Effect of the High-k Dielectric/Semiconductor Interface on Electronic Properties in Ultra-Thin Channels

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Abstract Submission

As logic devices continue to downscale, an increasing fraction of the channel atoms are in close contact with oxide atoms of the gate. These surface atoms experience a chemical environment that is distinct from the bulk-like environment found in thicker channels. Using the non-orthogonal tight-binding method Extended Huckel Theory (EHT), III-IV/High-k dielectric interfaces are constructed and electronic structure in the two transverse directions in the plane of the interface is calculated.

Introduction

In the ultra-small channels predicted by the continued scaling of transistors, an ever increasing fraction will be in contact with the gate oxide material as seen in Fig 1 based on ITRS projections for single gate devices[1]. However, most existing atomistic models of semiconductor nanowires (NW) and ultra-thin bodies (UTB) use hydrogen termination[2-4] to approximate the oxide semiconductor interface. Semiconductor/oxide interfaces are constructed using AtomistixToolKit (ATK)[5], minimizing strain between the two surfaces as in Fig. 2. The structure is then relaxed using ATK's LDA DFT implementation. Electronic structure is then computed within our own nanoelectronic modeling tool NEMO5. Where available, existing EHT parameters are for semiconductors[6]. For oxides with no existing parameterization, EHT parameters are fitted to band structure and wave function DFT targets (Fig 3) following the process described by Y. Tan et al[7].

Discussion

Electronic structure (Figs. 3 and 4) is calculated in the two transverse directions in the plane of the interface using EHT. Density of States (DOS) (Fig. X) for the interface cases are increased relative to the hydrogen-terminated UTB case due to the coupling of the semiconductor with the oxide. It is noted that though the DOS is increased for the interface case (Fig. 6), the conduction bands become nearly flat away from the Γ-point.

Summary

EHT calculations were performed on semiconductor/oxide interfaces and band structure and DOS results were obtained. These results are then compared with corresponding results for hydrogen-terminated UTB's.

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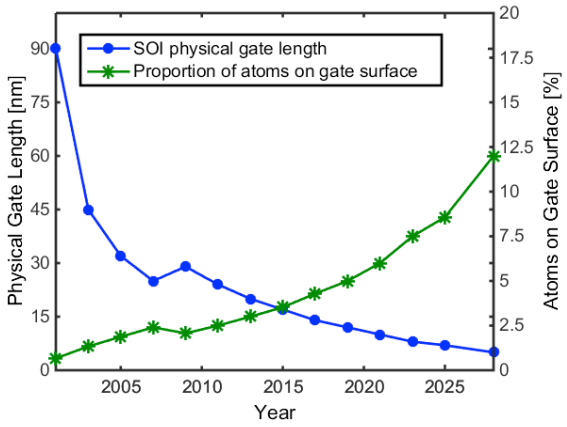

Fig. 1. Band structure comparison of $InAs/TiO_2$ with H-terminated UTB

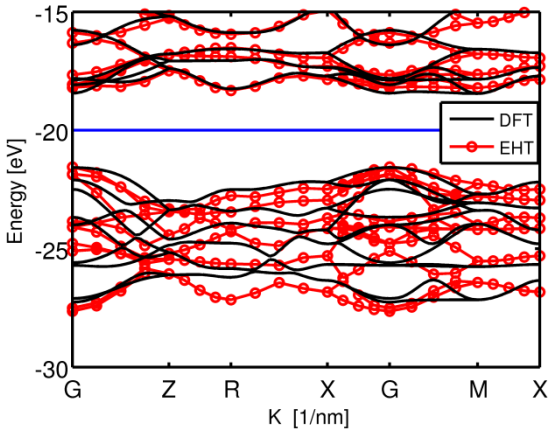

Fig. 3 .Example fitting of EHT parameters to DFT Targets for rutile phase of bulk TiO_2

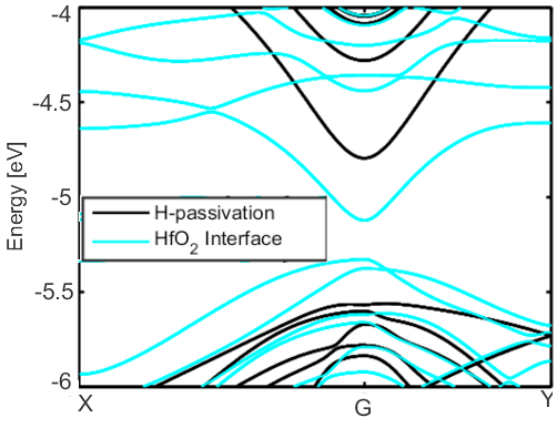

Fig. 5. $InAs/HfO_2$ interface

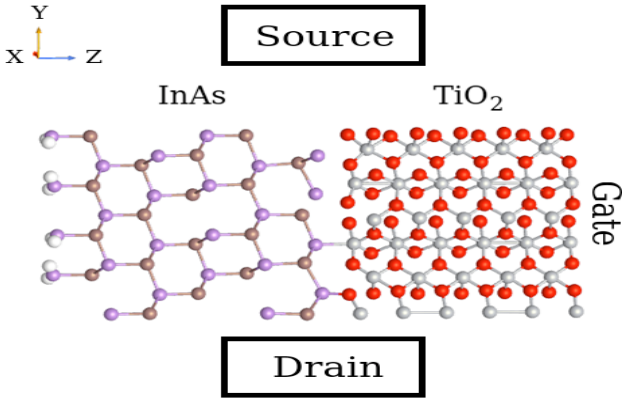

Fig. 2 .$InAs/TiO_2$ (rutile crystal phase) interface. This structure was structurally relaxed with LDA DFT

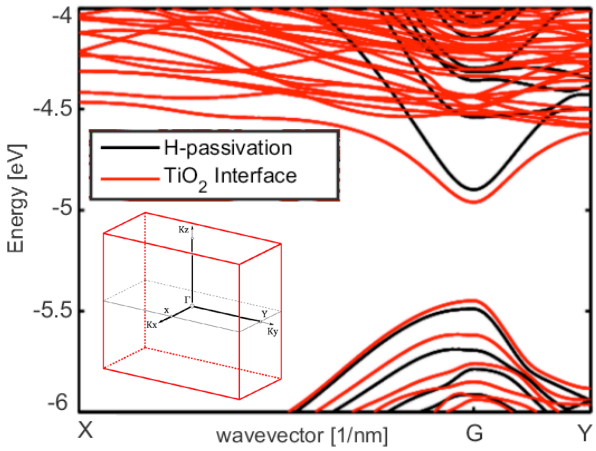

Fig. 4. Band structure comparison of $InAs/TiO_2$ with H-terminated UTB. Inset: Interface coordinate system and Brillouin zone

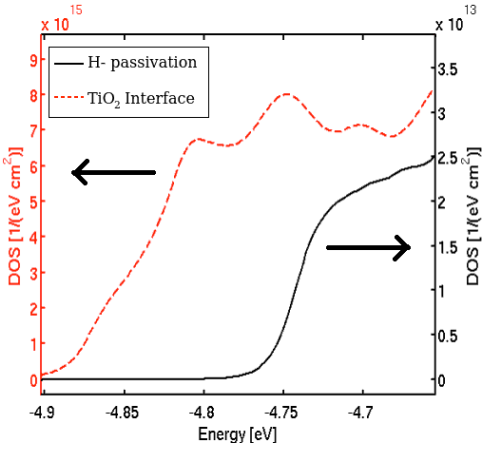

Fig. 6. Density of states comparison of $InAs/TiO_2$ with H-terminated UTB.