Crystal Field Analysis, Electron-phonon Coupling and Spectral Band Shape Modeling in MgO:Cr^{3+}

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A crystal field analysis of the energy level structure of Cr^{3+} in MgO crystal is performed, using the exchange charge model of the crystal field theory. The crystal field parameters acting on the optical electrons of Cr^{3+} are calculated from the crystal structure data; good agreement between the calculated and observed energy levels of Cr^{3+} in the title host is demonstrated. The Stokes shift $S = 5.9$ and the energy of the phonons effectively interacting with the impurity center $\hbar\omega = 405$ cm^{-1} are derived from the experimental spectra of absorption and emission. The obtained values of S and $\hbar\omega$ were used for the computer modeling of the Cr^{3+} $^4T_{2g} \rightarrow {}^4A_{2g}$ emission and $^4A_{2g} \rightarrow {}^4T_{2g}$ absorption bands. From this modeling, the zero-phonon energy for the considered transitions was estimated to be 14,000 cm^{-1}.

Key words: Crystal Field Theory; 3d-Ions; Electron-phonon Coupling.