

# First principles study of the degradation of silicon-dioxide gate dielectrics

Andreas Domdey, Kristian Hafkemeyer, Timor Knudsen, Wolfgang Krautschneider

**Abstract**—An approach to investigate the atomistic mechanisms leading to degradation and breakdown of silicon-dioxide gate dielectrics is presented. These mechanisms concern the reliability of modern MOSFET devices.

**Index Terms**—MOSFET, reliability, degradation, breakdown, silicon-dioxide gate dielectrics, first-principles studies

## I. INTRODUCTION

Current MOSFET devices exhibit very thin gate dielectrics in the range of  $1 \dots 2nm$  which corresponds to only a few atom layers. Due to the small thicknesses, these devices are prone to quantum mechanical effects like tunnelling through and hot charge carrier injection into the dielectric. This causes weakening, breaking, and thus restructuring of its atomic bonding.

Macroscopically, an irreversible deterioration of the electrical MOSFET parameters – e.g. threshold voltage, subthreshold current and noise – as a function of time by virtue of the degraded gate dielectric can be observed. In an advanced state of degradation, the further declined electrical characteristics can cause malfunctions of the circuit culminating in the gate dielectric breakdown which means a conducting path from the channel to the gate and total loss of the device.

Since future MOSFET devices will be continuously scaled down and feature even thinner gate dielectrics, the influence of quantum mechanical effects on the reliability increases. Therefore, a comprehensive understanding of the processes on atomic level is essential.

Earlier research work focussed on the phenomenological description of the electrical parameter changes depending on time. In many cases, a theoretical model has been developed on the basis of the thus obtained empirical function. This explains the variety of models for gate dielectric degradation that can be found in literature. But none of them covers all aspects of the atomic mechanisms finally leading to breakdown.

Our project aims at the analysis and accurate description of the physical mechanisms responsible for gate dielectric degradation. In a first step, we concentrate on silicon-dioxide ( $SiO_2$ ) as a representative. An  $SiO_2$  layer has been modelled using *Molecular Dynamics* (MD) simulations (Section II). The

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$SiO_2$  will become part of a complete atomic MOSFET model and the whole ensemble will then be applied to first principles calculations (Section III). Conclusions of our project so far will be drawn in Section IV.

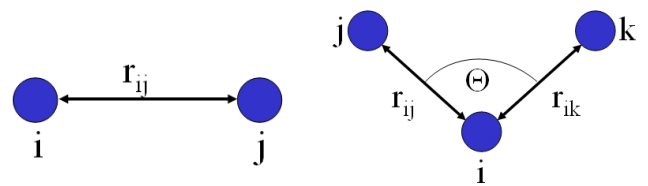
## II. MODELLING OF SILICON-DIOXIDE GATE DIELECTRICS

Silicon-dioxide is an amorphous (vitreous) material. I.e. there is no long distance order in  $SiO_2$ . In contrast to e.g. monocrystalline silicon ( $Si$ ) where each atom position is defined by the lattice (diamond structure) and its constant ( $5.43102\text{\AA}$  at  $300K$  [1]), the modelling of  $SiO_2$  is more complicated and requires extensive calculations.

A self-evident solution to this problem consists in performing *Molecular Dynamics* (MD) simulations. This computational method is based on the classical treatment of atoms (Born-Oppenheimer approximation) and the numerical integration of Newton's equation of motion

$$\vec{a}_i = \frac{d^2 \vec{r}_i}{dt^2} = \frac{\vec{f}_i}{m_i} = -\frac{\vec{\nabla}_i V(\vec{r}_1, \dots, \vec{r}_N)}{m_i} \quad (1)$$

in order to obtain the position  $\vec{r}_i$ , and the velocity  $\vec{v}_i$  of each atom  $i$  (mass  $m_i$ ) out of  $N$  total atoms at time  $t$ . The potential energy function  $V(\vec{r}_1, \dots, \vec{r}_N)$  implicitly contains the principles of quantum mechanics like the Pauli exclusion principle and is time-invariant. It can be derived by fitting certain sample functions to measurements (semi-empirical potential energy function, e.g. Stillinger-Weber potential [2]), or by performing quantum mechanical calculations (ab-initio potential energy function, e.g. EDIP [3]).



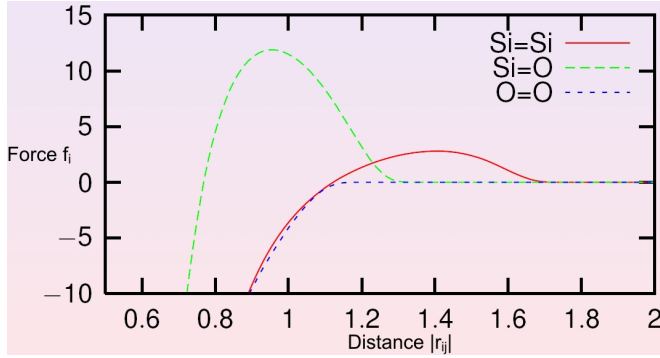
1: Two-body interaction

2: Three-body interaction

A potential energy function suitable for condensed systems composed of silicon and oxygen ( $O$ ) atoms was proposed by T. Watanabe and co-workers in [4]. This potential energy function consists of a two-body and a three-body term. The two-body term (Fig. 1) contains the pairlike interaction between two atoms due to attracting as well as repulsive interatomic forces and is of Stillinger-Weber type. Since the range of interatomic forces is infinite, a so-called cut-off function has been incorporated into the two-body potential for computational purposes

(Fig. 3). This means atoms within the cut-off distance are considered to interact while interactions exceeding the cut-off distance are neglected. The three-body term (Fig. 2) covers – also within a certain cut-off – angular dependencies between three atoms. By applying this potential energy function to MD simulations, the user is able to handle

- $Si-Si$ ,  $Si-O$  pairs ( $O-O$  is considered to be repulsive),
- $Si-Si-Si$ ,  $Si-Si-O$ ,  $Si-O-Si$ ,  $O-Si-O$  triplets,
- mixed  $Si$ ,  $O$  systems from bulk  $Si$  to  $SiO_2$  including interface,
- different silica phases.



3: Two-body term with reduced units

One possibility to model silicon-dioxide by MD simulations is the quenching of an  $Si$  and  $O$  melt. For that purpose, an initial position  $\vec{r}_i$  and velocity  $\vec{v}_i$  is assigned to each atom  $i$  of the  $N$  total atoms. Then, the position  $\vec{r}_i(t + \Delta t)$  of each atom  $i$  at time  $t + \Delta t$  is derived from the position  $\vec{r}_i(t)$ , velocity  $\vec{v}_i(t)$  and force  $\vec{f}_i(t)$  at the previous time  $t$ . This is done by numerically integrating Newton's equation of motion using an algorithm like Verlet. With the new position  $\vec{r}_i(t + \Delta t)$ , the new velocity  $\vec{v}_i(t + \Delta t)$  and force  $\vec{f}_i(t + \Delta t)$  for each atom  $i$  are calculated. A thermostat scales the velocity under consideration of a Gaussian shaped velocity distribution in order to quench the melt. The latter three steps are repeated until the solidification point is reached.

### III. FIRST PRINCIPLES STUDY OF SILICON-DIOXIDE GATE DIELECTRICS

The model of  $SiO_2$  (Sec. II) – or more precisely the locations of the atoms of both species – are fed into *Density Functional Theory* (DFT) and later on into *Time-Dependent Density Functional Theory* (TD-DFT) calculations. The DFT is a method to determine the quantum-mechanical ground-state of many-electron systems. It relies on the *Hohenberg-Kohn-Sham* (HKS) theorem which states that the ground-state energy of a many-electron system is a unique functional of the space-dependent electron density  $n(\vec{r})$  and that this functional has its minimum at the equilibrium electron density  $n_0(\vec{r})$ . The electron density is to be computed. All other system properties in the ground-state can be derived from  $n(\vec{r})$  then. The availability of the Born-Oppenheimer approximation is implied. This means only the electrons are treated quantum-mechanically.

The main advantage of the DFT consists in the fact that it is not necessary to solve the complete Schrodinger's equation of the many electrons system. Thus, the computational effort decreases and the calculation of systems with considerably more than ten electrons is possible. Nowadays, powerful computers can handle systems with up to 1000 atoms. The TD-DFT is an enhancement of the DFT with regard to the computation of excited-states.

In order to determine the electron density  $n(\vec{r})$ ,  $N$  single-electron wave functions  $\phi_i$  – the so-called Kohn-Sham functions – are assumed to be the  $N$  solutions of the one-electron Schrodinger's equations (Kohn-Sham equations) in an effective potential  $V_{eff}$ :

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + V_{eff}(\vec{r}) - E_i \right) \phi_i(\vec{r}) = 0. \quad (2)$$

The electron density  $n(\vec{r})$  can be derived from the Kohn-Sham functions corresponding to

$$n(\vec{r}) = \sum_{i=1}^N |\phi_i(\vec{r})|^2. \quad (3)$$

The effective potential  $V_{eff}(\vec{r})$  depends on the electron density according to

$$V_{eff}(\vec{r}) = V(\vec{r}) + V_H(\vec{r}) + V_{xc}(\vec{r}). \quad (4)$$

The first term, the external potential  $V(\vec{r})$ , is essentially created by the (ionic) nuclei (Hellmann-Feynman theorem). The second term  $V_H(\vec{r}) = f[n(\vec{r})]$  describes the repulsive electrostatic interaction of the electrons (Hartree). The third term, the so-called exchange and correlation potential  $V_{xc}(\vec{r})$ , ensures for the correct treatment of the many-electron system.

The exchange and correlation potential functional  $V_{xc}(\vec{r})$  is not exactly known and must be approximated. The *Local Density Approximation* (LDA) is the simplest approximation for this functional. It is local in the sense that the exchange and correlation potential at any point of the space is a function of the electron density at that point in space only. The LDA functional is derived from a model assuming that the per-electron exchange and correlation potential at every point in space is equal to the per-electron exchange and correlation potential of a homogeneous electron gas. In many cases, the LDA is sufficiently accurate although LDA calculations overestimate the bond strenghtes which leads to too short bond lengths of 1...2% (overbinding).

The effective potential  $V_{eff}(\vec{r})$  appears in the Kohn-Sham equations (Eq. 2) on the one hand. On the other hand, it depends through  $V_H(\vec{r}) = f[n(\vec{r})]$  on the electron density  $n(\vec{r})$  and thus on the solutions of the Kohn-Sham equations. Therefore, the effective potential  $V_{eff}(\vec{r})$  and the Kohn-Sham function  $\phi_i(\vec{r})$  have to be calculated iteratively. In case of valence and conduction band electrons in solids, the Kohn-Sham functions  $\phi_i(\vec{r})$  can be of plane wave type. They are advantageous in respect of the fast solution of the Kohn-Sham equations with efficient Fourier transform algorithms. In case of electrons close to the nucleus, plane waves are unsuitable and additional methods for this region are required. Solutions to this problem can be the completely separated treatment

of these electrons (*Augmented Plane Waves*), the addition of extra wave functions – so-called *Projector Augmented Waves* (PAW) – or the application of pseudopotentials. The *Vienna Ab-Initio Simulation Package* (VASP) has been chosen for performing our ab-initio *Quantum-Mechanical Molecular Dynamics* (QMMD) computations. It is based on the DFT with LDA and supports pseudopotentials as well as the PAW method and a plane wave basis set. [6], [7]

#### IV. CONCLUSION

The MD simulations described in Section II have been chosen for programming complexity reasons. But they reveal two major problems. Unrealistic cooling rates many orders of magnitude higher than observed experimentally are the first problem. High cooling rates in MD simulations are required due to finite simulation time and lead to questionable solid structures with regard to defect density and overcoordination [5]. The result is an undercooled liquid. The second problem is found in the minimisation of the potential energy during MD simulations and the energy landscape of amorphous materials like  $SiO_2$ . Typically, an energy landscape of an amorphous material possesses a multitude of local minima. The local minima are separated by barriers with energies considerably higher than the thermal energy  $k_B T$ . MD simulations usually transfer such a system into one of these local minima from which it cannot get out in most cases [5]. The simulations then freeze. To overcome these problems, the application of the *Activation Relaxation Technique* (ART) [8] has been taken into consideration for future simulations. Further work is required to implement this technique.

The next major step consists in the assembly of the whole atomic MOSFET model including poly- $Si$  gate,  $SiO_2$  gate dielectric, crystalline  $Si$  bulk and interfaces. The chosen simulation technique currently allows for structures up to 1000 atoms. This might appear to be a rather small amount. In consideration of the persistently minimised MOSFET devices with layer thicknesses of a few atom diameters, 1000 atoms already is a promising number nevertheless. Enhancements of computer performance, simulations techniques and simulation software will allow for an ever rising amount of atoms so that the simulation of realistic MOSFET devices appears to be feasible.

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