Scanning tunneling microscopy of the Si–SiO$_2$ interface in a metal-insulator-semiconductor structure

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The relief at the Si–SiO$_2$ interface in a high-quality metal-insulator-semiconductor structure has been studied for the first time by scanning tunneling microscopy. Large-scale irregularities with a typical height of 10–20 Å and a length of 300–600 Å have been found. The scattering of electrons by these irregularities is predominant and must be considered in the corresponding theory.

Reaching an understanding of the properties of metal-insulator-semiconductor (MIS) structures requires knowledge of the relief at the Si–SiO$_2$ interface in them. Irregularities of the relief have their greatest effect on the low-temperature mobility of the electrons of the inversion layer when the surface density of these electrons is[1,2] $n_S \gtrsim 10^{12}$ cm^{-2}. They also influence the quantum Hall effect, the localization of electrons, etc., although they have been discussed only at a qualitative level.[3] Extremely scanty information on the actual irregularities at an interface is based for the most part on studies of samples by transmission electron microscopy, despite the fact that this method is poor in bringing out irregularities with a typical length $\gtrsim 100$ Å (Refs. 4 and 5).

An excellent tool for studying surface relief is a tunneling microscope which scans over a relatively large area, $10 \times 10\ \mu\text{m}^2$, with a resolution near the atomic scale.[6] In this letter we report the use of this microscope to study the irregularity $\Delta(r)$ of the silicon surface in silicon MIS structures, on which we have already carried out a multifaceted study of the properties of the inversion layer.[3,7]

The samples. We studied high-quality MIS structures[8] fabricated on the (100)

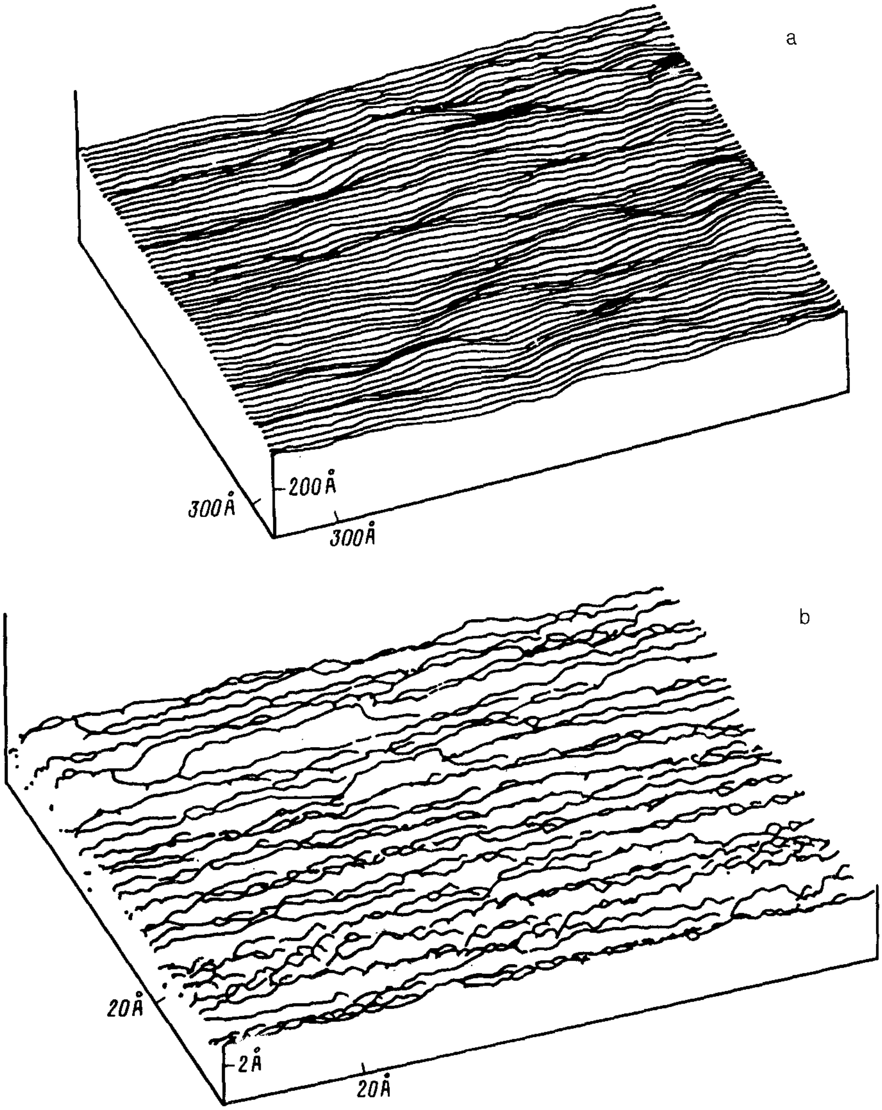

FIG. 1. Scanning tunneling micrograph of a silicon surface at different magnifications. The mean square deviation from a plane is $\langle \Delta^2 \rangle^{1/2} \simeq 17$ Å for Fig. 1a.

surface of p-Si with a boron impurity concentration $\simeq 7 \times 10^{14}$ atoms/cm^3. To expose the Si surface of the MIS structure, we etched away the Al film (the gate) and then used a 48% HF solution to etch away (in 10 min) the SiO_2 layer (2000 Å). Since pure silicon is essentially insoluble in HF, we expected that the exposed surface of the crystal would correspond to the Si–SiO_2 interface. After the etching, the samples were placed in the scanning tunneling microscope,[6] which operated in a vacuum of 0.1 torr at room temperature.

Results of the measurements by the scanning tunneling microscope. Figure 1 shows an example of the topography of a part of the Si surface, in two scales. The topograms consist of 64 rows, each of 128 points. We see that the short-period surface irregularities (Fig. 1b) are at the atomic scale, with a height δ on the order of a few angstroms. The long-period variations in the relief have typical amplitudes $\delta \sim 10$–30 Å and a length Λ of hundreds of angstroms.

The irregularity of the surface can be characterized quantitatively by its Fourier spectrum (Fig. 2). In constructing this spectrum, we first found the mean plane by the

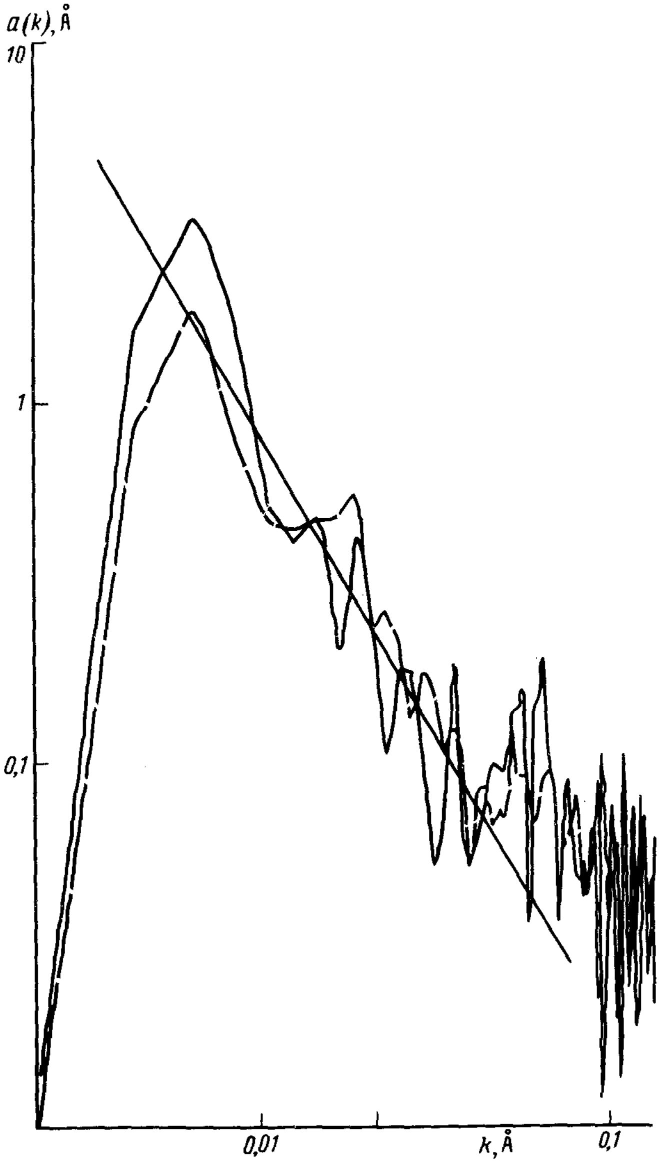

FIG. 2. Representative Fourier spectra of the irregularities on various parts of a silicon surface. The solid curve is the spectrum corresponding to Fig. 1a; the straight line shows $a(k) \propto k^{-n}$ with $n = 1.7$.

method of least squares. We used this mean plane as a reference plane. We then calculated the one-dimensional Fourier expansion of each row i in spatial harmonics, up to wave vectors $k = 2\pi\cdot 64/L$, where L is the length of a row:

$$\Delta(x, y_i) = \sum_k a_i(k)\cos(kx);$$

then the spectra of all 64 rows were averaged. The very first part of the spectra at small k, over the first two or three harmonics, is distorted because of two factors: A common reference plane was chosen for all the lines, and the statistical base is small. This wavelength interval, however, is not of major interest, since it contributes little to the scattering of the electrons, for reasons which we will see below.

A comparison of our results with data obtained previously shows that the long-period oscillations, which were undetected in those previous studies, have a large amplitude, which increases with descreasing k (Fig. 2). At the same time, according to Refs. 4 and 5, we could expect the amplitude of the components with $k \lesssim 0.1$ Å^{-1} to depend only weakly on the wavelength. Quantitatively, the scale size of the components with $k \sim 0.1$ Å^{-1} in our case is slightly smaller (by a factor of two or three) than that found in Refs. 4 and 5.

Effect of the surface irregularity on the mobility of the electrons of the inversion layer. It appears that the surface irregularities which are observed can be linked with aspects of the mobility μ of the electrons of the inversion layer, measured for similar samples from the same wafer. In contrast with several other studies (see, e.g., Figs. 65 and 67 in Ref. 1 and the bibliography there), at densities $n_S \gtrsim 10^{12}$ cm^{-2}, where μ is determined by the scattering of electrons by surface irregularities, we observed in Ref. 7 a dependence $\mu^{-1} \propto n_S$ (see Fig. 3), not $\mu^{-1} \propto n_S^2$. A similar dependence has been observed previously (Fig. 119 in Ref. 1).

Since the Fermi momentum of the electrons has a behavior $k_F \propto \sqrt{n_S}$, and their velocity has a behavior $v_F \propto \sqrt{n_S}$, we conclude that the behavior $\mu = e\tau/m \propto 1/n_S$ corresponds to the situation that the electron mean free path is described by $l \propto 1/\sqrt{n_S} \propto k_F^{-1}$. A relationship of this sort arises in a natural way in an "extremely dirty" situation, where the Ioffe-Regel' rule, $l \approx 2\pi/k_F$, applies. Numerically, however, the mean free path ($l \simeq 3 \times 10^3$ Å at $n_S = 10^{12}$ cm^{-2}) is an order of magnitude greater than the de Broglie wavelength for the motion of the electrons along the surface. We thus need an accurate solution of the scattering problem based on the Fourier spectrum of the surface relief in Fig. 2.

We can make some qualitative estimates which establish the relationship between the mean free path and the relief at the interface. For this purpose, we use a simple expression which describes the time (τ) of the scattering of electrons by a surface irregularity in the Born approximation [Eq. (4.55) in Ref. 1]:

$$1/\tau \propto \sum_k < |a(k)|^2 > \left|\frac{\Gamma(k)}{\kappa(k)}\right|^2 . \tag{1}$$

Here $a(k)$ and $\kappa(k)$ are Fourier components of the surface irregularities and the dielectric constant, and $\Gamma(k) \propto n_S$.

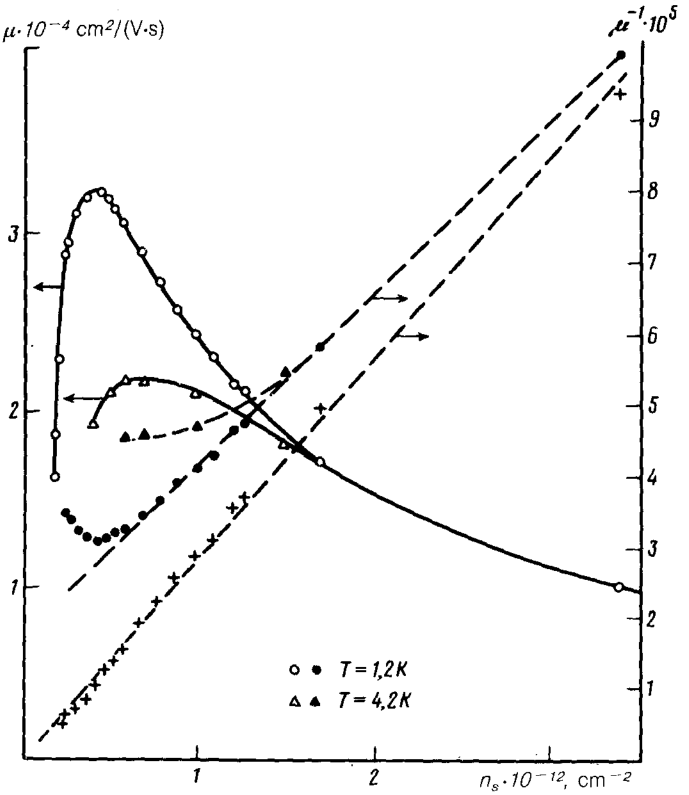

FIG. 3. The mobility μ and its reciprocal μ^{-1} of the electrons of the inversion layer at various temperatures. The plus signs show values of μ^{-1} after subtraction of the component due to scattering by ionized impurities, which is described by $\mu_{\text{imp}}^{-1} \underset{\sim}{\propto} n_S^{-0.6}$, according to Ref. 2.

Most of the scattering in (1) should come from the components with $k \simeq k_F$ (provided, of course, that they are of sufficient amplitude). The reason is that the scattering by larger inhomogeneities is relatively ineffective, since that is a small-angle scattering, and the scattering cross section is small at $k \gg k_F$. In the wavelength interval of interest here, $k \sim k_F = 0.01$–0.02 Å^{-1}, the expression $\kappa(k) \propto q_S/k \sim q_S/k_F$ would apply (q_S^{-1} is the screening length). As we see from Fig. 2, the amplitude of the Fourier components in this region falls off as $a(k) \propto k^{-1(1.5\text{–}2)}$. Substituting these estimates into (1), we find $1/\tau \propto 1/\mu \propto n_S$. We can thus conclude that the irregularities with dimensions on the order of $2\pi/k_F$ are indeed responsible for the electron scattering.

We note in conclusion that the long-period irregularities of the relief should also be taken into consideration in a study of localization processes, level broadening in a magnetic field, etc. We hope that the direct observation of the relief of the Si–SiO$_2$ interface which we are reporting here will serve as a starting point for a corresponding theory.

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