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Energy Spectrum of YAG:Cr^{3+} and Thermal Shifts of Its R Lines

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Abstract: Traditional ligand-field theory has to be improved by taking into account both "pure electronic" contribution and electron-phonon interaction one (including lattice-vibrational relaxation energy). By means of improved ligand-field theory, R_1, R_2, R'_3, R'_2, and R'_1 lines, U band, ground-state zero-field-splitting (GSZFS) and ground-state g factors as well as thermal shifts of R_1 line and R_2 line of YAG:Cr^{3+} have been calculated. The results are in very good agreement with the experimental data. In contrast with ruby, the octahedron of ligand oxygen ions surrounding the central Cr^{3+} ion in YAG:Cr^{3+} is compressed along the [111] direction. Thus, for YAG:Cr^{3+} and ruby, the splitting of $t_2^3 4A_2$ (or $t_2^3 2E$) has opposite order, and the trigonal-field parameters of the two crystals have opposite signs. In thermal shifts of R_1 and R_2 lines of YAG:Cr^{3+}, the temperature-dependent contributions due to EPI are dominant.

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Key words: improved ligand-field theory, electron-phonon interaction, Stokes shift, energy spectrum, thermal shift, g factor

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