystals is discussed too.