

Atomistic study of Metal/High-K interface

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Abstract

This paper describes our ab initio method to evaluate the effective work function of a MOS metal gate on HfO₂ oxide which is different from the vacuum one because of the Fermi pinning. The computation relies on Density Functional Theory (DFT) and Many Body theory. Firstly a monoclinic cell is computed using DFT to obtain a band structure; this one is corrected using the GW approximation. Then a stack made of W + HfO₂ is computed and using Van de Walle and Martins method, the energy bands alignment along the stack is obtained. Finally HfO₂ energies in the stack are corrected according to our previous computation on the HfO₂ cell. This calculation brings an evaluation of the valence band offset at the W/HfO₂ interface and the effective work function of W on HfO₂.

1 Introduction

In order to follow the ITRS road map, the gate oxide has to be replaced by a « high-k » material. The material which has shown the most interesting properties is the hafnium dioxide. However the use of this new MOS stack involves new challenges, namely concerning the comprehension of its electronics properties. Our work focuses on the energy bands alignment at the metal/oxide interface. More precisely the effective work function of a tungsten slab on an HfO₂ film is obtained by ab initio techniques. Due to the Fermi pinning phenomena [1], this work function is usually not equal to the vacuum work function. Here we will study a W/HfO₂ stack using DFT [2] and many body theory based methods (GW), thanks to the Abinit program [7]. To the best of our knowledge our way to tackle the issue of the effective work function hadn't been used yet for any metal/HfO₂ stack.

2 The Preliminary DFT Study

Using DFT energy minimization techniques within the local density approximation and Hartwigsen-Goedecker-Hutter (HGH) pseudopotentials, we have obtained the cubic, the tetragonal, the orthorhombic, and the monoclinic phases of HfO₂ crystal. They are very closed in energy (tab. 1), so that they all may crystallise in thin film. This accounts for the possibility of a polycrystalline phase in thin HfO₂ film. The most observed being the monoclinic phase [9, 10].

Phases	Volume per HfO ₂ (Å ³)	Energy difference per HfO ₂ from monoclinic phase (eV)
Cubic	31.1	0.19
Tetragonal	31.7	0.13
Orthorhombic	32.0	0.03
Monoclinic	33.2	0

Tab. 1: data from energy minimizations in DFT computation using GHG pseudopotential

Although experimentally the aim is to grow an amorphous oxide (in order to avoid leakage current), the cost to compute such a system using a GW based method is out of reach. So the monoclinic phase (fig.1) has been preferred here.

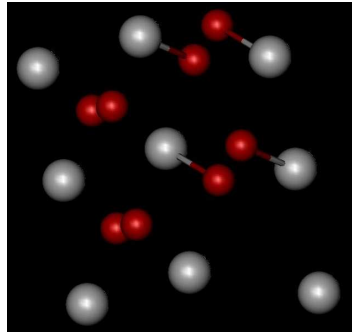


Fig. 1: HfO₂ monoclinic structure is a deformed fcc
Hf atoms in grey, O atoms in red

Firstly its energy band structure has been obtained using DFT. Unfortunately the energetic values resulting from a DFT computation are not accurate enough to be predictive, for example the indirect band gap is underestimated at 4.0 eV, whereas the experimental one is between 5.6-5.9 eV [11]. So correcting the DFT eigenvalues is a necessity to predict a band alignment, this is done with the GW formalism.

3 The GW Approximation

Although the Kohn-Sham (KS) approximation [5] gives no physical meaning to the DFT eigenvalues, the work on Many Body Theory led by Hedin [6] filled this lack with the GW formalism. The DFT eigenvalues are then seen in Abinit code, which we are using here, as the zero-th order of the GW eigenvalues. In DFT one solves the following Schrödinger equation:

$$(T + V_{ext} + V_{hartree} + V_{xc})\psi_i(r) = \epsilon_i\psi_i(r) \quad (1)$$

The lack of accuracy is due to the exchange correlation potential V_{xc} which does not describe precisely enough the mutual interaction between electrons.

So, to correct it we use the GW approximation based on the self-energy Σ to reappraise the exchange correlation:

$$\Sigma = G_0 W \quad (2)$$

where G_0 is the Green Function giving the transitions of the system, and W is the screening Coulomb potential (details of the computation will be published elsewhere).

4 The Bands Structure and Bands Alignment

For an insulator, near the band gap, the GW correction mainly yields to a shift of the electrons energy levels from the one obtained with DFT. Thanks to this correction we showed (fig.2) the necessity to include the semicore electrons in the pseudopotential in order to obtain a very realistic bandgap of 5.9 eV.

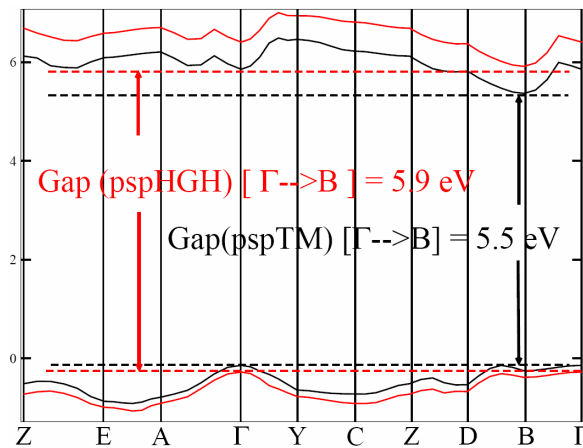


Fig. 2: Monoclinic HfO₂ - DFT band structure corrected with the GW approximation. Using Troullier-Martins pseudopotential (in black) considering only valence electrons, and HGH pseudopotential (in red) including the semicore electrons for hafnium. This shows that the semicore electrons are not frozen and interact with valence electrons.

Then a band alignment of a W bcc (110) on a m-HfO₂ (001) stack was computed with DFT based methods (fig. 3) [3; 4]. This gives an effective work function of 3.3 eV for tungsten, which is quantitatively wrong. Eventually using the assumption that the charge density is well described by DFT, as in ref. 8, the bands alignment is corrected using our computed GW shifts for the valence and the conduction bands. So the new bands alignment (fig. 3) affords us to evaluate the effective work function of the metal to be equal to a more realistic value of 4.9 eV.

5 Conclusion

Several phases of HfO₂ have been highlighted. The monoclinic phase has been used to study the band alignment at a given W/HfO₂ interface. We corrected the underestimated DFT bandgap and obtained a realistic bandgap thanks to the GW correction. This correction also allows us to correct the DFT band alignment at the

interface. This realistic new band alignment allows namely to give trends for the effective metal work function.

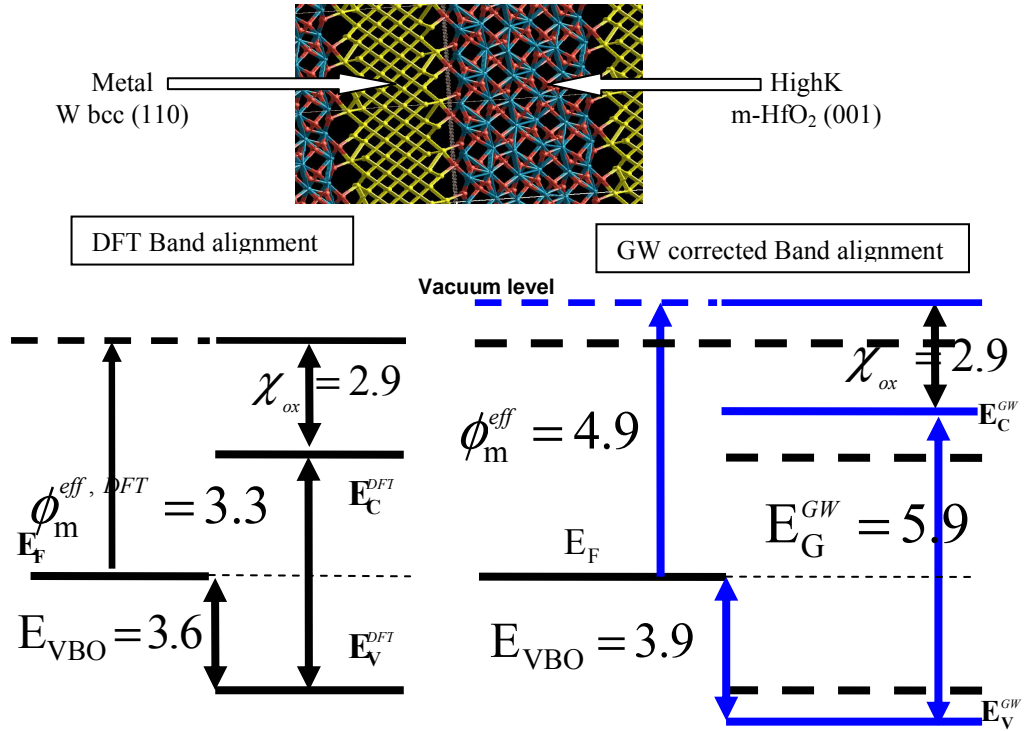


Fig 3: DFT band alignment and GW corrected band alignment of metal/HfO₂.

6 Acknowledgment

We are very grateful to Leonardo R.C. Fonseca for his help on the atomistic band alignment techniques applied to a metal / oxide interface.

7 References

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