Tunneling Properties of MOS Systems Based on High-k Oxides

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Abstract

In this work, we show full-band calculations of the tunneling properties of ZrO_2 and HfO_2 high-κ oxides. First, we have determined semiempirical sp^3s^*d tight-binding (TB) parameters which reproduce ab-initio band dispersions of the high-κ oxides; then we have calculated transmission coefficients and tunneling currents for Si/ZrO_2/Si and Si/HfO_2/Si MOS structures. Results show a very low gate leakage current in comparison to SiO_2-based structures with the same equivalent oxide thickness. The complex band structures of ZrO_2 and HfO_2 have been calculated; based on them we develop an energy dependent effective tunneling mass model. It is shown that this model can be used to obtain effective mass tunneling currents close to full-band results.

1 Introduction

Gate insulating films less than 2 nm thick, as required by the present scaling of Si-based technology [1], show quantum mechanical tunneling which results in excessive gate leakage current. In order to avoid this limitation, several alternative high-κ gate dielectrics have been studied; among these, ZrO_2 and HfO_2 have attracted great interest and selected for MOSFET applications, due to their relatively large dielectric constant, high band gap and sufficient band offset [2].

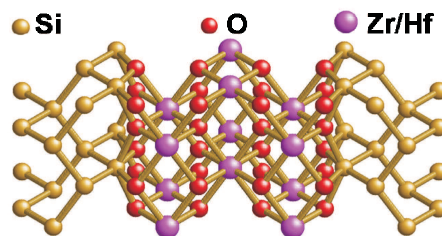

Figure 1: Microscopic model for Si/high-κ oxide/Si heterostructure.

2 Theoretical Methods

In this work, we investigate the tunneling properties of ZrO_2 and HfO_2 high-κ oxides, by applying quantum mechanical methods that include the full band structure of Si and oxide materials. First, electronic band structures of cubic crystalline forms of ZrO_2 and HfO_2 have been calculated using ABINIT code [3], in the frame of Density Functional Theory (DFT). Then, emiempirical $sp^3s^*d^5$ tight-binding (TB) parameters have been determined to reproduce the band dispersions obtained with DFT calculations and the experimental band-gap of the two oxides $E_g \approx 5.7$ eV [4]. Microscopic atomic Si/ZrO_2/Si and Si/HfO_2/Si MOS structures (see Fig. 1) have been constructed by applying the interface model described in Ref.[5], basing on the crystalline cubic forms of the oxides. This model assures that neither dangling bonds nor interface states are present, so that there are no states in the bandgap of Si. The structures have been relaxed in the frame of DFT approximation (SIESTA) by minimizing the atomic forces in the crystal. Calculations have been performed with our multi-scale multimodel integrated simulation tool TiberCAD [6]: a non-equilibrium Green function based-approach [7] in conjunction with TB have been used to calculate tunneling properties of Si/high-κ oxide/Si MOS structures. Complex band structures of ZrO_2 and HfO_2 have been calculated and investigated. From complex band, the dispersion of the evanescent imaginary band (IB) with imaginary k vector has been derived. With the assumption that IB determines completely the decay of the electron tunneling wave function in the relevant range of energy [8], we have determined an energy dependent electron tunneling mass $m_t(\varepsilon)$ for the IB. We find that, if this model is implemented, standard EMA calculations can give a good agreement with TB [9].

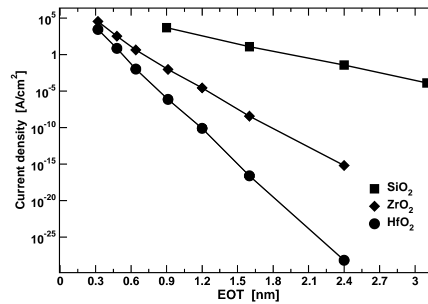

Figure 2: TB tunneling currents through ZrO_2 and HfO_2 for several values of EOT, compared to a SiO_2-based MOS.

3 Tunneling properties: ideal structures

Transmission coefficients and tunneling currents for Si/ZrO_2/Si and Si/HfO_2/Si MOS heterostructures have been calculated. Very low gate leakage currents are found for

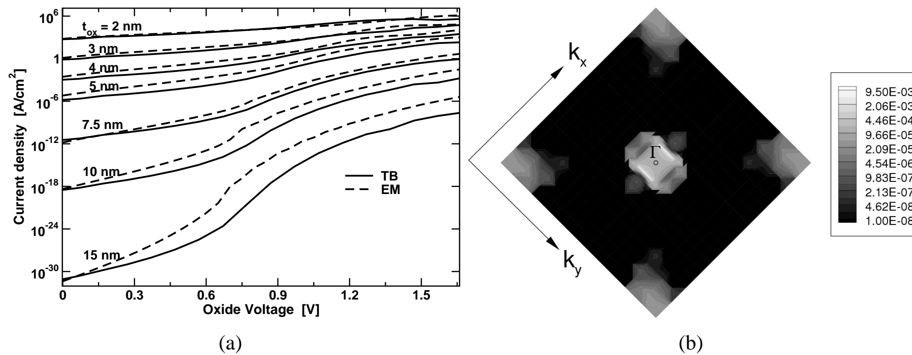

Figure 3: a) TB tunneling currents for a ZrO_2-based MOS structure (solid line) compared to EM with energy-dependent tunneling mass model (dash line); b) Transmission coefficient for 2 nm-thick ZrO_2 in the first planar Brillouin zone, for energy E=0.5 eV (above Si CB bottom).

high-κ oxide MOS systems, in comparison to SiO_2-based structures with an equivalent oxide thickness and the same bias (see Fig.2) [9].

Fig. 3a) shows tunneling currents for a n^+Si/ZrO_2/p-Si MOS diode biased in accumulation region, for several oxide thicknesses: the EM model with energy dependent tunneling mass is in close agreement with TB results. In Fig. 3b) the transmission coefficient $T(E,k_\parallel)$ in the first planar Brillouin zone is shown, for 2 nm-thick ZrO_2 and for an energy E = 0.50 eV above the Si conduction band minimum. It can be seen that at this energy the dominant contribution to transmission is very close to Γ point ($k_\parallel$=0).

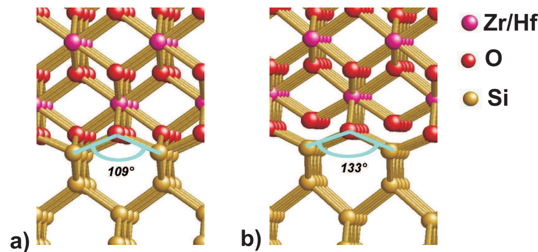

Figure 4: Microscopic model for Si/high-κ oxide interface: a) in ideal case and b) after relaxation.

4 Tunneling properties: relaxed structures

The effect of relaxation on ideal $Si/ZrO_2/Si$ and $Si/HfO_2/Si$ structures is shown in Fig. 4 a) (ideal interface) and b) (relaxed interface). Half of the interface oxygen atoms relax towards the Si layer, and form Si-O-Si bridges. Si-O-Si angle increases from 109° to 133° and O-Si bond length reduces from 2.3 $\AA$ to 1.9 $\AA$. Other interface oxygens relax

getting closer to ZrO_2. After relaxation, forces on the atoms converge to 0.04 eV/Å. Tunneling properties have been studied for the relaxed Si/high-κ oxide/Si structures: the transmission coefficients, integrated in the two-dimensional Brillouin zone, for 1 nm and 2 nm-thick ZrO_2 barriers, are reported in Fig. 5 (solid line). The comparison with the results obtained without structure relaxation (dash line) shows that relaxation does not seem to change the fundamental features of tunneling.

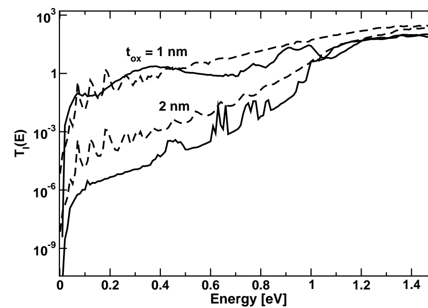

Figure 5: TB integrated transmission coefficient for a 1 nm and a 2 nm-thick relaxed ZrO_2-based structure (solid line) compared to results for a structure without relaxation (dash line).

Acknowledgements

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