Atomistic simulation of a III-V p-i-n junction

Comparison of density functional and tight-binding approaches

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***Abstract*—We compare the results of calculations based on tight-binding and density functional theory (DFT) for the description of an ultra-narrow two-dimensional (2D) InAs system. We first investigate the electronic structure of the 2D system to understand the effect of different surface terminations and how they are modeled using tight-binding and DFT approaches. We next set up a gated 2D InAs p-i-n junction and calculate the transistor characteristics of the system using the two different approaches.**

Keywords—atomic-scale modeling; InAs; p-i-n junction; tight-binding; density functional theory; surface effects

I. INTRODUCTION

In order to fully understand the intrinsic behavior of novel ultrascaled devices, it is necessary to employ both quantum mechanics (due to the small sizes involved, which e.g. lead to tunneling effects) and to model the systems atomistically, since the systems are so small that bulk parameters, as commonly used in TCAD models or simple effective mass theory, are no longer valid. A popular approach is to use the tight-binding method for simulating the atomic-scale properties of such system [1,2]. This approach is an approximation to the full quantum-mechanical description of the device, and it is interesting to know the importance of the missing details. In particular, the tight-binding parameters are usually fitted to bulk properties and may not be transferable to accurately describe surface and interface properties, even if experience generally indicates that they work rather well to describe systems of reduced dimensionality.

On the other hand, formally more accurate methods like DFT are well known to have problems reproducing the band gaps of semiconductors, which also creates problems when a predictive model is desired. In this paper we simulate a 2D InAs device using both tight-binding and first-principles DFT in order to get an impression of the difference in the description of the system using the two approaches.

Furthermore we will investigate different types of surface termination to understand the effect of such atomistic details and how they are described by different levels of theory.

II. METHODOLOGY

For the calculations we use the ATK-DFT [3] and ATK-SE [2] simulation engines. ATK-SE is a self-consistent tight-binding (TB) code, and to describe InAs we use the Vogl parameter set [4]. ATK-DFT is based on density functional theory and applies a local atomic orbital (LCAO) basis set. For the calculation of InAs we use the generalized gradient approximation (GGA) of Perdew, Burke and Enzenhofer [5]. For the device simulation we use the NEGF approach for calculating the electronic structure under device conditions [6] and use a real space Poisson solver for handling electrostatic gates [3].

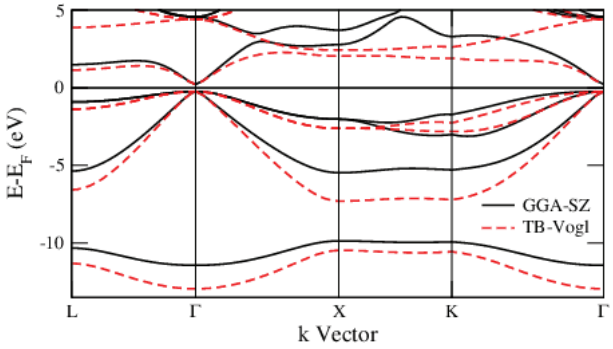

Fig. 1. Bandstructure of InAs obtained with the special DFT-GGA basis set and the Vogl TB model. Note the similar bandgap obtained with the two methods. The Fermi level is positioned in the middle of the band gap, and defines the energy zero level.

GGA does not generally describe the band gap of InAs well – in fact it typically gives a zero gap at the experimental lattice constant. However, for this calculation we have used a tailored minimal (SingleZeta) basis set, with one basis orbital per valence electron, which does give the same band gap as the Vogl TB model. Another option is to strain the InAs crystal, which can bring the band gap into agreement with experiments [7], however this approach is not suitable here since will later consider reconstruction of the surface of InAs nanowires, so the In–As bond length is not a free parameter.

The band structure of InAs obtained with the two different methods is show in Figure 1. In the relevant energy region for device simulations, i.e. from say –2 to +2 eV around the Fermi level, the two models agree reasonably well, even if the deviation increases away from the Fermi level, partly due to shortcomings of the sp^3 Vogl TB set, and partly because of the small DFT basis set.

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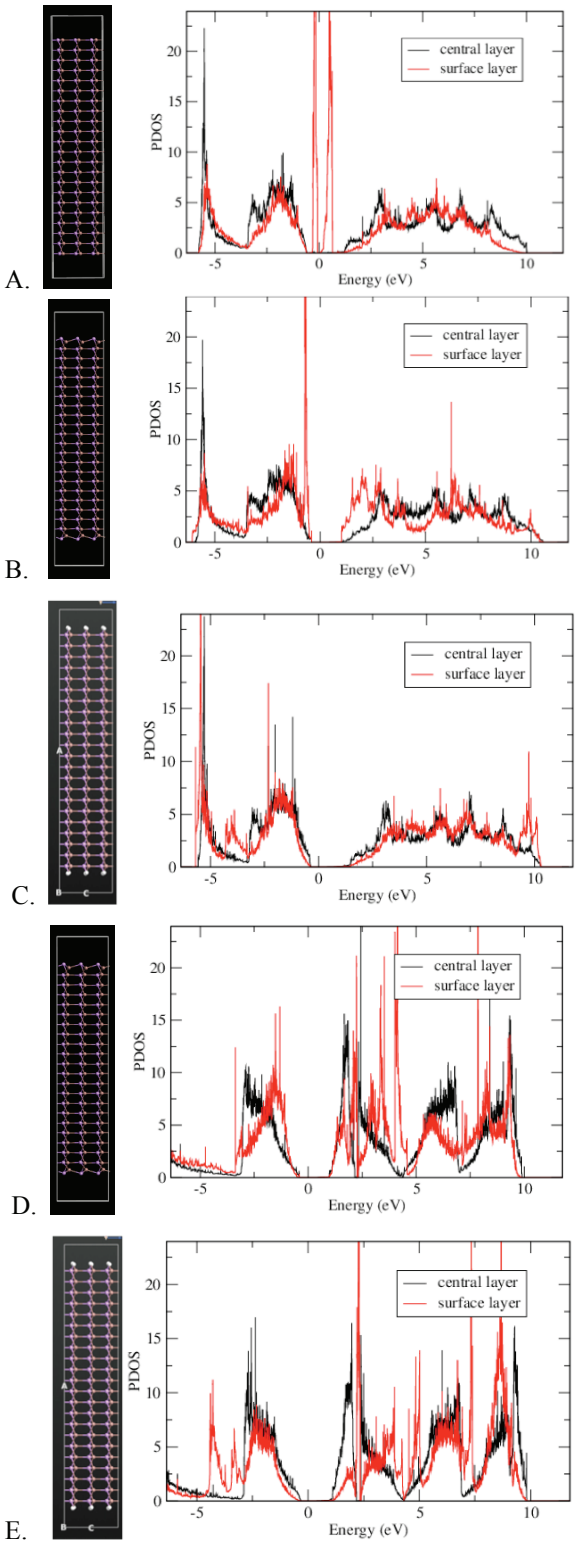

Fig. 2. Projected density of states (PDOS) for the surface and bulk layer of a 46 Å wide InAs 2D system with different surface passivation, and using different methods. A) Bulk surface, DFT, no passivation; B) Relaxed surface, DFT, no passivation; C) H-passivated surface, DFT; D) Relaxed surface, TB, E) H-passivated surface, TB.

III. INAS 2-D WIRES

We next calculate the band gap of a 2D InAs system using both the TB and DFT approaches. Figure 2A shows the projected density of states (PDOS) for the surface and the bulk layer of a 46 Å wide InAs 2D system, where the surface is not passivated. We see that there are surface states in the band gap; these will be strongly reactive and drive the surface to reconstruct. We next relax the surface geometry using DFT; Figure 2B shows the equilibrium geometry and the corresponding PDOS of the surface and bulk layer. The surface atoms relax inwards and after this reconstruction there are no longer any surface states in the band gap. However, there is an increased number of surface states just at the edge of the band gap.

It is common practice in simulations of this type to attach hydrogen atoms to the dangling bonds of surface atoms to passivate these states. The effect of such passivation is shown in Fig. 2C. The figure shows that in this case the surface states are completely removed and the density of states of the surface layer is very similar to the bulk. Thus, the surface PDOS is significantly different from the reconstructed surface case.

Figures 2D and 2E show the PDOS calculated with the TB approach, using the geometries from Figs. 2B and 2C, respectively. We see that for both systems the surface PDOS is quite similar to the central PDOS, in particular Fig. 2D does not show the same surface states close to the band edges as are apparent in Fig. 2B.

We next investigate the effect of the different models on the band gap for 2D systems of varying widths. The result is shown in Fig. 3. The geometries corresponding to Figs. 2B, C, D, E are given by the four data points at width = 46 Å.

For the systems with a width above 50 nm, the gaps are rather similar. However, below 50 nm there is a significant difference. In particular we notice that the H-passivated system when described with the TB model exhibits a lower band gap than the other systems. We believe that this difference is related to a difference in the description of the charge transfer between the surface and bulk in the 2D system. For systems B, C, D there is an additional confinement potential from the charge transfer between the bulk and the surface and this slightly increases the band gap.

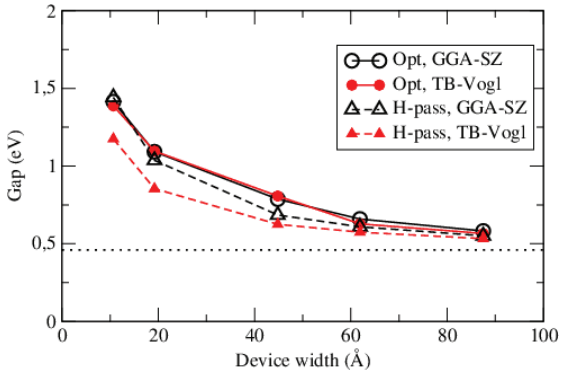

Fig. 3. Bandgap as function of the width of the InAs device system.

IV. InAs 2-D p-i-n junction

We next investigate how the different models translate into the description of the electronic structure in a device simulation. For the device system we have selected a 2D system of width 13 Å. This will be the system where the surface effects are strongest and will give an upper limit on the surface effects. The device system to be investigated is the p-i-n junction illustrated in Fig. 4. The system consists of p and n doped electrodes (10^{19} electrons/cm^3) with an intrinsic region in between. It has a width of 13 Å and a total length of 166 Å. The surface of the 2D system is either relaxed or passivated by hydrogen atoms. In the central part of the system we add a 60 Å long top and bottom electrostatic gate. The gate is separated from the InAs by a 6 Å thick dielectric region with dielectric constant 4.

Figure 4 shows the local density of states (LDOS), computed with DFT, along the z-direction, i.e. averaged over the x, y directions, for zero gate potential and no applied bias (zero gate, defined by the vacuum level of the left electrode). The formation of the p-n junction, as a result of the alignment of the two electrode Fermi levels and the corresponding band edge shifts, is clearly visible. The LDOS also illustrates the penetration of hole states from the left electrode into the gap region in the range 100-170 Å above the valence band. Similarly, electron states from the right electrode propagate into the gap region just below the conduction band. If the intrinsic region is sufficiently short – or, modified by the gate potential, as we shall see soon – it is evident that these states can make a connection and a tunneling current flow. All of this is of course nothing new, it's the basic operation of a p-n junction, but it's reassuring to see the results come out of a first-principles calculation instead of these effects being encoded into the model *a priori* – the only input parameters to the DFT model are the atomic coordinates and the doping levels. We also get a qualitative picture of the lengths of the exponential tails that extend into the gap, both energetically (at a fixed z-coordinate) and spatially (for a fixed energy).

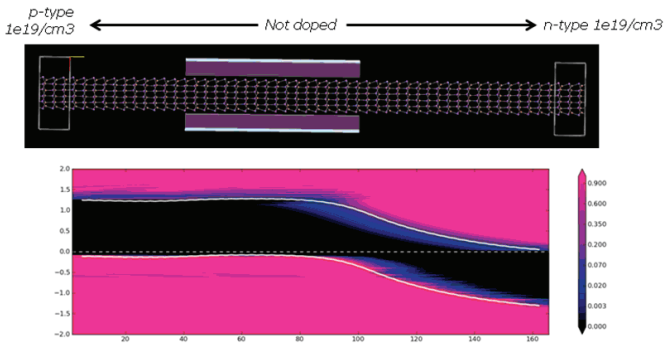

Fig. 4. Geometry of the 2D InAs p-i-n junction of width 13 Å and length 166 Å. Periodic boundary conditions are used in the direction perpendicular to the viewplane. An electrostatic double gate is placed in the center of the device, and a 6 Å thick dielectric is inserted between the gate and the device. The lower figure shows the DFT LDOS of the device at zero applied bias and with the gate potential grounded to the left electrode. The dashed line shows the Fermi level of the system.

We next calculate the I-V characteristics of the device at zero gate potential. The results for our four different models are shown in Fig. 5. The qualitative behavior of the models is the same. For the forward bias case the current grows exponentially with a $1/k_BT$ slope, corresponding to thermionic emission over the barrier. At reverse bias there is an onset at about –0.25 V; at this bias the valence band of the left electrode has sufficient overlap with the conduction band of the right electrode to allowing an elastic band-to-band tunneling current to flow. At –1 V bias the tunneling current is > 1 A/m. The different models exhibit a quantitative level of the current spanning more than 5 orders of magnitude at the same bias. This difference seems to be mainly associated with the band gap, viz. the TB-Vogl model has lowest bandgap and shows the highest current.

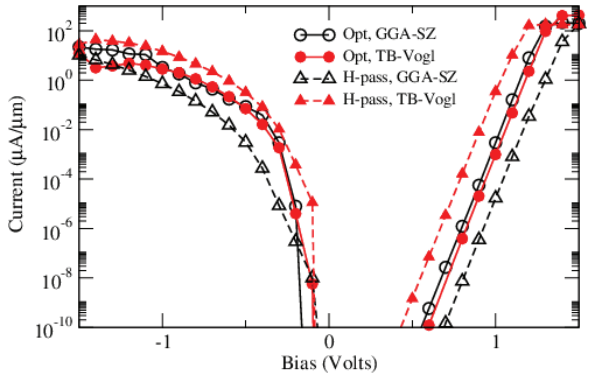

Fig. 5. Current-voltage characteristics for the p-i-n junction, with the gate grounded to the left electrode (zero gate). A positive bias corresponds to forward bias of the p-n junction. The current is calculated for different surface passivation models and with both the DFT and the TB method.

We next calculate the dependence of the current on the gate potential when operating at reverse bias –0.5 V. The results are shown in Fig. 6. We see that qualitatively the different models show the same behavior; in all cases the effect of the gate potential is to control the length of the tunneling gap and thereby the matrix element for the band-to-band tunneling current. At low gate potential the valence band below the gate aligns with the left electrode, and band-to-band tunneling will take place at the drain electrode, this is the situation illustrated in Fig. 4. For high gate potential, the conduction band below the gate will align with right electrode conduction band and the band-to-band tunneling will take place at the source electrode. For gate potentials in between these situations there will be an additional tunnel barrier below the gate and thereby a reduced current.

There are rather large differences in the quantitative behavior of the different models. For the hydrogen-passivated systems, the DFT and TB curves are however more or less just scaled by a factor 20, and this can be explained by the different band gaps of the two models. For the surface-reconstructed systems, on the other hand, the curves are more complex and the shapes differ. Combined, this shows that the TB model gives the same description of the band-to-band tunneling matrix elements as the DFT model (with account taken for the band gap). However, the effect of a gate potential produces rather different results and we relate this to a different

electrostatic response of the DFT model compared to the TB model. In particular, the DFT model also includes exchange-correlation contributions which might play an important role for ultrascaled devices. Moreover, the TB matrix elements are assumed to follow a simple scaling law with the bond length [4], however at the surface the bonds not only have different lengths but also angles, due to the reconstruction. The DFT model can be expected to account for these effects more accurately. This system is currently under investigation to further pinpoint the difference between the TB and DFT models.

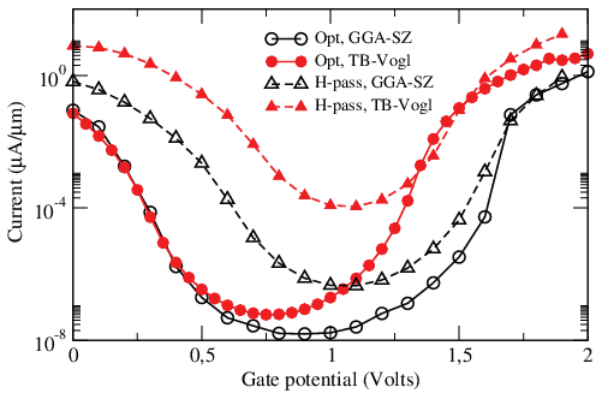

Fig. 6. Current-gate characteristics for an applied bias of –0.5 V. Zero gate potential corresponds to the gate grounded to the left electrode. The ground of the right electrode is at 1.58, 1.68, 1.78, 1.53 V for the different models, respectively.

We also note that the difference between the different surface terminations is of the same order of magnitude as the different models, thus, any improvements of the computational model itself will be in vain unless there is better certainty in the description of the surface.

V. Conclusions

In this paper we have compared the description of ultra-scaled 2D devices using an atomic-scale description based on density functional theory and a semi-empirical tight-binding model. Often the surface termination of the free surface in the 2D device is unknown, and in this paper we investigated two different models: a surface-reconstructed model and a hydrogen-passivated model. None of the models describe realistically a real device, however, they seem to provide two extreme situations, i.e. the surface-reconstructed model has a large number of surface states at the band edges, while the surface atoms are all bulk-like in the passivated model. In a real device the situation is most likely somewhere in between these situations, thus, the study of these two surface models can give an indication of the effect of the surface.

The TB and DFT models gave quantitative different results for the I-V characteristics of the two systems. For the I-V characteristics at zero gate bias, the curves were similar and the difference could be explained by a different band gap of the two different methods. For the gate dependence of the current there are larger discrepancies between the two models, most likely due to additional exchange-correlation contributions to the electrostatic screening in the DFT model.

The discrepancy of the TB and DFT models are of the same order of magnitude as the difference between the surface termination models. Thus, it might not be worth while to use more elaborate DFT models if the structure of the surface is unknown. It will be interesting to perform the same comparison for wider 2D devices, where the surface effects are smaller. Such studies are more computationally challenging, and a new version of our software which will allow such studies is under development.

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