2001 Vol.36 No.3 pp.357-364 DOI:

Theoretical Calculations of Thermal Shifts of Ground-StateZero-Field-Splitting for Ruby

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(Received: 2000-11-13; Revised:)

Abstract: 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 thermal shifts (TS) of the ground-state zero-field-splitting (GSZFS) due to EPI for ruby have microscopic-theoretically been calculated; the contribution to TS of GSZFS from thermal expansion has also been calculated. The results are in very good agreement with experiments. It is found that the contributions from the first-order perturbation of the second-order term in EPI Hamiltonian are dominant in the Raman term and optical-branch term for TS of GSZFS; the different between the TS due to EPI of $t_2^3\ ^4A_2 \pm (1/2)\ e_2\ (G_2)$ level and the TS due to EPI of $t_2^3\ ^4A_2 \pm (3/2)\ e_2\ (G_1)$ level gives rise to the TS due to EPI of GSZFS, which is very small in comparison with the TS due to EPI of G_2 or G_1 level. Among various terms in TS of GSZFS, Raman term is the largest one and the signs of the Raman term and optical-branch term are opposite to the sign of the thermal-expansion term; the optical-branch term plays an important role in TS of GSZFS and increases rapidly with temperature; all various contributions to TS of GSZFS have to be taken into account, since the subtle balance among them determines the total result. The comparison between the features of TS of GSZFS and those of TS of R_1 and R_2 lines has been made. For TS of GSZFS, the contribution from thermal expansion is especially important; the neighbor-level term is insignificant.

PACS: 63.20.Mt, 63.20.Kr, 71.70.Ch, 75.10.Dg
Key words: optical materials, crystal fields, electronic paramagnetic resonance, phonons, thermal expansion

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