2001 Vol.35 No.5 pp.627-634 DOI:

Energy Spectra, g Factors and Their Pressure-Induced and/or Thermal Shifts of SrTiO_3:Cr^{3+} and SrTiO_3:Mn^{4+} II: Pressure Effects on Ground-State g Factorand Splittings of t^3_2{}^2E and t^3_2{}^4A_2 of SrTiO_3:Cr^{3+}

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(Received: 2000-10-24; Revised:)

Abstract: By using the wavefunctions obtained from diagonalizing the complete d^3 energy matrix at normal and various pressures, the g factor of the ground state of $SrTiO_3:Cr^{3+}$ and its pressure-induced shift have been microscopically calculated. Only by taking the local strains around Cr^{3+} in $SrTiO_3:Cr^{3+}$ (which are about twice the bulk ones) and corresponding P-χ dependence, can we obtain a good agreement between the calculated result of pressure-induced shift of ground-state g factor and the experimental one. The physical origins of this pressure-induced shift have been explained. It is found that the change of Dq^{-1} with pressure makes main contribution to the pressure-induced shift of ground-state g factor of $SrTiO_3:Cr^{3+}$. By using the wavefunctions obtained from diagonalizing the complete d^3 energy matrix at normal pressure, the relevant matrix elements and accordingly strain-induced splittings of $t_2^3{}^2E$ and $t_2^3{}^4A_2$ of $SrTiO_3:Cr^{3+}$ have been calculated. The important results of Y_c, Z_c, P_c and Q_c have also been evaluated. It is the admixtures of basic wavefunctions resulted from the spin-orbit interaction and/or Coulomb interaction and/or Kramers degeneracy that make the strain-induced splittings of the levels nonzero. It is found that there are nonvanishing matrix elements of operators $T_2\xi$, $T_2\eta$ and $T_2\zeta$ between wavefunctions with positive M_s and those with negative M_s', which have important effects on the strain-induced splittings of the levels.

PACS: 71.70.Ch, 71.70.Fk, 76.30.Fc, 78.20.Hp
Key words: crystal fields, energy spectrum, g factors, high-pressure effect, strain-induced splitting

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