Title: Growth of hBN crystals from metal solutions under high N_2 pressure – modeling the thermodynamic properties of Me-B-N systems and experimental verification

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Institute: Institute of High Pressure Physics Polish Academy of Sciences

Unit: Laboratory of Nitride Semiconductor Physics (NL-2)

WWW of the unit: https://www.unipress.waw.pl/en/labs/laboratory-of-nitride-semiconductor-physics

Background [max 1500 characters]:

The scientific concept of the project is based on the controlled crystallization of hBN from metallic solutions under high nitrogen pressure, under conditions close to thermodynamic equilibrium. The key issue is to determine how the composition of the metallic solvent, for example Fe-, Ga-, or Mg-based systems, the activity of boron, and the chemical potential of nitrogen affect the stability of hBN and the course of crystallization.
The PhD project will combine thermodynamic modelling with experimental verification of selected hBN stability limits in Me–B–N systems. The theoretical part will include the determination of boron activity in metallic solutions using literature data, simplified thermodynamic models, and, where justified, ab initio calculations of boron–metal interaction energies.
The experimental part will involve participation in the preparation and analysis of selected high-pressure experiments aimed at testing model predictions and linking equilibrium conditions with the observed growth or absence of growth of hBN. The obtained results will be used to construct quantitative hBN stability maps and to identify favourable conditions for crystallization from metallic solutions.

Aim of the project [max 500 characters]
The aim of the project is to develop and experimentally verify a thermodynamic description of hBN stability in selected Me–B–N systems under high nitrogen pressure. The outcomes will include hBN stability maps, assessment of the influence of solvent composition on boron activity and hBN formation equilibrium, and identification of conditions favourable for controlled crystallization by combining modelling with experiment.

Requirements:

The candidate should hold a Master’s degree in physics, materials science, chemistry, or a related discipline. Required qualifications include a solid background in solid-state physics, thermodynamics, or computational materials science. The candidate should be familiar with basic concepts of ab initio modelling or numerical simulations and demonstrate the ability to develop and apply theoretical models to interpret experimental data. Prior experience with density functional theory (DFT), thermodynamic calculations, or scientific programming will be considered an advantage. The candidate is expected to work independently on theoretical tasks, actively collaborate with experimental researchers, and communicate results effectively within a multidisciplinary research team. Good command of English is required (min. B2 level).