Ministry of Education and Science of Ukraine

Institute of Physics of NASU

V.E. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine

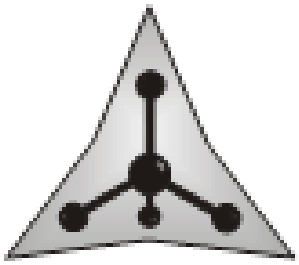
Scientific Council "Semiconductor and Dielectric Physics" at Physics and Astronomy Department of NASU

Academy of Sciences of Higher Education of Ukraine

Drohobych Ivan Franko State Pedagogical University

XII-th International Conference

TOPICAL PROBLEMS OF SEMICONDUCTOR PHYSICS



Prykarpattya,

Drohobych, UKRAINE

MAY 25–29, 2026

“Topical Problems of Semiconductors Physics” / Edited by Ihor Stolyarchuk. – Drohobych : Drohobych Ivan Franko State Pedagogical University, 2026. – 93 p.

Actual problems and important achievements of modern semiconductors physics are presented in the Proceedings of the XII-th International Conference “Topical Problems of Semiconductors Physics”. The abstracts are grouped into 7 sections, according to the Conference Thematic: “A. New frontiers in semiconductors and their based structures for electronics, optoelectronics, spintronic and sensing”, “B. Semiconductor low-dimensional structures: advances in synthesis, characterization, theoretical modeling and applications”, “C. The semiconductors for LEDs, solar and related energy technologies and sensor materials”, “D. Synthesis, processing and characterization of multifunctional oxide materials”, “E. Advanced strategies for smart functional and multifunctional bionanomaterials and biointerfaces”, “F. Laser material processing: from fundamental interactions to innovative applications”, “G. Modern computational methods and their applications in materials science: Synergy of theory and experiment”. The Proceedings were prepared for publication by the Conference Program Committee and presented in the author’s edition.

Recommended for publication by the Academic Council of Drohobych Ivan Franko State Pedagogical University.

ISBN 978-617-8591-12-0

Dependence of thermophysical and thermoelectric properties of lead diiodide nanofilms on their thickness

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The thermophysical and thermoelectric properties of nanometer planar structures (nanofilms) based on lead diiodide have been theoretically investigated with an emphasis on their changes when the nanofilm thickness changes. The heat capacity, entropy, free energy, thermal diffusion coefficient, lattice thermal conductivity, and thermoelectric figure of merit have been calculated as functions of the film thickness. For this purpose, analytical expressions for the dispersion dependences of acoustic phonon frequencies and group velocities in hexagonal quasi-two-dimensional nanostructures, obtained in [1] in the elastic continuum approximation [2], were used.

It is shown that a pronounced size effect is observed for ultrathin nanofilms, where all the considered quantities demonstrate a nonlinear dependence on the thickness. The dominant contribution to the thermodynamic functions is provided by transverse shear and bending modes of acoustic phonons; while the dilation mode mainly determines the heat transfer and thermoelectric processes.

The obtained results are in satisfactory agreement with the available experimental data and first-principles calculations of other researchers. The obtained results demonstrate the potential of phonon engineering to tune the thermophysical and thermoelectric properties of PbI_2-containing nanostructures by controlling their thickness.

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