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Microscopic Theoretical Calculations of R-Line ThermalShifts and Broadenings of $MgO:Cr^{3+}$

MA Dong-Ping,[1,2] LIU Yan-Yun,[1] MA Ning[3] andCHEN 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
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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 basic wavefunctions within d^3 electronic configuration, the values of all the parameters in the expressions of thermal shift (TS) and thermal broadening (TB) due to EPI for the ground level, R level and R line of $MgO:Cr^{3+}$ have microscopically been evaluated; and then, TS and TB of R line and various contributions to them have uniformly been calculated. The results are in very good agreement with the experimental data. It is found that all the three terms of TS due to EPI are red shifts; the Raman term is the largest one, and the optical-branch term and neighbor-level term are important for TS; the contribution to TS from thermal expansion is blue shift, which is also important. The R-line TS of $MgO:Cr^{3+}$ comes from the first-order term of EPI. The elastic Raman scattering of acoustic phonons plays a dominant role in R-line TB of $MgO:Cr^{3+}$. For both TS and TB, it is very important to take into account all the admixtures of basic wavefunctions within d^3 electronic configuration.

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