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Energy Spectra, g Factors and Their Pressure-Induced and/or Thermal Shifts of $SrTiO_3:Cr^{3+}$ and $SrTiO_3:Mn^{4+}$ III: R-Line Thermal Shifts of $SrTiO_3:Mn^{4+}$

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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 the parameters in the expressions of thermal shift (TS) from EPI for the ground level, R level and R line of $SrTiO_3:Mn^{4+}$ have been evaluated; the R-line TS and various contributions to it have been calculated in the low-temperature region. It is found that all the three terms of R-line TS from EPI relevant to the lattice vibration are red shifts. The Raman term is the largest, the neighbor-level term is the second, and the optical-branch term is very small over the range of $T \leqslant 80$ K. The contribution to R-line TS from thermal expansion has been approximately neglected in this work. The very strong EPI relevant to its lattice vibration for $SrTiO_3:Mn^{4+}$ causes its R-line TS to be an unusually large red-shift. Only by taking into account the strong softening of the low-frequency acoustic modes of the lattice vibration at low temperatures, can we successfully explain the variation of R-line TS of $SrTiO_3$\$:Mn^{4+} with temperature.

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