Defect Structure of the Tetragonal Cu²⁺ Center in PbTiO₃: Cu²⁺ Crystal

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The defect structure of the tetragonal Cu^{2+} center in PbTiO₃: Cu^{2+} crystal is studied by analyzing the EPR g factors and hyperfine structure constants. From the study, we suggest that an oxygen vacancy occurs in the nearest-neighbors site of Cu^{2+} due to charge compensation, and that the off-center displacement of Cu^{2+} is smaller than that of the replaced host ion Ti^{4+} . The reasonableness of the defect structure is discussed.

Key words: Defect Structure; Electron Paramagnetic Resonance; Crystal-field Theory; $\mathrm{Cu^{2+}}; \mathrm{PbTiO_3}$