2007 Vol.47 No.5 pp.937-943 DOI:

Improved Ligand-Field Calculation of Energy Spectrum and R-Line Thermal Shift of $MgO:Cr^{3+}$

ZHANG Zheng-Jie[1] and MA Dong-Ping[2]

[1] College of Information Engineering, Chengdu University of Technology, Chengdu 610059, China
[2] Department of Applied Physics, Sichuan University, Chengdu 610065, China
(Received: 2006-6-6; 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, the R-line, $t_2^{3}{}^2T_1$ lines, t_2^2 ($^3T_1$) e^4T_2, and t_2^2 ($^3T_1$)e^4T_1 bands, ground-state g factor, four strain-induced level-splittings, and R-line thermal shift of $MgO:Cr^{3+}$ have been calculated. The results are in very good agreement with the experimental data. It is found that for $MgO:Cr^{3+}$, the contributions due to electron-phonon interaction (EPI) come from the first-order term. In thermal shift of R-line of $MgO:Cr^{3+}$, the temperature-dependent contribution due to EPI is dominant.

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

[Full text: PDF]

Close