

Photoluminescence studies of the futuristic SnSe semiconductor

M. Szot^{1,2}, P. Wojnar¹, J. Korczak^{1,2}, W. Zaleszczyk^{1,2}, L. Kowalczyk¹, S. Chusnutdinow¹,
R. Minikayev¹, W. Wołkanowicz¹, T. Story^{1,2}, G. Karczewski¹

¹ *Institute of Physics, Al. Lotników 32/46, PL-02668 Warsaw, Poland*

² *International Research Centre MagTop, Institute of Physics Polish Academy of Sciences, Al. Lotników 32/46, PL-02668 Warsaw, Poland*

SnSe semiconductor belongs to the family of binary IV-VI chalcogenide compounds (Sn-X; X=Se,S), which owe the interest of researchers to the similarity of their layered crystal structure to molybdenum dichalcogenides - a prototype 2D systems. In particular, SnX₂ chalcogenides have been extensively studied as they exhibit high optical absorption coefficient and strong photo-responsivity in the near infrared spectral range allowing their wide application in a new generation of optoelectronic and photonic systems. Unlike rock salt lead monochalcogenides tin-based chalcogenides crystallize in hexagonal and monoclinic phases for SnX₂ or orthorhombic phase for SnX compounds. The layered orthorhombic structure (distorted rock salt structure) of SnSe leads to anisotropy and anharmonicity of chemical bonds responsible for extremely low thermal conductivity along the plane with zig-zag ordering of ions and finally for the very high value of the thermoelectric figure of merit parameter *ZT* reaching 2.6 [1]. The excellent thermoelectric properties of monocrystalline SnSe have become a new inspiration for research on SnX materials. Therefore, tin chalcogenides appear as a family of semiconductors with the possibility of dual use in the field of photovoltaic and thermoelectric energy conversion, important from the point of view of environmental protection. In addition, the exciton binding energy and the energy gap of SnSe significantly depend on dimensionality of the structures (due to strong quantum confinement) and on the method of material preparation. For SnSe bulk samples an indirect bandgap of about 0.9 eV is expected, while for single-layer material the indirect and minimum direct gap differs slightly and amount to 1.63 eV and 1.66 eV, respectively [2]. Since SnX chalcogenides are generally less investigated than SnX₂ compounds, systematic study of their optical properties is needed. In particular, the results of luminescence (PL) studies of these compounds are rarely reported.

In this paper we discuss the results of PL measurements of monocrystalline SnSe synthesized in a direct reaction between the elements in a vacuum-sealed quartz ampoule at 950 °C. Orthorhombic structure of the resulting crystal was confirmed by XRD analysis. For these crystals excited with a 405 nm laser at cryogenic temperatures we observed several PL lines with energies of 0.9 eV, 0.94 eV and 1 eV, the position of which is weakly dependent on temperature. We assign the weakest line with the lowest energy to the indirect bandgap transition expected for bulk SnSe material. Higher energy lines, which are 5 to 10 times stronger, we associate with direct transitions in layered terraces-like structures (revealed on the surface of our SnSe crystals in SEM microscopic measurements), because the energy positions and amplitudes of these lines depend on the spatial position at the sample in which measurement has been taken. Our interpretation of the obtained PL spectra will be discussed in detail, taking into account the results of micro- and cathodo-luminescence measurements.

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References

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