Theoretical Interpretation of the EPR Parameters for Dy^{3+} Ion in $LuPO_4$ Crystal

Hui-Ning Dong[a,b], Hui-Ping Du[a], Shao-Yi Wu[b,c], and Peng Li[d]

[a] Institute of Applied Physics & College of Electronic Engineering, Chongqing University of Posts and Telecommunications, Chongqing 400065, P. R. China

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

[c] Department of Applied Physics, University of Electronic Science and Technology of China, Chengdu 610054, P. R. China

[d] Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, P. R. China

Reprint requests to Dr. H.-N.D.; E-mail: donghn@163.com

Based on the superposition model, in this paper the EPR parameters $g_\parallel$ and $g_\perp$ of Dy^{3+}, and the hyperfine structure constants $A_\parallel$ and $A_\perp$ of $^{161}Dy^{3+}$ and $^{163}Dy^{3+}$ in $LuPO_4$ crystal are calculated by perturbation formulas from the crystal-field theory. In the calculations, the contributions of various admixtures and interactions such as J-mixing, mixtures among states with the same J-value, two-order perturbation, covalency as well as local lattice relaxation are considered. The calculated results agree reasonably with the observed values.

Key words: Electron Paramagnetic Resonance; The Superposition Model; $LuPO_4$; Dy^{3+}.