The Studies of Geometrical Microstructure of Tetragonal Co\textsuperscript{2+}-V\textsubscript{O} Centers in KNbO\textsubscript{3} and KTaO\textsubscript{3} Crystals from EPR Data

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From the perturbation formulas for the EPR $g$ factors $g_\parallel$ and $g_\perp$ of a 3d\textsuperscript{7} ion in tetragonal octahedral crystal field based on a cluster approach, the geometrical microstructures of tetragonal Co\textsuperscript{2+}-V\textsubscript{O} centers in KNbO\textsubscript{3} and KTaO\textsubscript{3} crystals are obtained by fitting the calculated $g_\parallel$ and $g_\perp$ to the observed values. It is found that the Co\textsuperscript{2+} ion in Co\textsuperscript{2+}-V\textsubscript{O} centers is displaced away from the oxygen vacancy V\textsubscript{O} by 0.3 Å in KNbO\textsubscript{3} and by 0.29 Å in KTaO\textsubscript{3}. These results are comparable with those of Fe\textsuperscript{3+}-V\textsubscript{O} centers in ABO\textsubscript{3} perovskite-type crystals obtained from both the shell-model simulations and the embedded-cluster calculations, and from theoretical studies of EPR data. The experimental values of $g_\parallel$ and $g_\perp$ for the tetragonal Co\textsuperscript{2+}-V\textsubscript{O} centers in both crystals are also explained reasonably.

\textit{Key words:} Electron Paramagnetic Resonance (EPR); Crystal- and Ligand-Field Theory; Defect Structure; Co\textsuperscript{2+}; KNbO\textsubscript{3}; KTaO\textsubscript{3}. 