The electronic band structure of highly mismatched semiconductor alloys for their use in optoelectronic devices.

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Abstract

Highly mismatched semiconductor alloys (HMAs), dilute bismides in particular, are a relatively new group of materials. The term *highly mismatched*, comes from the differences in sizes and electronegativity of the atoms in the alloyed compounds. As a consequence, these materials have extraordinary properties, much different from those in regular semiconductor alloys such as a very high reduction of the band gap even for low Bi composition and drastic changes in the electronic band structure. Alloying with bismuth, is the only way to obtain III-V materials with a band gap lower than that of pure InSb, which is very desirable from the point of view of applications in infrared devices, lasers in particular. Due to necessary changes in the growth process of these materials, the structures may additionally include unwanted defects. The information on both the electronic band structure as well as defect properties is very limited so far. A comprehensive and consistent study of the electronic band structure as well as defect properties would provide a significant help in the interpretation of the experimental results and materials design.

In this thesis. an entirely original and thorough first-principle study of the electronic properties of III-V-Bi alloys was conducted. All III-V zinc-blende semiconductors alloyed with bismuth were studied, i.e. AlPBi, AlAsBi, AlSbBi, GaPBi, GaAsBi, GaSbBi, InPBi, InAsBi and InSbBi. State-of-the-art DFT methods were employed in order to calculate the electronic band structure of those materials in the whole Brillouin zone, and parameters describing the changes in the band structures were obtained and presented.

The band structure calculations were followed by the investigation of defect properties in these systems. In this case, native as well as Bi-related defects in form of point or pair defects were studied, in the low Bi composition (diluted regime). Hybrid functionals together with the FNV correction scheme for charged defects were used in order to obtain the most accurate results of formation energies, binding energies and charge-state transition defect levels. In order to obtain the values for every studied defect, a regression model based on the obtained results was built, allowing for accurate prediction of the values without employing computationally expensive tools. The calculated properties of all 9 materials and all 27 defects for each were collected and presented in a form of tables and figures.

The chemical trend for the materials were then discussed in terms of the applicability of the materials in optoelectronics.