Investigations of the Defect Structure for Cu^{2+} in $SrLaAlO_4$

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The defect structure for Cu^{2+} in $SrLaAlO_4$ is theoretically investigated by the perturbation formulas of the spin Hamiltonian parameters (g factors $g_{\|}$, $g_{\perp}$ and the hyperfine structure constants $A_{\|}$ and $A_{\perp}$) for a $3d^9$ ion in tetragonally elongated octahedra. Based on these studies, the tetragonal center may be attributed to Cu^{2+} occupying the host Al^{3+} site, associated with one hole delocalized at the four oxygen ligands in planar coordination. Furthermore, the four Cu,O bonds (perpendicular to the four-fold axis) are found to suffer an outward stretch of about 0.06 Å due to (i) the local tenseness in this plane, arising from the size mismatching substitution of the smaller Al^{3+} by the larger Cu^{2+} and (ii) the weaker electrostatic attraction of the less charged Cu^{2+} acting upon the four oxygen ions containing the delocalized hole. The calculated spin Hamiltonian parameters agree well with the experimental data. The defect structure of this center is discussed.

Key words: Electron Paramagnetic Resonance (EPR); Defect Structure; Crystal-field and Spin Hamiltonians; Cu^{2+}; $SrLaAlO_4$.