INVESTIGATION OF INP-SI INTERFACE BAND STRUCTURE USING DENSITY FUNCTIONAL THEORY

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Introduction

To achieve monolithic integration of III-V devices into Si-based photonic circuits, a comprehensive understanding of the band alignment for epitaxially grown III-V semiconductors on Si is crucial. This knowledge is essential to accommodate the effects of carrier transport through the interface (Fig. 1a) into the device design. The goal of this research is to gain insight into the stress-induced band shifts between largely mismatched materials and, therefore, the band alignment relative to the stress caused by the lattice mismatch.

Methods

To minimize defect formation in InP grown on Si, a single nucleation seed condition on a well-defined (111) Si plane should be satisfied. In this study, we aim to investigate the effect of the lattice mismatch on a thin layer of InP, by means of DFT calculations and deformation potential theory. To have an absolute reference level for the deformation potential, we resort to construction of a supercell, which contains the same material in different strained states.

Summary

In this contribution, we present our first results for the deformation potentials, calculated using DFT, for an InP bulk crystal strained in the directions perpendicular to the <111> direction, as seen in Fig. 1b, simulating the experimental direction of growth. The results are compared to the available literature values. Furthermore, we discuss the results of the DFT calculations in the context of band alignment for the Si-InP interface.