

# Theoretical Studies on the Gyromagnetic Factors and the Hyperfine Structure Constants for the Tetragonal Copper Center in $\text{KTaO}_3$

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The gyromagnetic factors  $g_{\parallel}$ ,  $g_{\perp}$  and the hyperfine structure constants  $A_{\parallel}$  and  $A_{\perp}$  of the tetragonal  $\text{Cu}^{2+}$  center in  $\text{KTaO}_3$  are theoretically studied in this work. Based on the analyses of the electron paramagnetic resonance results of this center, it is found that the impurity  $\text{Cu}^{2+}$  occupies the octahedral  $\text{Ta}^{5+}$  site, associated with a nearest-neighbouring oxygen vacancy  $\text{V}_\text{O}$  along the  $C_4$  axis. Due to the electrostatic repulsion of  $\text{V}_\text{O}$ ,  $\text{Cu}^{2+}$  is displaced away from  $\text{V}_\text{O}$  by  $\Delta Z (\approx -0.29 \text{ \AA})$  along the  $C_4$  axis. The theoretical values of the  $g$  and  $A$  factors based on the above defect structure and the impurity displacement agree reasonably with the experimental data.

*Key words:* Electron Paramagnetic Resonance; Defect Structures; Crystal-field Theory;  $\text{Cu}^{2+}$ ;  $\text{KTaO}_3$ .