The Warsaw Doctoral School in Natural and Biomedical Sciences and
the Institute of High Pressure Physics PAS cordially invites you to a **SPOTLIGHT TALK**

Numerical Simulations in Bulk Crystal and Layer Growth

given by

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on 3rd July 2023, 14:00

at the IHPP PAS New Technologies building ul. Prymasa Tysiąclecia 9
Durations: 60 min + more

All Warsaw-4-Phd students (and others) very welcome!

Crystalline materials are the basis for electronic, optical and opto-electronic devices and thus the foundation for the today-world. Bulk crystals are required as substrates for epitaxial layers or directly for optical devices.

Requirements for structural perfection, homogeneity in doping etc. have been increased over the years when going to smaller and smaller structures on the devices. Since the nineties the process development has been accompanied by numerical simulations, which has become more and more elaborate with the increasing computer power. Nevertheless, crystal growth a complex process and numerical simulations of the process are still challenging. In principle one would like to cover from the furnace scale (up to meter for industrial production) down to atomistic scale for defects.

For bulk crystal growth an overview will be given on the methods for global simulations. The broad ingredients of physics involved will be discussed and the engineering approach in such computations.

Specific examples will be given for the Czochralski growth of germanium and the Czochralski growth of Ga_2O_3 . The latter is used to make homo-epitaxy of

$Ga_2O_{3,}$, a material which is of great interest for power electronics and thus in this context of importance for electro mobility as well as for energy conversion in renewable energy production.

In the second part the epitaxial growth of layers is considered. Here we focus on microscopic and atomistic approaches such as phase field methods, density functional theory calculations and kinetic Monte Carlo simulations.

Specific examples will be given for the homo-epitaxial growth of Ga_2O_3 as well as of AlN and AlGaN layer growth on AlN(0001). The latter can be used for power or UV photonic devices.