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Development of a Multi-Scale Time Dependent Dielectric Breakdown Simulator Based on TBQC and KMC Method: Application to the Evaluation of a Gate Oxide Film for CMOS Technology

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1. Introduction

Time dependent dielectric breakdown (TDDB) is a key failure mechanism in gate oxide films in complementary metal oxide semiconductors (CMOS) devices used in large-scale integrated circuits [1-3]. To enable further reduction in the equivalent oxide thickness for technology downscaling and simultaneous reduction in the leakage current, various high-*k* dielectrics are being explored as a replacement to the conventional silicon oxides or oxinitrides. Moreover, to improve the adhesion characteristics of the high-*k* material to the silicon substrate an intermediate silicon oxide interfacial layer in between is needed. In fact the presence of the interfacial layer is unavoidable as it tends to form during the annealing steps of the fabrication process. Consequently, understanding the physics of TDDB phenomena for silicon oxides as well as high-*k* materials is an issue of the outmost importance related to the design and construction of better CMOS devices.

A fair number of studies have been performed so far in this field including both, macroscopic reliability assessment techniques using the power law model to fit experimental data [4-6], as well as microscopic studies oriented to understand the phenomena based on quantum chemical approaches [7,8]. However few of them combine the macro- and microscopic aspects to obtain a rather complete solution to the problem. Studies considering multi-scale simulations linking the device scale behavior with the atomistic analysis are critical in the design of electronic devices.

Here, to bridge this gap, we report on the development of a computer methodology for device scale simulation that uses a kinetic Monte Carlo (KMC) method to evaluate the voltage-current characteristics, together with an atomic scale simulator that can evaluate the probability for a KMC movement analyzing the respective energy diagrams. The latter combines our originally developed tight-binding quantum chemical (TBQC) program.

2. Computational method

The development of the new pair of simulators (micro- and macro-scale) is thus performed with the microscopic part consisting of our original TBQC simulator "Colors". In this TBQC simulator, the level of theory corresponds to that of the extended Hückel method. To determine the off-diagonal elements of the Hamiltonian matrix, the corrected distance-dependent Wolfsberg-Helmholz formula was used [9]. In order to solve the Shrödenger equation in this simulator, parameters are used for the Hamiltonian matrix elements that are derived on the basis of first-principles calculation results. The details of the parameterization have been published elsewhere [10].

On the other hand, the macroscopic part consists of our original KMC simulator. This simulator is realized using a 250×250×90 nm silicon oxide model divided into 5,625 cells, each of which are of 10 nm of edge. The upper and the lower sides of the model were poly-silicon and silicon substrate respectively. Electrons were injected from the upper side to the silicon oxide layer and the holes were generated near the substrate side and were caused by impact ionization. The injected electron can move along the cells according to the Fowler-Nordheim tunneling probability,

$$T_{TunnelingProbability} = AE^2 \exp\left(-\frac{4\sqrt{2m^* q\phi_{barrier}^3}}{3\hbar E}\right) \qquad (1)$$

here, A is a fitting parameter, E is the strength of the electric field, m^* is the effective mass, q is the elementary electric charge, ϕ is the barrier height and $\hbar$ is Planck's constant respectively. The model includes the electric field caused by the applied drift field and the Coulombic effects resulting from interaction of ambient electrons and holes.

First-principles density functional code "DMol[3]" and "CASTEP" were used to verify the reliability of the parameters.

3. Results and discussion

To verify the reliability of the parameter set for the TBQC calculation, the TBQC and first-principles calculation were firstly executed using a SiO_2 model. The calculated atomic charges, bond orders and the total binding energy are shown in Table I. It can be observed that the values of the TBQC calculation are in good agreement with the first-principles results.

Table I TBQC results for the atomic charges, diatomic bond order and total binding energy compared with first-principles results.

	Charge(-)		Bond order (-)	Binding energy (kcal/mol)
	Si	O	Si-O	Si-O
First-principles calc.	0.541	-0.271	0.57	7286.4
TBQC calc.	0.541	-0.271	0.53	7217.2

Since it is known that the electron trap site involves a hydrogen-terminating silicon dangling bond related to an oxygen defect [3,11], we adopted the β-quartz model containing an oxygen defect and two Si-H terminations for the quantum calculation, as shown in Fig. 1. The calculated molecular orbital corresponding to the hydrogen terminations is also shown in Fig. 1. The energy level of this molecular orbital around the hydrogen atoms was located 0.569 eV under the bottom of the conduction band. Since we obtained 1.019 eV for the electron trap depth from the calculation model containing two oxygen defects, the minimum and maximum energy levels of electron trap sites were set to these values in the macro-scale simulation.

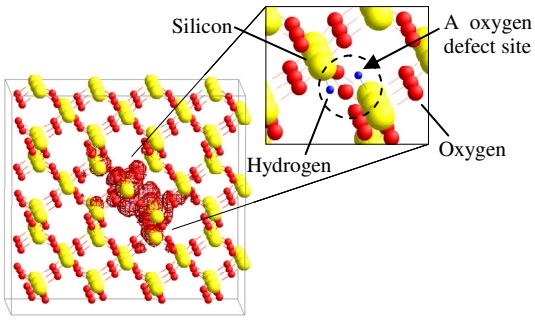

Fig. 1 Molecular orbital around a oxygen defect. Energy level at 0.569 eV under the bottom of conduction band.

Finally the macro-scale TDDB simulation was performed using the barrier height obtained as described above. The flow chart of this simulator is shown in Fig. 2. We simulated the effect of hole generation near the silicon substrates caused by impact ionization. Since the holes promote a steep inclination of the electric field, the Fowler-Nordheim tunneling potential barrier lowers substantially and there is a net increase in the current flow [3]. As illustrated in Fig. 3, the results of the constant current TDDB simulation reflect this tendency quite well.

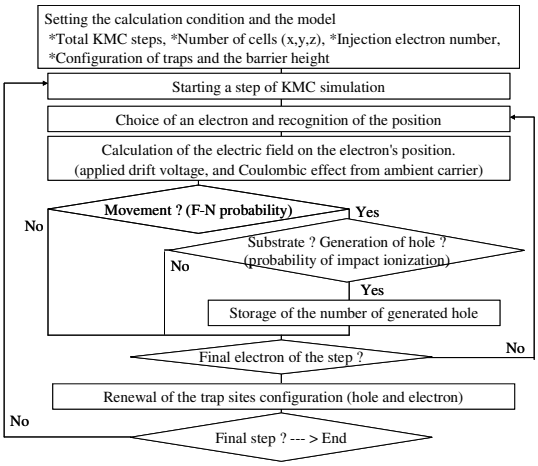

Fig. 2 The flow chart of TDDB simulator

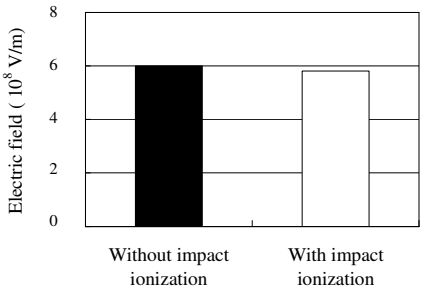

Fig. 3 Results for the constant current TDDB simulation

Consequently, we have succeeded in the development of a new multi-scale TDDB simulator. Although the comparison was made only on one model and more examples are of course needed to validate our new method, it should be emphasized here that our methodology is a non-empirical one and thus might be applicable to a wide range of complex systems.

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