2002 Vol.37 No.2 pp.247-252 DOI:

# Thermal Shifts and Electron-Phonon Interactions of $^4T_2$ and $^4T_1$ Broad Bands for Ruby

MA Dong-Ping,[1,2] MA Ning[3] and CHEN Ju-Rong[1]

[1] Department of Applied Physics, Sichuan University, Chengdu 610065, China
[2] International Centre for Materials Physics, The Chinese Academy of Sciences, Shenyang 110015, China
[3] Department of Computer Science, Sichuan University, Chengdu 610064, China
(Received: 2001-6-25; Revised: )

Abstract: For the first time, by taking into account all the irreducible representations and their components in the electron-phonon interaction (EPI) as well as all the levels and the admixtures of wavefunctions within $d^3$ electronic configuration, the values of parameters in expressions of Raman and optical-branch terms of thermal shifts (TS) due to EPI for three levels, $^4T_2$ band and $^4T_1$ band of ruby have been evaluated; the contributions to TS of $^4T_2$ and $^4T_1$ broad bands from thermal expansion have also been calculated; and then, the TS of the peak energies of $^4T_2$ and $^4T_1$ broad bands have been calculated. The results are in satisfactory agreement with observed data. The values of single-electron reduced matrix elements representing the strengths of EPI of $^4T_2$ and $^4T_1$ bands have respectively been determined. For TS of the peak energies of $^4T_2$ and $^4T_1$ bands, it is found that the contribution to TS from the second-order term in EPI Hamiltonian is dominant; TS due to EPI of acoustic branches are over two times as much as those of optical branches, and both of them increase rapidly with temperature; the neighbor-level term is insignificant; the contribution to TS from thermal expansion is specially important, and all the three terms of TS of $^4T_2$ or $^4T_1$ band are red shifts.

PACS: 78.20.Nv, 71.70.Ch, 63.20.Mt, 63.20.Kr
Key words: crystal fields, optical spectral bands, electron-phonon interaction, thermal expansion, thermal shift

[Full text: PDF]

Close