First-Principles investigation of polytypic defects in InP

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Introduction

III-V materials are widely researched as channel material candidates or for photonic applications, but integration of III-Vs leads to numerous defects, such as threading dislocations or Rotational Twin Planes (RTPs). Defects usually degrade the performance of the device they appear in, but they can potentially also be useful if their formation is controlled. For example, RTPs are predicted to work as atomically thin, shallow quantum wells in GaN. In this work we continued the studies of defects in III-Vs, by specifically investigating RTPs and phase-mixing defects in Indium Phosphide (InP). The work reported here is a condensation of the study published in Scientific Reports.[1]

Simulation Methodology

The results were acquired using the state-of-the-art first-principles methods implemented in the T-2022.03 version of QuantumATK by Synopsys. We used the "High" version of the PseudoDojo basis sets and their correponding pseudo-potentials. For the exchange/correlation functional we used the Generalized Gradient Approximation (GGA), by Perdew, Burke and Ernzerhof for solids (PBES). All systems were constructed from supercells of minimal bulk InP systems, which were relaxed until the forces between the atoms were smaller than $0.05\,\mathrm{eV\,\AA^{-1}}$ and the stress was less than $0.1\,\mathrm{GPa}$.

InP crystallises in the Zincblende (ZB) phase, Fig. 1a but can also form the meta-stable Wurtzite (WZ) phase, Fig. 1b. Random transitions between ZB and WZ often occurs, the smallest transition region in a ZB phase, is called a Rotational Twin Plane (RTP), Fig. 1c. If two RTPs form sequentially, the layers form a well-defined WZ phase, Fig. 1d. The stacking sequence of ZB and WZ is shown in Fig. 1, together with an RTP superlattice and a maximally intermixed ZB/WZ system.

Results

Fig. 2 shows the local band gap in a periodic ZB/WZ interface, with different cutoffs of the Local Density of States (LDOS). We see that the transition is far from abrupt, it takes approximately $7\,\mathrm{nm}$, making atomically thin quantum wells from RTPs in InP impossible.
In Fig. 3, the same transition is investigated with a LDOS obtained from a non-equilibrium Greens function calculation. This eliminates the effect from the periodic image of the supercell. Here we found that the transition requires $15\,\mathrm{nm}$.
We next investigated the defects effect on the conductivity. In Fig. 4 the conductivity across the defects are reported, with an intrinsic n-type doping of $1\times10^{17}\,\mathrm{cm^{-3}}$. We see that WZ has a 5% higher conductivity than ZB, and that the ZB systems with defects have higher conductivities the higher their fraction of WZ is.
In Fig. 5 the relative conductivities are shown again, but with zero bias voltage and varying doping levels instead. We see that increasing the n-doping have similar effects to increasing the applied voltage. But at p-doping levels higher than $4\times10^{19}\,\mathrm{cm^{-3}}$, the conductivities fall sharply to a mere 5-40% of the ZB reference.
In Fig. 6 we show the conductivities of the systems along the defects. We here see that the defects function as pathways of lesser resistance, thereby increasing the conductivity.

Acknowledgement

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References

1. Vedel, C., Smidstrup, S. & Georgiev, V. First-principles investigation of polytypic defects in InP. *Scientific Reports* **12** (Nov. 2022).

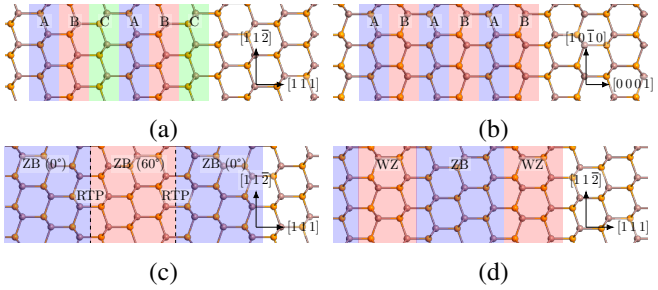

Fig. 1 The 4 different kinds of InP systems investigated in this paper. **(a)** Pristine Zincblende (ZB). **(b)** Pristine Wurtzite (WZ). **(c)** A Rotational Twin Plane (RTP), here shown with a periodicity of 1 RTP every 3 layers of ZB. **(d)** A mixture of WZ and ZB, here shown with a periodicity of 2 layers WZ every 3 layers ZB.

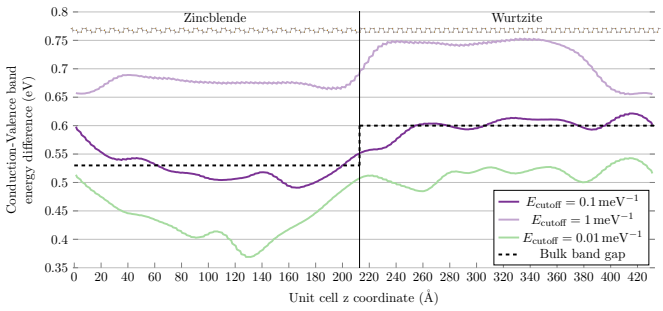

Fig. 2 Conduction-Valence band energy difference in 127 atomic layer long InP ZB/WZ interface system for three different DOS cutoff values.

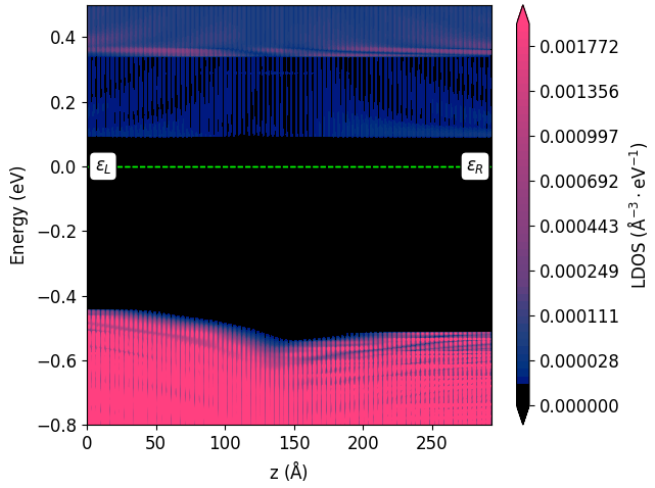

Fig. 3 LDOS of InP interface between Zincblende (on the left) and Wurtzite (on the right).

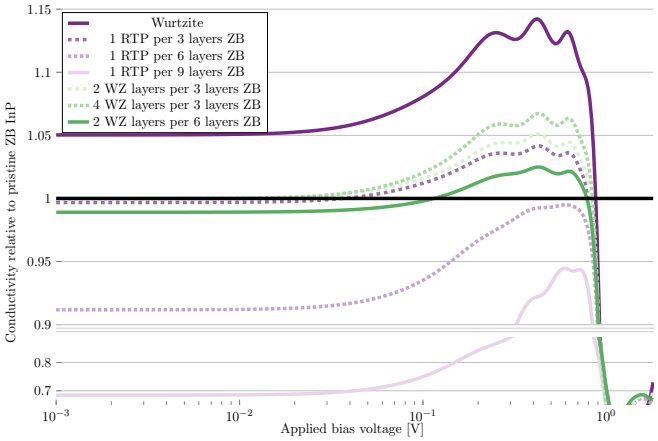

Fig. 4 Conductivity of InP systems along $[1\,1\,1]/[0\,0\,0\,1]$, relative to pristine ZB InP, at intrinsic doping levels.

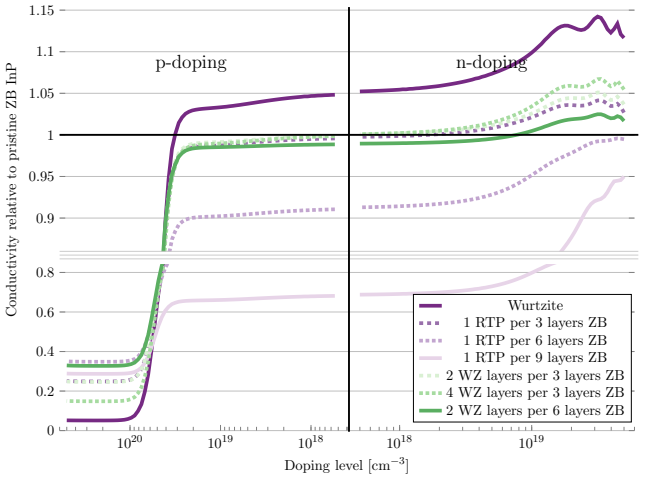

Fig. 5 Conductivity of InP systems along $[1\,1\,1]/[0\,0\,0\,1]$, relative to pristine ZB InP, at zero bias voltage.

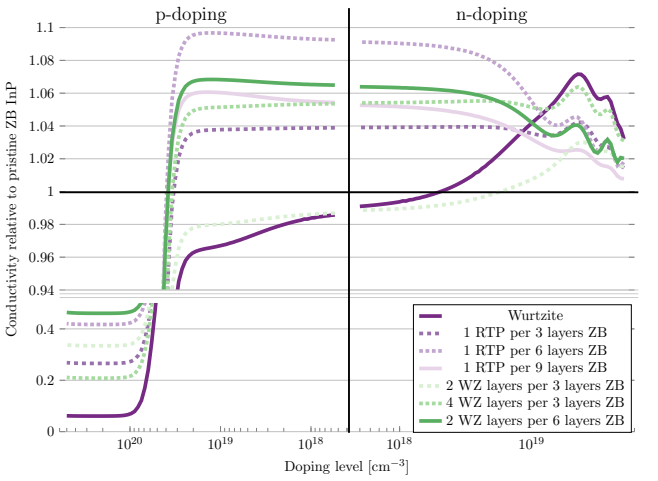

Fig. 6 Conductivity of InP systems along $[1\,1\,\bar{2}]/[1\,0\,\bar{1}\,0]$, relative to pristine ZB InP, at zero bias voltage.