Investigation of the Electric-field Effect in EPR Spectra of Fe³⁺ in KTaO₃

Wen-Chen Zheng a,c , Sheng Tang a , and Xiao-Xuan Wu a,b,c

a Department of Material Science, Sichuan University, Chengdu 610064, P. R. China
b Department of Physics, Civil Aviation Flying Institute of China, Guanghan 618307, P. R. China
c International Centre for Materials Physics, Chinese Academy of Sciences, Shenyang 110016, P. R. China

Reprint requests to W.-C. Z.; E-mail: zhengwc1@163.com

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The displacements of Fe^{3+} (at the Ta^{5+} site) along the [001] direction in KTaO3 crystal, caused by the electric field, have been studied by calculating the electric-field-induced zero-field splittings from the microscopic mechanisms and the empirical superposition model. It is found that the Fe^{3+} displacements obtained by the two methods at the same electric-field strength and temperature are close to each other. These displacements are also close to that estimated from the force-balance equation. It is suggested that the electric-field-induced zero-field splitting can be attributed primarily to the above displacement and the temperature dependence of the electric-field-induced zero-field splitting is mainly due to the change in the dielectric constant of KTaO3 with temperature.

Key words: Electron Paramagnetic Resonance; Electric-field Effect; Crystal-field Theory; Fe³⁺; KTaO₃.