Physics Final Year Project 2019/2020

„Properties of wurtzite Boron Nitride and Boron containing III-Nitride alloys: Insights from density functional theory "

Supervisor: Stefan Schulz

Project description:

Given their large band gaps, see Fig. 1, the nitride semiconductors aluminum nitride (AlN) and gallium nitride (GaN) have attracted considerable interest for energy efficient light emitting diodes (LEDs) operating in the ultraviolet (UV) spectral range. The nitride alloy AlGaN is in this sense unique, since by modifying the GaN content in AlGaN, in principle, its emission wavelength can be „tailored" from 200 nm to 400 nm. This UV wavelength window is of strong interest for a wide range of applications such as water purification, sensing, plant lighting and manufacturing (e.g. 3D printing). However, in contrast to LEDs operating in the blue spectral range, the efficiency of UV LEDs is very low. Therefore, there has been strong research interest around the world to gain insight into fundamental limitations but also to find ways to improve the efficiency of UV LEDs based on AlGaN. Despite many years of efforts, progress is slow on this. Recently, a new and more radical approach has been proposed to tailor electronic and optical properties of AlGaN emitters, namely by adding small fractions of Boron Nitride (BN) to these alloys. Given the smaller lattice constant of BN in comparison to AlN and GaN, see Fig. 1, „strain management" in AlGaN-based heterostructures, where thin AlGaN layers are sandwiched between AlN layers, is within reach. By tailoring the lattice constant of AlGaN by adding BN, for several different reasons, the performance of a device utilizing the heterostructure described above should benefit from the reduced strain in the layer. However, several fundamental properties of wurtzite BN, such as the band gap for instance, are still not well known, resulting from difficulties in growing these materials. As a consequence, how properties of BAlGaN change with BN content is still a matter of debate.

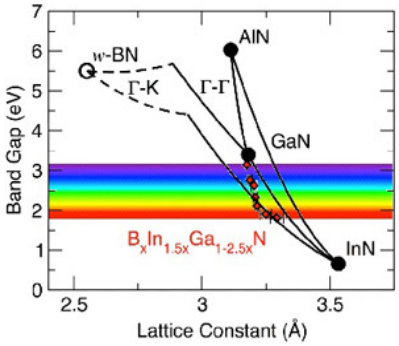

Fig. 2: Energy/Band gap of wurtzite BN, AlN, GaN and InN as a function of the lattice constant. (Appl. Phys. Lett. 111, 211107, (2017)).

Aim of this **Final Year Physics Project** is to **theoretically study**, in a first step, the **electronic and optical properties** of wurtzite **BN**.

Method: Here these properties shall be studied in the framework of **first-principles density functional theory (DFT)**. Initially different functionals shall be used to investigate the bulk band structure of BN. In a second step strain/pressure dependent DFT calculations shall be performed. The aim of this study is first to gain insight into the so-called deformation potentials of BN. Secondly, once the pressure dependence of the band gap at the center of first Brillouin and for the fundamental, indirect gap of BN is know, this information might help to distinguish states in BGaN alloys. If time permits, supercell calculations for BGaN alloys shall be targeted to study the evolution of the band

gap of BGaN alloys with BN content. The outcome of these studies shall help to provide first insights into the potential benefit of Boron containing nitride-based system for optoelectronic device applications with improved performance; they shall also facilitate in the longer run the development of semi-empirical models to treat BAlGaN heterostructures.