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# A method for reducing surface roughness during the thermal desorption of silicon

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#### Abstract

An in situ method for inhibiting surface roughening during the thermal removal of the silicon native oxide layer is explored and developed. The method entails depositing a thin sacrificial silicon film at low temperature directly exterior to the native oxide, following which the sample is heated such that the native oxide preferentially reacts with the sacrificial film reducing wafer etching. The results indicate a significant improvement in surface smoothness, from an RMS roughness of 2.70 to 0.84 nm, while leaving an exposed surface which has been demonstrated to be suitable for epitaxial growth.

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### 1. Introduction

As dimensions in ultra-large scale integration metal-oxidesemiconductor technology are decreased, the removal of the native oxide layer becomes an increasingly important process. Silicon (Si) wafers supplied by wafer manufacturers are covered with a protective UV/ozone native oxide layer with a typical thickness between 1 and 2 nm [1]. This native oxide and suboxides are electrically inferior to thermally grown oxides and therefore must be removed prior to device manufacturing. Furthermore, requirements for high quality SiO<sub>2</sub>/Si interfaces also place importance on native oxide removal [2,3]. There currently exists several classifiable methods for native oxide removal: chemical etching, ion milling, and thermal desorption. Chemical etches, such as the plasma and reactive ion etching methods, can cause appreciable surface roughening and involve significant amounts of hazardous materials which can lead to higher concentrations of impurity contaminants on the substrate surface [3,4]. Ion milling is a mechanical technique in which the removal of surface material is accomplished thru ion bombardment of the substrate resulting in a pristine surface, but is characterized by

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several rather nontrivial drawbacks including high cost, complexity, and low throughput [2].

In contrast, the thermal desorption of oxide species utilizing heat treatment in a reduced or non-reactive atmosphere. This method, however, suffers from the thermally driven reaction between constituents of the oxide species and the underlying Si substrate leading to damage to the substrate in the form of surface roughening. This can be explained by examining the following reaction which occurs at approximately 800 °C [5–9]:

$$Si + SiO_2 \Rightarrow 2SiO\uparrow$$
 (1)

As noted from this equation, the stable Si-oxide reacts, consuming bulk Si to produce the unstable SiO reaction product, which is evaporated at these temperatures. This thermally driven chemical reaction for the evaporation of oxide species utilizes bulk Si material in an inhomogenous way such that the resulting substrate surface is characterized by either voids or central silicon columnar structures. The kinetics of this surface damage and the necessary temperature for this reaction to occur is strongly dependent upon the chemical method of oxide formation, its thickness, surface contaminants, and the presence of excess Si atoms near the Si/SiO<sub>2</sub> interface, and has been extensively studied [1,5,8–13]. These changes in surface morphology are dependent on



Fig. 1. 10  $\mu$ m atomic force microscopy images of substrates subjected to (a) normal thermal desorption and treatment thicknesses of 0.28 and 0.43 nm, (b) and (c), respectively.

Eq. (1) and are thus reliant on the presence of  $SiO_2$  within the oxide layer. It is desirable to minimize this surface roughness due to its effect on electron mobility, which is currently accomplished by growing micron-thick homoepitaxial buffer layers after desorption [14].

In this letter, we report a method that acts as a preventative measure to surface roughening by feeding reaction (1) with additional Si, such that the substrate is less damaged. This is accomplished by depositing a very thin Si layer directly onto the native oxide surface prior to thermal treatment. The required thickness ( $t_{Si}$ ) of this thin layer is dependent on both the oxide thickness and its SiO<sub>2</sub> incorporation, and can readily be calculated from Eq. (1) as:

$$t_{\rm Si} = 0.48 \times t_{\rm ox} \times \eta \tag{2}$$

where  $t_{ox}$  is the native oxide thickness, and  $\eta$  is the percentage of SiO<sub>2</sub> in the native oxide, assuming densities of 2.3 and 2.4 g/cm<sup>3</sup> for amorphous silicon and SiO<sub>2</sub>, respectively. Furthermore, the structure and deposition method of the thin film is inconsequential, however the uniformity and coverage is paramount. This method is similar at least in ideology to methods reported previously which utilize a sacrificial material other than Si

[15,16], and similar studies utilizing silicon transported to the native oxide during heating as molecular beam flux [17-19]. However, utilizing Si flux during thermal desorption invokes the problem of depositing silicon on both the oxide surface and exposed wafer portions, resulting in the formation of polycrystalline films with large voids [19]. However, previous works [15-19] have been focused mainly on fundamental studies such as silicon–oxygen bonds breaking dynamics and the activation energy difference for thermal desorption of SiO<sub>2</sub> with and without Si beam, but no study on the surface roughness with and without Si beam has been done. This problem is circumvented in the current method by depositing a solid sacrificial film of calculated thickness prior to heating thus reducing the possibility of excess polycrystalline material following heating.

#### 2. Experimental

For this study, a pulsed laser deposition system with a base pressure of  $\sim 10^{-7}$  Torr was utilized to deposit an amorphous Si layer, as shown by reflection high-energy electron diffraction (RHEED), onto a 2 nm native oxide layer (as measured by ellilpsometry) present on a n-type Si(100) substrate at a temperature of 200 °C. The sample was subsequently heated to a temperature of 850 °C and held at temperature for 30 min, during which time RHEED was utilized to monitor the oxide desorption process. Following this heating, the sample was rapidly cooled to reduce post process surface modification, then removed for ex situ examination under contact mode atomic force microscopy.

#### 3. Results and discussion

Fig. 1(a) shows the typical sample surface morphology obtained from heating an untreated substrate, characterized by large Si structures as a result of reaction (1) etching away at the substrate surface. For a sample treated with a 0.28 nm thick amorphous Si layer prior to heating, the size of these silicon structures is increased by a factor of  $\sim$ 2, as shown in Fig. 1(b). Fig. 1(c) illustrates a sample which has been subjected to a 0.43 nm thick Si film prior to heating. The resulting surface morphology is significantly smoother as a result of being subjected to the discussed treatment. For all three samples



Fig. 2. Height profiles obtained from AFM scans for samples subjected to treatment thicknesses 0.0, 0.14, 0.28, 0.24, and 0.43 nm demonstrates the film thickness effect on the resulting surface morphology.

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