# Multi-scale Simulation of Interfacial Roughness Effects in Silicon Nanowires

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Abstract—Using a unique multi-scale simulation approach combining an atomic scale simulation of silicon nanowires (SiNWs) oxidation with an interfacial roughness characterization technique and the non-equilibrium Green's function (NEGF) calculation, the interfacial roughness effect on the transport characteristics was investigated. The calculated interfacial roughness, such as the root-mean-squared (RMS) roughness and correlation length was found to be in good agreement with the previous experimental work. The RMS roughness and correlation length increased linearly during the oxidation process. The NEGF calculation result revealed the decrease of the mobility with the increase of the charge density in the oxidized SiNW with 10 nm diameter.

Keywords-multi-scale simulation; silicon nanowires; interfacial roughness; TCAD

# I. INTRODUCTION

Silicon nanowires (SiNWs) have been considered as the most manufacturable nanostructured building block [1-4]. Various prototype devices based on SiNWs were reported such as field effect transistors (FETs), photodetectors and biosensors [5-7]. In the nanometer scale devices with sub-10 nm gate length, atomic scale roughness at the dielectric/channel interface significantly affects the device performance and reliability [8]. Thus, understanding and controlling the interface

morphology of  $Si/SiO_2$  in SiNWs is an essential issue, especially, in optimizing the device performance of SiNW field effect transistors (FETs). However, experimental methods to characterize the interfacial roughness are highly limited at present. Previous analyses on the effect of the interfacial roughness in SiNWs were thus based on pure speculation [9-11]. In this work, we proposed a unique multi-scale simulation method combining an atomic scale simulation of SiNW oxidation with an interfacial roughness characterization technique and the non-equilibrium Greens' function (NEGF) calculation. Using this approach, the effect of the interfacial roughness on the transport behavior in 10 nm SiNW was investigated.

## II. COMPUTATIONAL METHODS

The schematic diagram in Fig. 1 shows the simulation procedure. Reactive molecular dynamics (MD) simulation of SiNWs oxidation was performed using the reactive force field proposed by van Duin *et al.* [12]. After oxidation, the etching process was performed to expose the interface between Si/SiO<sub>2</sub>, then, the roughness profile of Si/SiO<sub>2</sub> interface was obtained by the virtual atomic force microscope (AFM) simulation. The statistical properties of the interfacial roughness were characterized by an autocorrelation function as follows:



Figure 1. Schematic diagram for our simulation procedure.

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$$C(\theta, z) = \left\langle \Delta(\theta, z + \theta_0, z_0) \Delta(\theta_0, z_0) \right\rangle = \Delta_m^2 e^{-\sqrt{2}\sqrt{\theta^2 + z^2}/L_m}$$
(1)

where  $\Delta_{\rm m}$  is the root-mean-squared (RMS) fluctuation of the roughness,  $L_m$  is the correlation length,  $\theta$  is the circumferential direction of SiNWs and z is the wire axis. Finally, surface-roughness (SR)-limited mobility was obtained by NEGF calculation. Each simulation method in detail will be discussed in the following sections.

# A. Oxidation Process for Silicon Nanowires

A SiNW of the [311] orientation with 10 nm diameter was prepared. The orientation of the simulation was chosen based on the recent experimental results [13]. The oxidation temperature was set to 1073 K to mimic a typical thermal oxidation. The SiNW with 10 nm diameter was relaxed for 100 ps before the oxidation process was performed. Then, the simulation box was filled with O2 molecules of which the partial pressure was set to be approximately 275 atm to investigate the rare events in the oxidation reaction (Fig. 2). However, the temperature of the system was rescaled to the oxidation temperature at every time step, 1 fs, to prevent overheating the system due to the high pressure during simulation. The periodic boundary conditions were applied in all directions. "Large-scale Atomic/Molecular Massively Parallelized Simulator" code was used for the MD simulations [14]. After the oxidation process of 80 ps, the oxygen molecules, which were not reacted with the silicon atoms in SiNWs, were removed in the system for further investigations.



Figure 2. Simulation box for Si [311] NW oxidation. Gray atoms are Si, and red ones are O.

## B. Interfacial Roughness Characterization

After MD simulation of the oxidation process, the oxide layer was etched by removing the silicon atoms of the Mulliken charge larger than 0.8e and the oxygen atoms associated with the etched silicon atoms as shown in Fig. 3. The number of atoms in the etched oxide layer during the oxidation process was calculated to validate our etching process as summarized in Table I.



Figure 3. (a) after MD simulation of the oxidation process of 10 nm SiNW at 80 ps. (b) after the etching process. Larger atoms are Si and smaller ones are O. All atoms are colored with the Mulliken charge analysis.

 
 TABLE I.
 The number of oxygen and silicon atoms in the etched oxide layer.

Time (ps)	# of Oxygen	# of Silicon	Ratio O/Si
10	19	11	1.73
20	111	54	2.06
30	235	105	2.24
40	258	120	2.15
50	1465	659	2.22
60	1512	675	2.24
70	1407	655	2.15
80	1657	762	2.17

Then, the virtual AFM simulation was performed to obtain the roughness profile of Si/SiO<sub>2</sub> interface by scanning the exposed surface of the etched SiNWs. In our virtual AFM code, the Lennard-Jones (LJ) potential was used to describe atomic forces between a virtual probe atom, which is considered as a single Si atom, and atoms on the interface of SiNWs. The zerocrossing distances in LJ potential was set to 4.2 Å for Si-Si and 3.62 Å for Si-O based on Van der Waals radii of Si and O, 2.1 and 1.52 Å, respectively. The statistical properties of the interfacial roughness were characterized by the principle of exponentially decaying autocorrelation function as described in (1). Finally, we obtained the values of RMS and  $L_m$  for 10 nm SiNW during the oxidation process.

#### C. NEGF Transport Calculation

The MD results are then linked to our in-house, fullquantum, self-consistent, three-dimensional NEGF-based transport simulator for an accurate calculation of the SRlimited electron mobility in SiNW FETs. In the device simulations, SiNW channel surrounded by oxides in the gated region has the SR patterns, generated by using the exponential autocorrelation function with RMS and  $L_m$  values from the MD results. All the six delta valleys of Si were included in our calculations, and to treat the [311] orientation, the full effective mass Hamiltonian was constructed, which has the coupling terms such as  $k_x k_y$  due to the non-zero off-diagonal terms in the 3x3 inverse mass tensor.

# III. RESULTS AND DISCUSSION

Fig. 4 shows the time evolution of interfacial roughness, RMS and correlation length for 10 nm SiNW during the oxidation process. As the oxidation proceeded, the RMS roughness and correlation length increased linearly, which indicates that the oxide growth leads to rough interface. It must be noted that the calculated values at 80 ps,  $\Delta_m = 1.96$  Å,  $L_m$  in  $\theta$ -direction = 7.23 Å, were found to be in consistent with the previous experimental work on Si (100) surface,  $\Delta_m =$  $1.39\pm0.06$  Å and  $L_m = 7.1\pm2.0$  Å [15]. This consistency would exhibit the validity of our simulation and interfacial roughness analysis.



Figure 4. The time evolution of RMS and correlation length in z and  $\theta$  directions for 10 nm SiNW.

We performed the NEGF-based transport calculation using the interfacial roughness values calculated from the MD simulation and interfacial roughness characterization. The mobility of SiNW FETs was then obtained by calculating the charge density in the channel region and the electrical conductivity. Typically 20 SR samples were generated to give statistically averaged values. Fig. 5 shows thus-calculated mobility of a 10 nm diameter SiNW FET as a function of the charge density, which exhibits the usual decrease of the mobility with the increase of the charge density.



Figure 5. Ballistic mobility and effective mobility of a 10 nm diameter SiNW FET.

It is expected that the use of the RMS and  $L_m$  values from the MD calculations, instead of values for bulk silicon could extend to other SiNWs systems with various conditions, such as diameters of SiNWs, oxidation temperature and pressure, etc.

## IV. CONCLUSIONS

In summary, we propose a unique multi-scale simulation approach to investigate the interfacial roughness effect on the transport characteristics through the reactive MD, interfacial roughness characterization technique and NEGF calculations. Especially, our simulation technique provides quantitative values of the interfacial roughness in the oxidized SiNWs which are hardly observed or characterized in experimental methods. The present work reveals that RMS and the correlation length increase with increasing the oxidation time in 10 nm SiNW. Using these values, RMS and correlation length from MD simulation and interfacial roughness characterization, the effect of the interfacial roughness on the transport behavior, especially electron mobility in 10 nm SiNW was investigated by the NEGF transport calculation.

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