Local Structure Determination of Tetragonal Cr^{2+} Center in CdS Semiconductor

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Z. Naturforsch. **64a,** 507 – 510 (2009); received August 28, 2008 / revised November 10, 2008

Recently, many studies for the local structure of $3d^5$ ions in octahedrally coordinated compounds are made by simulating the EPR parameters on the basis of the complete energy matrix. However, for the $3d^4$ ions in tetrahedrally coordinated compounds, the studies are relatively fewer. In this work, by diagonalizing the complete energy matrix for a d^4configuration in a tetragonal ligand-field within a strong-field representation, the local structure around Cr^{2+} in CdS crystal is studied. Our results show that there exists a compression distortion in the local lattice structure. From our calculations, the distortion parameters $\Delta R = -0.022$ Å and $\Delta\theta = -1.410^\circ$ are obtained.

Key words: Local Structure; Energy Matrix, EPR Parameters.
PACS numbers: 75.10.Dg; 76.30.-v