Galyna Puchkovska International School-Seminar Spectroscopy of Molecules and Crystals

EPR STUDY OF PARAMAGNETIC DEFECTS IN ZnSe:Cr CRYSTALS D. Savchenko¹, K. Lamonova², N. Kovalenko³, M. Hidulianov⁴, I. Ivanchenko⁴, N. Popenko⁴



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Introduction

ZnSe has received considerable attention due to its successful application in blue-green semiconductor lasers, mid-infrared lasers and other optoelectronic devices, doped with Cr2+, and Fe2+ have a significant lasing potential, demonstrated efficient, room-temperature lasing action near 2.5 µm, and have important potential applications in vibrational spectroscopy, trace gas detection, and medicine.

Research methods

EPR spectroscopy (Bruker ELEXSYS EPR E580 spectrometer (~9.4 GHz) The EPR spectra were simulated using the EasySpin 5.2.28 software package Modified Crystal Field Theory (MCFT) Quantum Espresso calculations on the base of the Density Functional Theory (DFT) Luminescence spectroscopy



Conclusion

The EPR spectra at T > 15 K consist of the intense line sextet with g ~ 2.005 and A ~ 6.5 mT due to hyperfine interaction with 55 Mn nuclei (I = 5/2) caused by Mn²⁺ ions along with a broad line with a linewidth of about 20 mT that varies its magnetic resonance position and intensity upon the temperature decrease. At 5 K, additional lines appear in the EPR spectrum of ZnSe:Cr. The spin Hamiltonian parameters $g_{\perp} = 1.98$, $g_{\parallel} = 1.961$, D = -2.48 cm⁻¹, a = 0.02 cm⁻¹. The symmetry of the center was taken as D₂₄. Thus, the lines that appeared in the EPR spectrum at 5 K should be related to Cr^{2+} ions in ZnSe. The character of the angular dependence could hint that the Cr^{2+} ions are located in the interstitial sites. The luminescence study of Cr doped ZnSe shows Cr^{2+} is in a tetrahedral coordination complexes and the luminescence transitions arise between $E_g \rightarrow T_{2g}$ levels.

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