First-principles calculations of band offset at InAs/InP interfaces

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We have performed first-principles calculations of the band alignment of InAs/InP heterojonctions on an InP substrate. A strained valence-band offset of 0.39 eV and 0.32 eV is calculated for the cubic and wurtzite phases respectively. The dependence of the band alignment on crystalline phases implicates a possible way of patterning quantum wire structures with thickness engineering.

Key words: **Band offset, nanowires, *ab initio* calculations**

I. INTRODUCTION

Recent years have witnessed increasing interest in III-V core-shell nanowires (NWs) as the building blocks for and functional components of future nanoscaled transistors, single photon sources, and chemical sensors [1]. This is due to unique optical properties that stems from combination of dielectric effects linked to aspect ratios with specific crystallographic structures differing from those of material constituents [2]. In this context, there has been considerable effort placed on developing high electron mobility NWs with InAs/InP heterostructure material systems to take advantage of the small electron effective mass of bulk InAs. These systems grown on hexagonal symmetry containing ultrathin wurtzite InAs surrounded by inner thick wurtzite InP [3]. In particular, they demonstrate an intrinsic mobility which is significantly higher than that of single-crystalline InAs nanowires [4], which is attributed to the band offset between InAs and InP bands. Conversely, from a structural perspective, the lattice mismatch between bulk InAs and InP is relatively large about 3 %, and places constraints on achieving defect-free NW structures. While the strain distribution in wurtzite InAs/InP nanowires is rather well known [4-5], the effect of strain on the band alignments generally has not been explored. In addition, although previous theoretical studies have focused on the electronic properties of single-crystalline InP and InAs nanowires [6-7], modeling of wurtzite InAs/InP interfaces is still lacking. In this paper, we present *ab initio* calculations of the InAs/InP heterojonction grown on InP (0001). For the sake of comparison, the valence-band offset of cubic InAs/InP superlattices grown along the [001] and [111] directions have also been simulated. In Sect. II we present the computational aspects. Results of bulk parameters and band alignments are given in Sec. III

II. COMPUTATIONAL DETAILS

Density functional theory (DFT) calculations are performed by using the ABINIT code [8] within the local-density approximation. A precise convergence of simulations has been obtained with a plane-wave energy cutoff of 70 Ry. The Brillouin zone integration for is performed with a Γ-centered Monkhorst-Pack grids with 8 x 8 x 6 mesh in reciprocal space for bulk InAs and InP. The non-local norm-conserving pseudo potentials are constructed from the Fritz Haber Institute (FHI) Format using the OPIUM using the OPIUM program [9]. The atomic shells of In ($4d^{10}5s^{2}5p^{1}$), P ($3s^{2}3p^{2}$) and As ($4s^{2}4p^{3}$) are explicitly included as valence electrons. InAs/InP interfaces are modeled within different super-cells containing up to 24 atoms i.e. 8 molecular layers for cubic (001), 6 molecular layers for cubic (111) and 6 for wurtzite (0001) interfaces. The supercell calculations are performed with an energy cutoff of 70 Ry, and using for the k-space integrations the 8 x 8x 1 Monkhorst-Pack grid for the (001) junction and the 12 x 12 x 2 grid for the (111) and (0001) interface. The procedure to obtain the lineups follows the model-solid approach of Van de Walle and Martin [10]. In this theory, the average energy of highest valence bands at the Γ-point E_v set on an absolute scale for bulk relaxed material. The valence band-lineup ΔE_v is obtained from the planar averaged *ab initio* potentials ΔV_{LDA} in a relaxed superlattice depending on growth condition.

III. RESULTS

Table I: Cell parameters and gap energies of InAs and InP compared to experimental data [11] for the wurtzite structure.

Parameters	InP		InAs	
	LDA	Exp.	LDA	Exp.
a [Å]	4.1266	4.1500	4.2717	4.2839
c [Å]	6.7291	6.7770	7.0195	6.9954
u [/]	0.3705	0.3749	0.3703	0.3750
E_g [eV]	0.428	1.645	-0.427	0.54
Δ_{cr} [eV]	0.086	0.110	0.068	0.195

Table I summarizes some band parameters of w-InAs and w-InP obtained from our calculations. The structural optimization gives the lattice parameters which are only 0.5% larger than the experimental results. A fairly good agreement is observed for the valence band splitting Δ_{cr} and discrepancy must be related

to inherent strain effects in the NW structures in the experimental side [11]. The LDA functional is well known to significant underestimate semiconductor band gaps or even to predict zero band gaps for small-gap semiconductors as observed for InAs. This is among reasons due to a missing derivative discontinuity and an incomplete self-interaction cancellation in the LDA exchange-correlation (XC) functional. Hybrid XC functionals that include a fraction α of Hartree–Fock exchange provide a promising alternative in modeling the electronic structure of bulk semiconductors [12]. However α is not a universal parameter and may differ between materials so that reliability of band offsets is questionable. The valence-band offset of (001), (111), and (0001) InAs/InP heterojunctions is summarized in Table II

Table II: Valence-band offset of InAs/InP junctions for different phase materials and growth orientation.

Crystals	Cubic (001)		Cubic(111)	WZ(0001)
	LDA	Exp.[13]	LDA	LDA
VBO [eV]	0.39	0.38	0.38	0.32

In our simulations, the in-plane lattice constant is that of bulk InP and the quantum structure can relax along the growth direction. The relaxed lattice parameters are obtained from a minimization of the total energy of the super-cell. For the (001) InAs/InP heterojunction, the LDA valence-band offset agrees very well the experimental result [13], which underlines the quality of the present modeling. The comparison between the zinc-blende (001) and (111) heterostructures, having the same substrate lattice constant, shows that for a comparable strain condition, the ordering direction slightly influences the band line-up. This is a direct consequence of the small differences of the charge readjustment at the [001] and [111] interfaces. Conversely, a marked difference of 0.06 eV is observed between the (111) and (0001) InAs/InP superlattices. The valence-band offset can be divided into a band-structure contribution which is the difference between the energies of the valence-band edges and the difference in the value of the average electrostatic potential in the supercell layers. Since the band edges of the individual wurtzite and zinc-blende semiconductors comprising the heterostructure behave differently when the system is stressed, i.e., having different deformation potentials, epitaxial strain is liable to have a significant effect on the band offsets as observed in our simulations.

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IV. CONCLUSION

In summary, we have investigated the influence of growth orientation and symmetry on the interface properties of InAs-InP based heterostructures. Different valence-band offsets are calculated between the wurtzite and zinc-blende structures and this can be related to the strain effects and crystal symmetry.

ACKNOWLEDGMENT

This work was performed using HPC resources from GENCI CINES and IDRIS 2013-2013096724. The work is supported through the participation of the INSCOOP ANR project.

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