One-dimensional periodic structure on high-index silicon surfaces

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A periodic structure in the form of a system of atomic steps, which may be the cause for the occurrence of superlattice effects on such surfaces, has been observed at the Si-SiO_2 interface on high-index silicon surfaces by using the method of low-energy-electron diffraction.

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It has been reported recently that the electronic inversion layers of high-index silicon surfaces exhibit effects such as channel-conduction anomalies,[1] a sharp anisotropy of IR absorption,[2] etc., which are associated with the presence of any energy gap in the electron spectrum. The existence of an energy gap can now be explained by two alternative models: the valley splitting model[3] and the crystal-potential effect attributable to a new translational symmetry on the high-index surfaces.[4] However, these two models, which are neither complete nor definitive,[5] disregard the real structure of the Si-SiO_2 interface in the high-index silicon surfaces, since such data, based on straightforward experimental investigation, have been unavailable until now.

The purpose of this paper is to report that a one-dimensional periodic structure in the form of a system of atomic steps with identical height h and width L of the terrace, which can be associated with the mentioned effects, is formed at the Si-SiO_2 interface

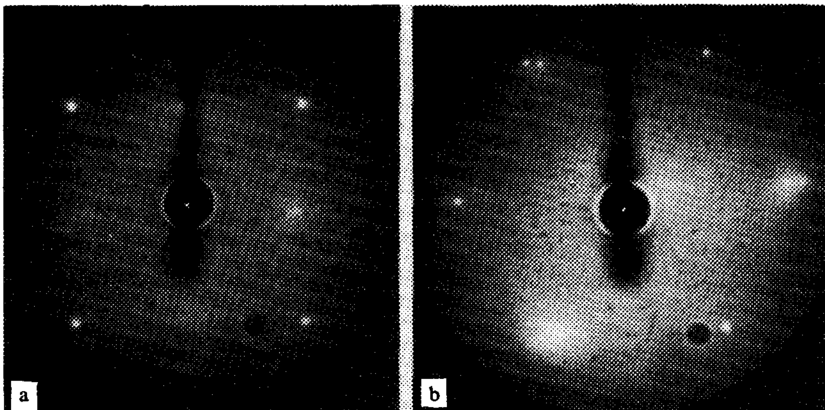

FIG. 1. LEED patterns of the silicon surfaces. (a) A 7°20′ angle with respect to the (100) plane. The electron energy is 53 eV; (b) a 4°40′ angle with respect to the (111) plane. The electron energy is 46 eV.

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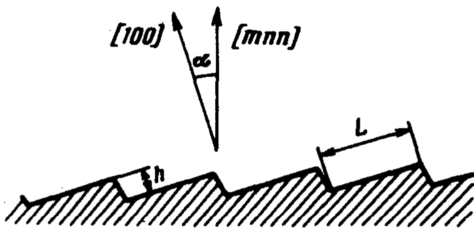

FIG. 2. A system of steps on the silicon surface with a (mnn) orientation under an oxide layer. (α) The slope angle of the surface with respect to the (100) plane.

on the high-index silicon surfaces during the oxidation process. This is indicated by the diffraction patterns of low energy electrons (LEED) from the silicon surfaces, which were deflected at different angles from the (100) and (111) planes after oxidizing the surface by using a standard procedure in dry and moist oxygen at 1050–1150 °C to a depth of about 1 micron and subsequently removing the oxide layer in concentrated fluoric acid.[6] The spots in these LEED patterns (Fig. 1) appear as singlets or doublets, depending on the energy of the primary electrons. The splitting of spots into doublets indicates the presence of ordered systems of atomic steps.[7] The orientations of terraces of the steps are (100) and (111), respectively. The condition for the appearance of a singlet is that the path difference, as a result of scattering from the neighboring terraces, must be equal to an integral number of waves. The ratio of the accelerating voltage for primary electrons V, at which the singlets can be observed, to the height h of the steps, can be obtained from the Bragg law, and for OO mirror reflection due to a normal incidence of the primary beam it has the form

$$V = \frac{37.5 n^2}{h^2},$$

where n is the diffraction order. The height of the steps was determined from the slope of the relations $n^2 = f(V)$ obtained experimentally. The width of the terrace, which was determined from the known angle of slope of the surface and from the height of the steps, was verified from the angular splitting of the spot.[8] The measured height of the steps on the surfaces of the $[01\bar{1}]$ band, which are oriented near the (100) plane, is equal to a twofold interplanar spacing d_{100}, i.e., 2.72 Å, but the height of the steps with a front in the $[11\bar{2}]$ and $[\bar{1}\bar{1}2]$ directions on the surfaces of the same band, which are oriented near the (111) plane, is equal to the interplanar spacing d_{111}, i.e., 3.14 Å. The same result was obtained by performing two and three cycles of oxidation and removal of oxide. As is known, fluoric acid can dissolve the oxide without etching the silicon surface.[9]

The described periodic structure should lead to the appearance of a superlattice potential, which can account for the effects described in Refs. 1–3. Since the height of the steps remains constant when the angle of slope of the surface is changed with repect to the (100) or (111) plane, while the width of the terrace, which determines the period of this potential (Fig. 2), changes, the latter can be changed by properly select-

ing the orientation of the surface.

Petrov[10] was the first person to predict theoretically the possibility of obtaining one-dimensional periodic structures by forming systems of atomic steps on the surface of semiconductors. An estimate of the first energy gap[10] gave a value of 10^{-3}–10^{-2} eV for the described periodic structure, consistent with the results observed experimentally.

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