

A combined DFT-scattering theory approach for transport properties calculation of $\text{HfO}_2/\text{Si}/\text{HfO}_2$ silicon-on-insulator FET

Giacomo Giorgi,^{1*} Leonardo R.C.Fonseca², Anatoli Korkin³, Koichi Yamashita¹

¹Department of Chemical System Engineering, Graduate School of Engineering, The University of Tokyo, Tokyo 113-8656, Japan, ²Werner von Braun Center for Advanced Research, Av. Alice CPN Mattosinho 301, Campinas, SP13098-392, Brazil, ³Nano & Giga Solutions, Gilbert, Arizona 85296, USA

By combining DFT calculations, *via* plane waves [1] and atomic orbital approaches [2], and the non-perturbative scattering theory method based on the solution of the Lippmann Schwinger [3] equation, we here report results of calculations of carrier transport in nanometer-thin atomistic silicon-on-insulator (NSOI) field effect transistor (FET) models.

To shed light on the impact of different crystalline phases of the dielectric on the transport characteristics of the channel, we have investigated different polymorphs of hafnia interfacing with silicon.

In particular, for the transport calculations we have employed both the experimentally and theoretically well-detected tetragonal and the purely theoretical detected anatase polymorphs in order to study the resulting NSOI films (*t*- $\text{HfO}_2/\text{Si}/\text{t}$ - HfO_2 and *a*- $\text{HfO}_2/\text{Si}/\text{a}$ - HfO_2 , see Fig.1).

In particular, the anatase polymorph of HfO_2 has been previously reported in recent papers [4] and its interface with silicon is characterized by a reduced amount of stress.

We found that transport is more efficient for *a*- $\text{HfO}_2/\text{Si}/\text{a}$ - HfO_2 NSOI. This result is related with anatase good lattice match to Si which does not create interface states in the Si band gap. At odds, the tetragonal polymorph creates scattering states in the Si band valence band edge through the presence of stretched Si-Si bonds at the interface, resulting in degraded transport characteristics.

This analysis suggests that different bonding arrangements along the channel length create regions of increased carrier scattering even in the absence of other scattering processes.

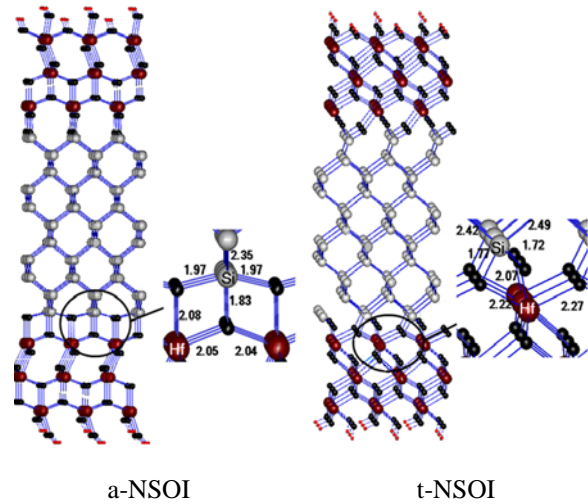


Fig.1: Optimized structure of the two NSOI, (left, *a*- $\text{HfO}_2/\text{Si}/\text{a}$ - HfO_2 ; right, *t*- $\text{HfO}_2/\text{Si}/\text{t}$ - HfO_2)

[1] Vienna *Ab Initio* Simulation Package (VASP), version 4.5.8, <http://cms.mpi.univie.ac.at/vasp/>, and references therein

[2] Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA), version 2.0, <http://www.uam.es/departamentos/ciencias/fismateria/c/siesta>, and references therein

[3] J. J. Sakurai, *Modern Quantum Mechanics* (Addison Wesley, Reading, 1994)

[4] G. Giorgi, A. Korkin, and K. Yamashita, *Comp. Mater. Sci.* 43 (2008), 930-937

* Email: giacomo@tcl.t.utokyo.ac.jp