First-principle Density-Functional Theory simulations for MOSFET devices.

E.P.Nakhmedov, M. Trentzsch, C. Schubert, I. Kabadshow, E.Nadimi, K. Wieczorek[1], and C. Radehaus

The ongoing trend of scaling down size in silicon based electronic device technology, in order to increase the device performance and functionality, requires to fabricate Si MOSFETs with gate lengths well below 50 nm and an oxide thickness below 2nm. This tendency highlights the challenges for the manufacturing industry due to the increased gate leakage current, which considerably increases the heat generation and the problem of dielectric breakdown. Key factors, playing a dramatic role in the reduction of the device reliability, are the character of defects, their concentration and distribution in the gate oxide, the interface quality etc.

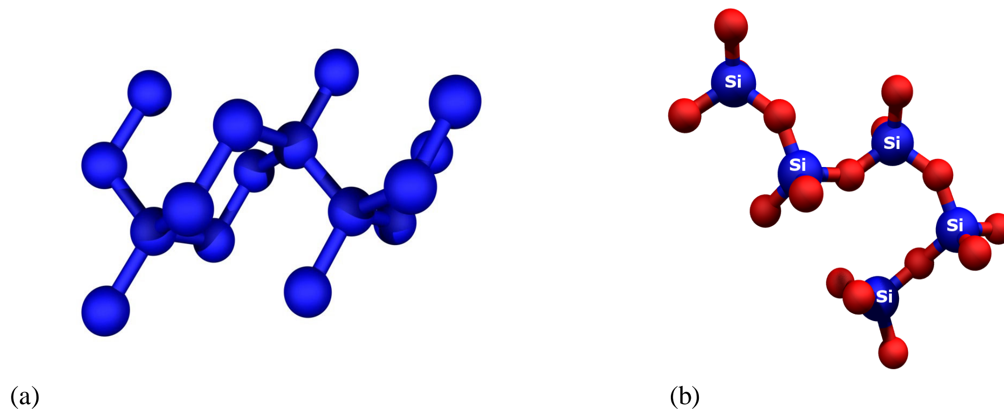
One topic of our current activity concerns investigations of the structure of silicon and silicon oxide, which are the basic elements of device technology, as well as studies of various defects in *Si* and SiO_2 crystals and the *Si*/ SiO_2 interface. For this purpose we use the Kohn- Sham Density Functional Theory (DFT) based on ab-initio simulation technique, [1,2], which is one of the powerful first-principle methods allowing to compute the ground state energy, the structure of crystal and amorphous materials, the band structure and the electron density.

Calculation of the total ground-state energy of the interacting system of electrons in the DFT is based on the Kohn- Sham energy functional, given as, [1]:

$$E^{KS}[\{\phi_i\}] = T_s[\{\phi_i\}] + \int d^3r V_{ext}(r)n(r) + \frac{1}{2}\int d^3r V_H(r)n(r) + E_{ex}[n]; \qquad (1)$$

which is an explicit functional of the electronic one-particle density $n(r) = \sum_i^{occ} f_i |\phi_i(r)|^2$ formed by the orthonormal one-particle Kohn-Sham orbitals $\{\Phi_i\}$ at *i*-th quantum state with f_i the occupation number. The first term in the Kohn-Sham functional (1) is the kinetic energy of non-interacting electrons, in the second term the external potential $V_{ext}(r)$ consists of internuclear interaction and electron- nuclear interaction. Electron-electron correlation effects are given by the last two terms in (1), representing the Hartree potential and the exchange functional.

We have employed in our computations the local density approximation (LDA) and gradient corrections for the exchange-correlation functional. Kohn- Sham orbitals are expanded in a plane wave basis set with a kinetic energy cutoff of 30 Hartree and a 2x2x2 grid in the *k*-space was used. In cartesian coordinates this grid is simple cubic, and actually corresponds to the 4x4x4 Monkhorst- Pack grid. For a structural optimization supercells with 16 and 72 atoms, respectively for *Si* and SiO_2 crystals, are chosen, which are then periodically repeated in three dimensions to represent the infinite nature of the crystalline solid.



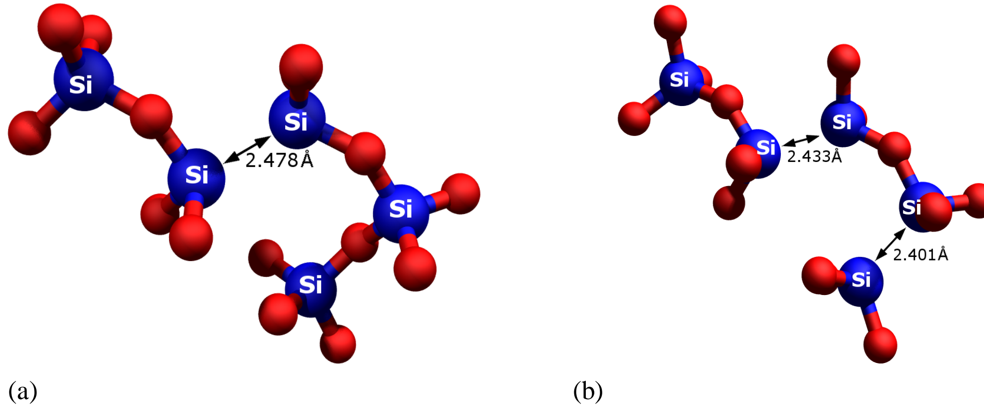
(a) (b)

Fig. 1:The structures of (a) Si crystal and (b) α-quartz.

The simulated topological structures of a clean *Si* crystal and α-quartz prototype of SiO_2 are presented in Fig.1. The elementary cell size for the silicon crystal is computed to be equal to 5.43 Å. For a clean α-quartz each oxygen atom is computed to form a short bond (SB) of 1.624 Å and a long bond (LB) of 1.628Å to a silicon atom which is in good agreement with experimental estimates of 1.607 Å and

[1] AMD Saxony LLC&Co.KG, Wilschdorfer Landstraße 101, D-01109 Dresden

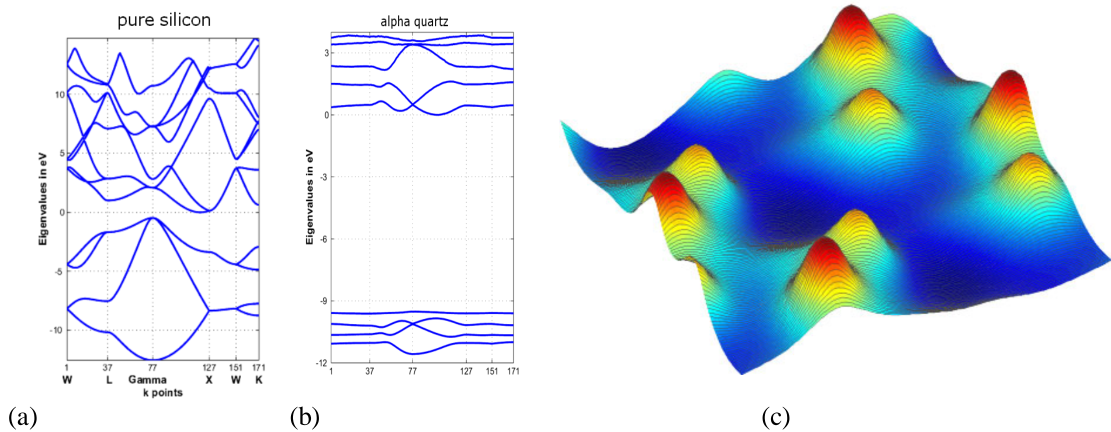
1.612 Å. To understand a mechanism of the SiO_2 gate degradation, we have studied different oxygen vacancies, which are the fundamental and most important defects in silica. Structures of α- quartz with one- and two- oxygen vacancies are shown in Fig.2.



(a) (b)

Fig. 2: The optimized structure of SiO_2 crystal with (a) one- and (b) two- oxygen vacancies.

One oxygen vacancy is created in two different structural conformations; as a neutral (V_0^0) and as a positively charged (V_0^+ or E') vacancy state. Creation of one neutral oxygen vacancy leads to the dimer configuration with the *Si-Si* distance of 2.478 Å. The positively charged state is obtained by removing one electron in addition to the oxygen vacancy, which has been usually identified with the radiation induced E' center in crystalline silica, and with the E_{δ}' center in amorphous silica. The *Si-Si* distance increases due to the charging to the value of 3.095 Å, approaching to a similar distance, as 3.08 Å, in pure α-quartz.



(a) (b) (c)

Fig.3: The band structure of (a) silicon crystal and (b) clean quartz; (c) the electron distribution in SiO_2 in the presence of one oxygen vacancy. These computations were done with the ABINIT program package.

The first-principle DFT method allows to compute the band structure and the electron distribution (see Fig. 3) in the presence of defects. Suggesting that a gate oxide degradation occurs due to the charge flow through percolative trajectories, formed in the oxide by connecting the channel with the poly-*Si* gate. The energetic states of defects in the band structure and electron distribution around vacancies in Fig.3 give useful information to compute the overlapp integral between two vacancies.

References:

[1]. W. Kohn and L. J. Sham, Phys. Rev. **A 140,** 1133 (1965).

[2]. M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias, and J. D. Joannopoulos, Rev. Mod. Phys., **64**, 1045 (1992).