EPR Theoretical Study of the Local Lattice Structure of Fe$^{3+}$ Doped in MgTiO$_3$ and LiTaO$_3$

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The EPR zero-field splittings of Fe$^{3+}$ doped in MgTiO$_3$ and LiTaO$_3$ are studied by diagonalizing the complete energy matrices of the electron-electron repulsion, ligand-field and spin-orbit coupling interactions for a d$^5$ configuration ion in a trigonal ligand-field. It is shown that, when Fe$^{3+}$ is doped in a MgTiO$_3$ or LiTaO$_3$ crystal, the local lattice structure around the octahedral Fe$^{3+}$ center has an obvious distortion along the C$_3$ axis. By simulating the second- and fourth-order EPR parameters $D$ and $(a - F)$ simultaneously, the local structure parameters of Fe$^{3+}$ doped in MgTiO$_3$ and LiTaO$_3$ crystals are determined, which reveal that Fe$^{3+}$ occupies both the Mg$^{2+}$ and Ti$^{4+}$ sites in the MgTiO$_3$:Fe$^{3+}$ system and occupies the Li$^+$ site rather than the Ta$^{5+}$ site in the LiTaO$_3$:Fe$^{3+}$ system. The results accord with the ENDOR and EPR experiments. – PACS numbers: 71.70.Gm; 75.30.Et; 71.70.Ch.

Key words: MgTiO$_3$:Fe$^{3+}$ and LiTaO$_3$:Fe$^{3+}$ Systems; Local Lattice Structure; EPR Spectrum.