2005 Vol.43 No.3 pp.529-538 DOI:

Improved Ligand-Field Theory with Effect of Electron-Phonon Interaction

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(Received: 2004-6-15; Revised:)

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 of ruby and/or GSGG:Cr^{3+} as well as thermal shifts of GSZFS, R_1 line and R_2 line of ruby have been calculated. The results are in very good agreement with the experimental data. Moreover, it is found that the value of cubic-field parameter given by traditional ligand-field theory is inappropriately large. For thermal shifts of GSZFS, R_1 line and R_2 line of ruby, several conclusions have also been obtained.

PACS: 71.70.Ch, 76.30.Fc, 78.20. Nv, 63.20.Mt
Key words: improved ligand-field theory, electron-phonon interaction, Stokes shift, energy spectrum, thermal shift, g factor

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