Studies on the Local Structure of the Tetragonal Er^{3+} Center in CaO

Shao-Yi Wu[a,b] and Hui-Ning Dong[b,c]

[a] Department of Applied Physics, University of Electronic Science & Technology of China,
Chengdu 610054, P. R. China
[b] International Centre for Materials Physics, Chinese Academy of Sciences, Shenyang 110016,
P. R. China
[c] College of Electronic Engineering, Chongqing University of Posts and Telecommunications,
Chongqing 400065, P. R. China

Reprint requests to S.-Y. W; E-mail: shaoyi-wu@163.com

The local structure of the tetragonal Er^{3+} center in CaO is theoretically studied by using the perturbation formulas of the g factors for a $4f^{11}$ ion in tetragonal symmetry. In these formulas, the contributions to the g factors from the second-order perturbation terms and the admixtures of various states are taken into account. Based on the investigations, this center is suggested to be the impurity Er^{3+} substituting the host Ca^{2+} site, associated with a Ca^{2+} vacancy V_{Ca} in the [100] (C_4) axis due to charge compensation. By studying the g factors of the tetragonal center, impurity Er^{3+} is expected to undergo an off-center displacement $\Delta Z (\approx 0.2 \text{ Å})$ towards the V_{Ca} along the C_4 axis because of the electrostatic attraction. The calculated g factors based on the displacement ΔZ show reasonable agreement with the observed values.