Investigation of group-III-nitride semiconductor nanostructures using an eight-band $k \cdot p$ formalism

OLIVER MARQUARDT, TILMANN HICKEL, JOERG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung — Despite its approximative nature, the $k \cdot p$-formalism provides a numerically efficient and accurate description of the electronic structure of group-III nitride semiconductor nanostructures with characteristic dimensions of few nanometers. [1] With the computational effort of this method being independent of the system size, it is possible to study an extensive set of zero-, one- and two-dimensional semiconductor nanostructures. We applied a plane-wave implementation of the 8-band $k \cdot p$ formalism and second-order continuum elasticity theory to various III-nitride nanostructures such as InGaN/GaN or GaN/AlN quantum dots in the characteristic wurtzite and zincblende crystal structures. We investigated the effect of strain and polarization effects on the charge carrier localization which typically leads to a spatial separation of electrons and holes in wurtzite nanostructures. Additionally, studies have been performed in order to evaluate trends when varying the alloy composition in InGaN/GaN nanostructures in order to understand light emission processes in realistic nanostructures.