Belarusian State University
of Informatics and Radioelectronics
R&D Department
BSUIR, 6, P. Brovki Str., Minsk 220013, Republic of Belarus

Development of combined methods and models for describing the thermodynamic properties of crystals, solid solutions and composite materials for devices operating at high temperatures

Tasks: creating a library of material parameters used in the development of devices that operate at high temperatures.

Research materials: AxB1-xC solid solutions, composite heterostructures, traditional bulk materials.

Expected results:

- thermal conductivity and heat capacity, taking into account the anisotropy of the properties, as well as the coefficient of thermal expansion, phonon spectra, force constants;
- distribution of thermal characteristics over the volume of the multilayer structure, including the allocation of the contact area of the two materials («λ1 material / λcontact(l) / λ2 material»), using molecular dynamics methods;
- electronic library with fundamental and thermal characteristics.

Methods:

- QM and MD modeling taking into account phonon-phonon and electron-phonon interaction (a new feature of the modeling environment),
- macroscopic models of thermal conductivity,
- quadratic interpolation for determining thermal conductivity in the solid solutions of AxB1-xC,
- a model of thermal conductivity that takes into account surface processes at the interface of two phases.

Type of collaboration

research cooperation

Key words

thermodynamic, composite, thermal conductivity, temperature

Contacts

Head of research
Viktor Stempitsky
PhD, Associate Professor
vstem@bsuir.by

Technology Transfer
science@bsuir.by