Scaling Analysis of SiO2/Si Interface Roughness by Atomic Force Microscopy

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The scaling behavior of SiO2/Si interface roughness was investigated by atomic force microscopy. The rms value of the roughness increased as a power of the scale up to 100nm with the scaling exponent of 0.3 - 0.5, and saturated at ca. 0.3nm above 100nm scale. The scaling behavior of the observed roughness was well described by an exponential autocorrelation function with the correlation length of ca. 15nm. The relevancy of the scaling behavior to MOSFET channel carrier mobility is discussed.

1. INTRODUCTION
With the development of integrated circuit technology, a precise control of surfaces and interfaces is getting more and more significant in fabrication of a submicron device, since the influence of roughness in such a small system might be crucial to the device performance. For example, it is known that the electron mobility in a metal-oxide-semiconductor (MOS) system is seriously affected by scattering due to the roughness of the SiO2/Si interface. Therefore, a quantitative characterization of roughness is required in evaluation of processes.

As a measure of surface roughness, the rms value has been conventionally employed in engineering. It is often overlooked, however, that the rms value is well-defined only at a macroscopic scale. The scaling behavior of roughness must be taken into account at a mesoscopic scale, where the fractal nature of the surface is noticeable.

In this study, the SiO2/Si interface is investigated by AFM to reveal the scaling behavior of roughness.

2. EXPERIMENTS
Specimens were prepared as follows. A p-type Si (100) wafer (p=100 cm) was cleaned in the RCA process, and the chemical oxide was etched off in 1% HF. Dry oxidation was performed at 900°C followed by 15min of annealing in N2, at 900°C. The thickness of the oxide was 16.0nm. Specimens were dipped in 5% HF for oxide removal just before the AFM measurement in air.

In order to investigate the scaling behavior, AFM measurements were carried out for various sizes of areas, i.e., 100x100nm2, 800x800nm2, 5x5μm2 and 20x20μm2. In each measurement, the height data were acquired at 256x256 pixels. The AFM instrument employed in this study is a SPA-300/SPI-3600 from Seiko Instruments Inc.

3. RESULTS AND DISCUSSION
To investigate the geometrical properties of the SiO2/Si interface, several statistical quantities were extracted from the AFM images.

Width of interface
The width of interface W(L) is defined as the rms value of roughness calculated in a square of size LxL. The procedure of calculation is as follows. For each AFM image, the linear trend in the height data (or the sample mounting error) is removed, and then the image is divided into 2x2 sections. The rms value is calculated in each section, and is averaged over all sections. In this way, a series of W(L) are calculated from an AFM image. Those series of values calculated from several different sizes of images are connected together so that they cover a wide range of scales.

Figure 1 shows the width of SiO2/Si
interface calculated from AFM images as a function of the scale. Two distinct regions with different scaling behaviors are clearly observed. At scales larger than 100nm, the width is constant at ca. 0.3nm, which corresponds to the conventional rms value. At scales smaller than 100nm, the width varies as a power of the scale with the scaling exponent of 0.3 - 0.5, i.e.,

$$W(L) = L^\alpha \ (\alpha = 0.3 - 0.5).$$

In this region, the geometry is identified as self-affine \(^{3}\) in the sense that the roughness scales anisotropically in horizontal and vertical directions.

Qualitatively, the scaling behavior described above is in good agreement with the theory of kinetic roughening of a growing interface under far-from-equilibrium conditions.\(^{4}\)

Fig.1 Width of SiO\(_2\)/Si interface vs. scale.

**Autocorrelation function**

The autocorrelation function is defined as

$$ACF(r) = \langle h(r) h(r+r) \rangle,$$

where

$$\hat{h}(r) = h(r) - \langle h(r) \rangle$$

is the height relative to the average plane at position \(r\).

The autocorrelation function has been conventionally assumed to be Gaussian, i.e.,

$$ACF(r) = \Delta^2 \exp(-r^2/Lc^2),$$

in theoretical estimation of the surface roughness scattering of electrons at a SiO\(_2\)/Si interface.\(^{5,6}\) On the other hand, recent experiments show that the exponential autocorrelation

$$ACF(r) = \Delta^2 \exp(-r/Lc),$$

gives a better fit of data rather than the Gaussian autocorrelation.\(^{7,8}\) As for the value of the correlation length \(Lc\), however, there is still a large discrepancy between experiments.\(^{7,9}\)

We consider such a discrepancy comes from the scaling behavior of the interface roughness itself. It is obvious from Fig.1 that low-frequency components of roughness are cut off in observation of a small area. Goodnick et al.\(^{10}\) were aware of the effect of finite picture-length (typically, 40 - 80nm) in TEM observations, and Khaitin et al.\(^{11}\) pointed out the existence of low-frequency components with a length of 30 - 60nm, based on the spectrum analysis of STM images.

Figure 2 shows the autocorrelation functions calculated from AFM images of different sizes. As is expected, the correlation length seems to be much smaller in a smaller image. Therefore, it is important to determine the roughness parameters by fitting to the autocorrelation function for the relevant length scale; e.g., the electron mean free path in the case of roughness scattering.

Fig.2 Autocorrelation functions calculated from AFM images of different sizes.

**Power spectral density**

The (one-dimensional) power spectral density can be obtained by calculating the Fourier transform of the autocorrelation function. Several AFM images of different sizes cover a wide range of spatial frequencies.

Figure 3 shows the power spectral density vs. spatial frequency. At frequencies higher than 10\(^{-2}\)nm\(^{-1}\), the power spectral density is dependent on the spatial frequency with a slope of ca. -2, which is a very commonly observed value for fractal surfaces.\(^{3}\) At frequencies lower than 10\(^{-4}\)nm\(^{-1}\), the power spectral density is almost constant.

The Fourier transform of the autocorrelation function (5) gives

$$PSD(f) = \frac{2\Delta^2 Lc}{(2\pi f Lc)^2 + 1},$$

which behaves as
be carried out on a scale at

in agreement with our overall PSD(f) results. The flection point of 10^-2nm^-1 in Fig.3 gives a correlation length L_c of ca. 15nm.

The rms roughness \( \Delta \) and PSD(f) has the relation

\[
\Delta^2 = \int_{-\infty}^{\infty} PSD(f) df.
\]

Therefore, the measurement of \( \Delta \) must be carried out on a scale at least larger than the correlation length, otherwise it is underestimated due to low-frequency cut-off of PSD(f).

Comparison with simulation

As described in the previous section, the observed power spectral density is in good agreement with the exponential autocorrelation function. In the case of the Gaussian autocorrelation function, the power spectral density falls much faster at higher frequencies.

Another comparison was made by calculating the width of interface from the roughness generated by computer simulation. The method of simulation is the same as described in Ref.6. The roughness parameters used here are \( \Delta = 0.3 \text{nm} \) and \( L_c = 15 \text{nm} \). The results are shown in Fig.4. The experimental value of \( \alpha = 0.3 - 0.5 \) agrees well again with the exponential autocorrelation.

Fig.4 Width of interfaces generated by simulation.

4. SUMMARY

In summary, the width of the SiO_2/Si interface increased as a power of the scale up to 100nm with \( \alpha = 0.3 - 0.5 \), and saturated at ca. 0.3nm above 100nm scale. The scaling behavior was well described by an exponential autocorrelation function with the correlation length of ca. 15nm.

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