Calculation of the emission spectrum of Er doped silicon carbide

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The rare earth erbium luminescence has a sharp peak at 1.54 μm and has been applied to lasers and light-emitting devices. The previous study have shown that the addition of erbium to SiC, a semiconductor with a wide gap, has a low temperature dependence and stable intensity at room temperature [1]. Theoretical calculations are currently widely performed due to the complexity and difficulty of calculating the emission spectra of rare earths with electrons in the 4f orbitals. Therefore, this study focuses on the simple calculation of emission spectra from a point-charge model for a material in which erbium is added to SiC with multiple structures.

The two structures used in this study were 3C-SiC and 6H-SiC, to which models with Er added at a concentration of approximately 1% were utilised. A point charge model was created, taking into account Er and even the first neighbouring atom, and the crystal field matrix was calculated. The obtained crystal field matrix was used to calculate the energy levels in the 4f orbitals using multiplet calculations [2]. In the present study, the energy difference between the 4f and 5d orbitals is used in the multiplet calculations, but the exact values are not known and three cases are calculated for E_{5d}-E_{4f}=1 eV, 5 eV and 10 eV. In rare-earth emission, the hybridisation effect between the 4f and 5d orbitals allows an electric dipole-magnetic dipole transition in the 4f intra-orbital level, called the f-f transition. Emission spectrum was calculated based on the transition probabilities from the energy level splitting.

The calculation results showed a high reproducibility of previous studies at 1 eV, although a simplified model was used. It is predicted that calculations of models with other rare earths added to ionic crystals will also be possible. In addition to ligand field theory, a molecular orbital approach could be incorporated for further discussion.

References

[1] W.J. Choyke *et al*, Applied Physics Letters. **65** No13. 1668-1670 (1994)