An agent-based common software platform applied to multi-scale device and process simulations

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Abstract

This paper describes a common software platform that allows users to combine multi-scale physical simulations in the form of agents. To demonstrate the benefit of combing multiple simulations, hydrogen desorption at the interface of gate oxide and Si-substrate due to hot electrons in a deep sub-micron device is analysed by coupling device and lattice Monte Carlo simulation. Deposition profiles on a large-scale wafer are studied by using particle method hybridised with continuum simulation. The desorption probability of hydrogen and the coverage of deposition layer are shown to be strongly dependent on the position under the gate and on the wafer respectively.

1 Introduction

It becomes increasingly important to study multi-scale and multi-physics phenomena[1],[2] in ultra-small devices for improving performance and reliability such as transconductance degradation due to defect generation and microscopic manufacturing process on a large-scale Si-substrate. However, the technique of a seamless computing to couple multiple simulations needs to be much improved to reduce time and effort, which essentially involves implementing spatial and time-scale transformation. This paper describes composite analyses using an agent-based common software platform that allows interdisciplinary simulations to be efficiently combined into a single program. The first demonstrates stochastic desorption of H-terminated dangling bonds due to hot electrons, in which a device window Monte Carlo (DMC) simulation is combined with a lattice Monte Carlo (LMC) simulation to analyse desorption probability of H bonds on the Hitachi SR2201 parallel machine and WS clusters. Furthermore, deposition profiles in sub-micron trenches distributed on a Si-substrate using plasma chemical vapour deposition (CVD), in which hydrodynamic simulation to analyze diffusive gas flow in a reactor is hybridised with dynamic simulation Monte Carlo (DSMC) method near the trenches for rarefied gas regime.

2 Agent-based common software platform

To mask the complexities involved in composite parallel simulations that employ FDM, FEM and particle method, the system provides agent library calls to define correlative specifications such as nearest points, first nearest neighbours(1NN) and in-sphere correlation between mesh points and particles. Using standard message passing library such as MPI(Message Passing Interface) and PVM(Parallel Virtual Machine), as schematically shown in Fig.1, the agent associated with each simulation process can automatically determine to which communication is required and transform physical values associated with correlated discrete points while conserving density, momentum and energy. The performance of agents on the Hitachi SR2201 to combine two parallel simulations which employ different kinds of N discrete points and are decomposed into the same M domains is shown in Fig. 2. The agents can detect the correlated discrete points automatically, of which transaction time is designed to be $O(N\log_2 N)$ using a bucket method[3].

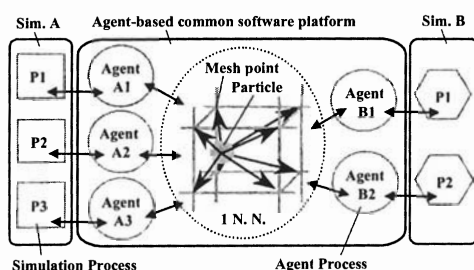

Fig. 1 Combination between different parallel simulations, in which physical values associated with discrete points are transferred and transformed by agents.

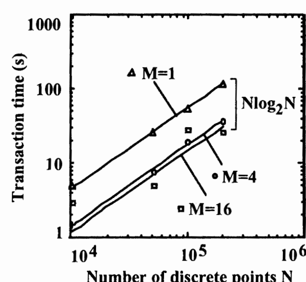

Fig. 2 Transaction time to detect correlated points of 1NN when simulations are decomposed in M domains.

3 Multi-scale composite simulations

The combination between device and lattice Monte Carlo simulations can be effectively realized using 34 agent library calls, together with some additional statements of 240 steps to convert the formats of the discrete points. The deposit simulation can be combined by using 24 agent library calls together with some additional statements of 100 steps, both of which are less than 1/10 of conventional development. Each simulation is easy to reuse and the optimum combination can be rearranged to improve physical accuracy and execution time on user demands.

3.1 Hydrogen desorption due to hot-electrons and multi-phonon interaction

The desorption probability P_{des} of H bonds is studied at the interface of Si/SiO_2 in deep sub-micron device of L_{eff} = 0.18um and oxide thickness of 5nm. In a window DMC, non-equilibrium electron distribution using 15000 electrons is calculated at V_d = 1.5V, V_g = 1.0V for 67ns. Desorption and diffusive migration of H atoms of 10^{17} m^{-2} due to hot electrons near the interface region, which is discretized by 250x15x30 FDM meshes of 1nm width, are analysed in the LMC. When combining two

simulations, the position of H bonds and defects is transferred to the DMC by the agents and used to identify the scattered electrons attributed to phonon absorption and emission at H bonds. As shown in Fig.3, the position of the scattered electrons is transferred back to the LMC on the two-way iterative communication. At low V_d less than the threshold energy E_{th} of 3.7eV for bond breaking, a multi-phonon process excited by hot electrons is considered to be one of the major mechanisms for H desorption leading to defects[4]. P_{des} due to hot electrons and multi-phonon interaction can be derived as a following equation.

$$P_{des} = \sum_{m} f(m,n) \{P_u(N_u, \varepsilon_u) P_d(N_d, \varepsilon_d)\}^{\frac{m}{2}} \{\frac{P_u(N_u, \varepsilon_u)}{P_d(N_d, \varepsilon_d)}\}^{\frac{n}{2}}$$

Where f(m,n) represents number of pathways from ground phonon state to n state at m times of electron scattering. P_u and P_d means effective scattering probabilities associated with emission and absorption of electrons, of which number is N_u, N_d and average energy is ε_u, ε_d respectively. H-Si bending phonon, of which energy is 0.29eV and n becomes 13, is assumed to be the typical phonon. In Fig. 4, P_{des} is dependent on the position under the gate and shows the maximum value at the drain side. Transconductance degradation can be evaluated using the position-dependent P_{des}, desorption time of H bonds and recombination rate with defects.

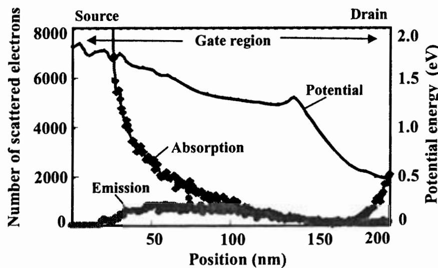

Fig. 3 Number of scattered electrons by a H bond at the interface of Si/SiO_2 under gate region

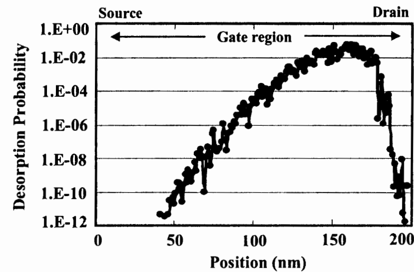

Fig. 4 Dependence of H desorption probability on the position under the gate electrode

3.2 Deposition profiles in sub-micron trenches on a large-scale Si-substrate

In the second composite simulation, the hydrodynamic simulation based on the Navier-Stokes equation is discretized by 5076 FEM meshes. As shown in Fig.5, a source region supplies raw reactive gases and a Si-substrate of 300mm exists at the bottom of a reactor. SiH_4 and reaction products of SiH_2 become major materials to form thin film in trenches. The partial pressure of SiH_2 at 973K is 6~7 orders smaller than that of SiH_4. On the other hand, the sticking coefficient of SiH_2 is 0.7 which is 6 orders larger than SiH_4 of 9.4×10^{-7}. The analytical region near the 0.1um trenches on the substrate should be analysed by the DSMC method[5], because the mean free path of molecules λ becomes larger than the size of the trenches D where $K_n = \lambda/D > 0.01$. Therefore, the DSMC is parallelized to different domains associated with each trench, which enables to analyse deposition profiles distributed on the Si-substrate

simultaneously. Using the agent-based system, the partial pressure of SiH_4 and SiH_2 obtained from the hydrodynamic simulation can be automatically transferred and transformed into 5000 gas molecules at each domain in the DSMC according to the Maxwell distribution. Because the normal component of gas flow at the bottom of the reactor is assumed to be zero in the hydrodynamic simulation. Fig.6 shows that coverage of the deposition profiles increases at the edge regime. Partial pressure of reactive production SiH_2 is too high at the central region to form a thicker layer on the surface due to high sticking coefficient. The composite simulation can be used to analyse microscopic manufacturing process by designing such as temperature and flow rate of reactive gases from hydrodynamic simulation.

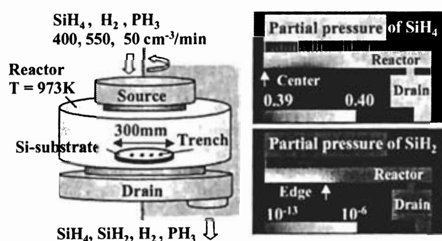

Fig. 5 Partial pressure of SiH_4 and SiH_2 obtained from hydrodynamic simulation using CVD

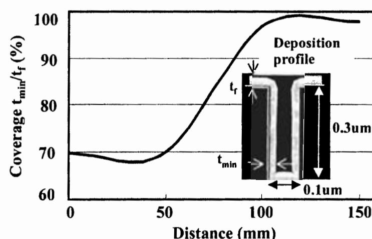

Fig. 6 Dependence of coverage in 0.1um trenches on the distance from the center of a Si-substrate

4 Conclusions

Taking account of the multi-phonon mechanism, the desorption probability of H bonds due to hot electrons is shown to be strongly dependent on the position under the gate electrode. The coverage of deposition profiles changes drastically according to the position on the large-scale substrate. It is shown that macroscopic characteristics and microscopic mechanisms are so intertwined that the agent-based software platform can be an efficient tool to analyse multi-scale simulations.

References

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