

Studies of EPR g -factors on Rutile (TiO_2) with Co^{2+} Ion

Shao-Yi Wu^{a,b} and Wen-Chen Zheng^{a,b,c}

^a Department of Material Science, Sichuan University, Chengdu 610064, P. R. China

^b International Centre for Materials Physics, Chinese Academy of Sciences,
Shenyang 110016, P. R. China

^c Key Laboratory for Radiation Physics and Technology of Ministry of Education,
P. R. China (in Sichuan University)

Reprint requests to S.-Y. W.; E-mail: wushaoyi.netease.com

Z. Naturforsch. **57 a**, 45–48 (2002); received November 19, 2001

The anisotropic g -factors g_X , g_Y , and g_Z for Co^{2+} in rutile crystal are studied from the second-order perturbation formulas based on the cluster approach. In the studies, the contributions due to covalency effects, the configuration interaction and the rhombic crystal field are taken into account. The calculated values are close to the observed ones. The small discrepancy between calculation and experiment is discussed.

Key words: Electron Paramagnetic Resonance; Crystal- and Ligand-field Theory; Co^{2+} ; Rutile.