1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Thermoelectric properties of II-VI superlattice : experimental and theoretical approach

1.1. Project goals

The goal of the project is to study and understand the thermoelectric properties of II-VI superlattices.

1.2. Outline

As part of phd student thesis, phd student plans to obtain a superlattice ZnO/CdO and ZnOMg/CdO at the Institute of Physics of the Polish Academy of Sciences in Warsaw as a first step. The doctoral student will participate in this. Further, the doctoral student will have to determine the thickness of the layers (SEM or optical profilometer). In the next stage, the doctoral student will perform measurements of thermal, electrical and thermoelectric properties in the range from -20C to 100C. Next, the doctoral student will analyze the thermoelectric properties using theoretical approaches. To study the thermoelectric properties of materials, a combination of density functional theory (DFT) and Boltzmann transport theory was used. The process began with structural optimization and electronic structure calculations using e.g. the CASTEP software. BoltzTrap2 was employed to calculate important thermoelectric properties such as the Seebeck coefficient, electrical conductivity and electronic thermal conductivity. However, since BoltzTrap2 does not calculate the lattice part of the thermal conductivity, the Slack model can be used to estimate it. These properties were analyzed over a range of temperatures to observe their behavior and to identify materials with high thermoelectric efficiency. The diffusive and ballisitic parts are respectively described by the Cattaneo and Guyer-Krumhansl equations that are rooted in the second law of thermodynamics. integrates these components into the variable space, offering a more rigorous framework for thermoelectric transport in superlattices [2]. The obtained insights can drive advancements in the design of thermoelectric materials and enhances the efficiency of heat-to-electricity energy conversion.

1.3. Work plan

1. Growing and structure characterization of superlattice

2. Thermal, electrical and thermoelectroci of superlattice

3. Use of DFT and Boltzmann equation for predicting thermoelectric, thermal and electrical properties of superlattice.

4. Use Machine learning to exhance results for point 4.

1.4. Literature (max. 7 listed, as a suggestion for a PhD candidate preliminary study)

Chatterjee Ankur, Swapna Mohanachandran Nair Sindhu, Mikaeeli Ameneh [i in.], Photothermal infrared radiometry and thermoreflectance : unique strategy for thermal transport characterization of nanolayers Nanomaterials, 2024, vol. 14, nr 21, s.1-18, Numer artykułu:1711

Required initial knowledge and skills of the PhD candidate

Required documented knowledge of DFT and Boltzmann calculation of thermoelectric properties.

Expected development of the PhD candidate's knowledge and skills

1. Experimental methods like SEM, AFM, PTR, TR, 4 probe method, Seebeck measurements

2. Calculation of thermoelectric properties using machine learning