EPR Theoretical Study of the Local Lattice Structure of Fe^{3+} Doped in $MgTiO_3$ and $LiTaO_3$

Lei-Lei Pan[a], Xiao-Yu Kuang[a,b], Guang-Dong Li[a], and Hui Wang[a]

[a] Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China
[b] International Centre for Materials Physics, Academia Sinica, Shenyang 110016, China

Reprint requests to X.-Y. K.; E-mail: panlei225@163.com

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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.