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Mechanism for Si island retention in buried SiO_2 layers formed by oxygen ion implantation

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The density of silicon islands trapped in buried SiO_2 layers produced by the implantation of oxygen into (001)Si substrates is monitored by atomic force microscopy for the oxygen dose range just above that required for continuous oxide formation. In addition to an exponential increase in the Si island density with oxygen dose, the regularly shaped remnants of an SiO_2 phase with a reduced HF etch rate were found. The formation of this additional oxide phase as a result of enhanced internal pressure inside the Si crystal is proposed to account for the retention of Si islands in the buried oxide. © *1997 American Institute of Physics.* [S0003-6951(97)00141-1]

Silicon-on-insulator structures produced by low-dose ($D<0.5\times10^{18}$ cm^{-2}) oxygen ion implantation (SIMOX) are superior to the standard ($D=2\times10^{18}$ cm^{-2}) SIMOX structures in terms of production cost and heat conductivity of the buried oxide (BOX). However, BOX layers of acceptable insulating quality are formed only within a narrow dose range around $D_{opt}=0.35\times10^{18}$ cm^{-2}.[1–3] Below D_{opt} no continuous BOX layer is formed, while $D>D_{opt}$ providing more oxygen leads, curiously, to the incorporation of Si islands into the BOX, thus degrading the electrical properties.[1] We will show that the density of Si islands in the SIMOX BOX increases exponentially for $D>D_{opt}$, and correlates with the formation of oxide inclusions having a reduced HF etching rate. The latter appear to originate from oxygen precipitation, not only in the form of amorphous SiO_2 but, also as coesite-like ribbons which trap Si islands inside the BOX.

The samples were produced by the implantation of 200 keV O^+ ions into (001)Si substrates at 590 °C with $D=(0.39-0.53)\times10^{18}$ cm^{-2}, followed by post-implantation annealing (PIA) in Ar+0.5% O_2 at 1310, 1330, or 1 350 °C for 4, 6, or 8 h. The BOX thickness was in the range of 77–115 nm. Subsequently, the top Si layer was removed, whereupon the exposed BOX layer was analyzed by atomic force microscopy (AFM) in a constant force mode after stepwise HF etchback.[4] The revealed inhomogeneities were additionally exposed to Si-selective etchant (KOH:H_2O at 60 °C) to distinguish between Si inclusions and the slowly etching SiO_2 phase. For electrical measurements, circular (∅≅0.8 mm) Au electrodes were evaporated onto the BOX.

AFM images of the sample surface after BOX removal (the sample becoming hydrophobic) are shown in Fig. 1 for three implantation doses and 8 h PIA at 1350 °C. The density of protrusions per unit area increases nearly exponentially with the dose for all three PIA temperatures [Fig. 2(a)]. This suggests a common protrusion generation mechanism. Shortening of the PIA time to 4 or 6 h was found to cause a significant increase in the density of protrusions ($>10^9$ cm^{-2} for $D=5.1\times10^{17}$ O^+ cm^{-2} and 4 h anneal at 1310 °C). Apparently, the protrusions are formed during the initial part of the PIA, and then slowly anneal as the duration of PIA increases. The mean protrusion height in the BOX annealed for 8 h is shown as a function of O^+ dose in Fig. 2(b). It is seen that the average height of the protrusions is only slightly less than the BOX thickness indicated by a solid line. In the samples annealed at 1330 and 1350 °C the protrusion height decreases with dose reduction, which suggests ''dissolution'' of the protrusions. Also shown in Fig. 2(b) (solid symbols) is the electric breakdown field of the BOX. Comparison indicates that the degradation of the BOX quality at $D>D_{opt}$ correlates with the presence of HF-resistant inclusions, pointing, in turn, to the presence of conductive silicon.

Indeed, there is evidence for the latter. On the samples with higher D ($\sim0.53\times10^{18}$ O^+ cm^{-2}) the Si portions of the inclusions are revealed by KOH etching performed after the removal of the upper 60 nm of the 110-nm-thick BOX layer. After the HF etch AFM shows regularly shaped inclusions (crystal) aligned with ⟨110⟩ directions of the Si substrate [Fig. 3(a)], which are similar to the Si islands observed by electron microscopy in the SIMOX BOX prepared at $D>D_{opt}$.[2,5] The subsequent KOH etch reduces the number of visible protrusions leaving in some places deep etch pits [see, e.g., *A* in Fig. 3(b)] reaching down to the Si substrate surface thus indicating the presence of Si. KOH etching, however, leaves some of the protrusions unattacked, indicating their oxide nature. In many cases these oxide protrusions have a rectangular shape with the sides aligned with the ⟨110⟩ directions of the Si substrate [see, e.g., *B* in Fig. 3(b)]. The largest amount of these slowly etched (both in HF and KOH) oxide particles are observed in samples with a high density of HF-resistant protrusions. It thus appears that the presence of Si inclusions in the BOX correlates with the presence of the low etch-rate oxide platelets.

With prolonged HF etch more and more protrusions are removed from the sample surface leaving some remnants at the BOX/Si interface. Two examples are shown in Fig. 4 for samples both implanted with 0.39×10^{18} O^+ cm^{-2} and an-

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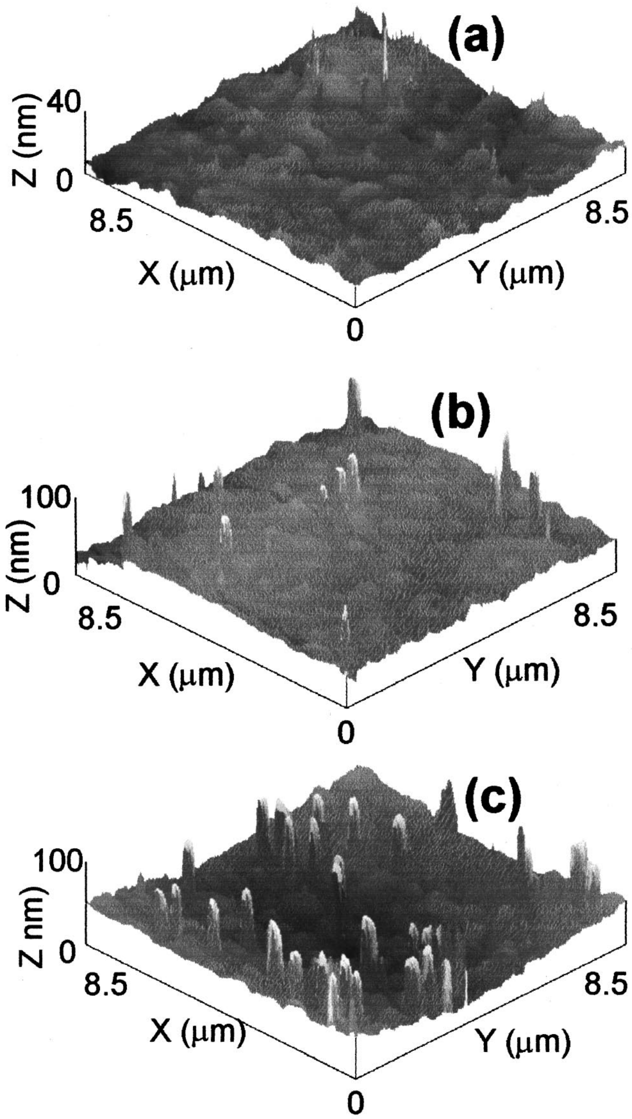

FIG. 1. AFM images (three dimensional view) of the Si substrate surface (after BOX etch-off) of SIMOX structures implanted with (a) 0.39, (b) 0.49, and (c) 0.53×10^{18} O^+ cm^{-2}, all annealed at 1350 °C for 8 h.

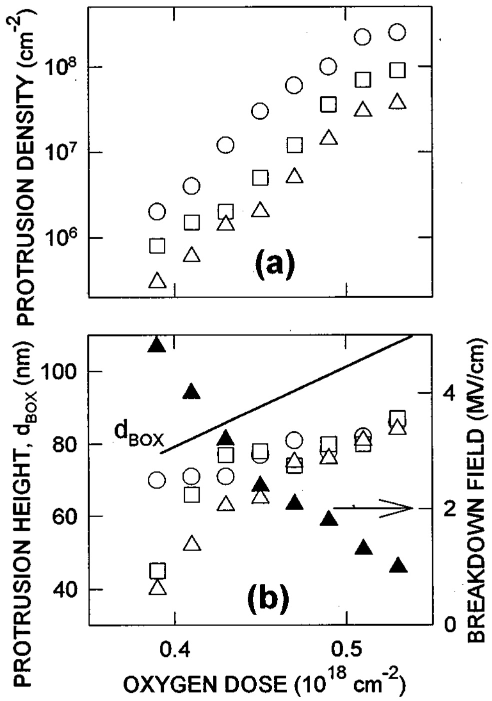

FIG. 2. Density of protrusions (after BOX removal in HF) with (a) a height larger than 40 nm and (b) the mean height of the protrusions as a function of O^+ dose in BOX layers annealed at 1310 (○), 1330 (□), and 1350 °C (△) for 8 h. In panel (b) the solid line represents the increasing BOX thickness (d_{BOX}) with implantation dose; the solid symbols show the electric breakdown field for the samples annealed at 1350 °C.

nealed at 1310 or 1350 °C. The former sample shows rectangular features aligned, again, along ⟨110⟩ substrate directions, composed of SiO_2, as revealed by their gradual elimination in HF. The second sample, in which ''dissolution'' of the inhomogeneities takes place, shows doublets (A), triplets (B), and quadruplets (C) of SiO_2 platelets elongated along the ⟨110⟩ direction [Fig. 4(b)]. Noteworthy in this image is the inhomogeneity of larger size (D) which appears to have a capping of HF resistant silicon. The regular shape of the oxide particles and their orientation in registry with the host Si crystal indicate the possibile epitaxial relationship between the slowly etching SiO_2 phase and the Si substrate.

The exponential increase of the protrusion density $N(D)\propto\exp(D)$ [see Fig. 2(a)] indicates that the formation of the Si islands is driven by the formation of the inclusions themselves: $dN/dD\propto N(D)$. A significant related observation coming from electron microscopy analysis indicates that incorporation of the Si islands in the BOX for $D>D_{opt}$ correlates with the appearance, in addition to the conventional SiO_2 precipitates, of ribbonlike oxide bands clearly visible near the final stages of the PIA.[1,2] The incorporation of Si islands may thus be pictured as a result of the oxide ribbon growth which, in turn, is driven by the volume increase associated with the Si→SiO_2 transformation. The latter results in the compression of the adjacent Si crystal,[6,7] and the ribbon formation can thus be pressure driven. Therefore, in addition to Si inclusions in the BOX and the oxide phase with reduced HF etching rate, this observation indicates that for $D>D_{opt}$ the oxide precipitation occurs in different SiO_2 phases. Two types of oxide precipitates are known to exist in Czochralski grown Si crystals: amorphous SiO_2 platelets with a (100) habit plane and ⟨110⟩-aligned coesite ribbons.[7,8] The formation of coesite, a high pressure dense SiO_2 polymorph,[9] is favored by a high O oversaturation and a low impurity content in the Si—conditions met in the SIMOX material.[7] Earlier we identified coesitelike oxide inclusions in standard-dose SIMOX BOX, indicating a polymorphic oxide transition.[4] Although the present data do not provide crystallographic identification, coesite appears to be the most probable candidate for the pressure-driven oxygen precipitation phase in Si.

A hypothetical scenario may be inferred from the present observations as follows. Initially, numerous amorphous SiO_2 precipitates form a discontinuous oxide; in the top silicon layer a high density of threading dislocations is produced allowing a partial accommodation of the internal strain. Next, upon the coalescence of the oxide precipitates into a continuous band, the dislocation density rapidly decreases[1] causing an increase of internal compressive stress (pressure)

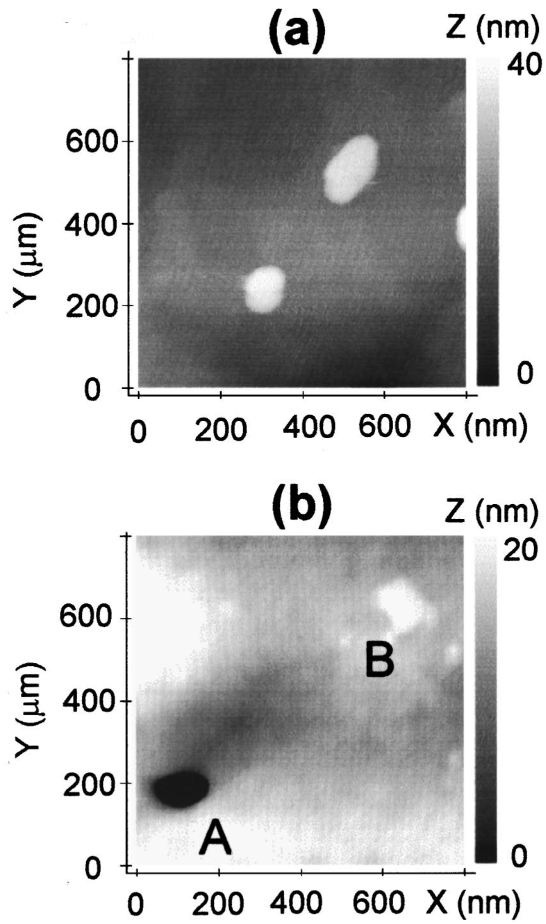

FIG. 3. AFM images (top view) of a BOX layer (a) thinned down from 110 to 50 nm and (b) subjected subsequently to a KOH etch in the structure implanted with 0.49×10^{18} O^+ cm^{-2} and annealed at 1330 °C for 8 h. Axis orientation: $x\|[100]$, $y\|[010]$, $z\|[001]$.

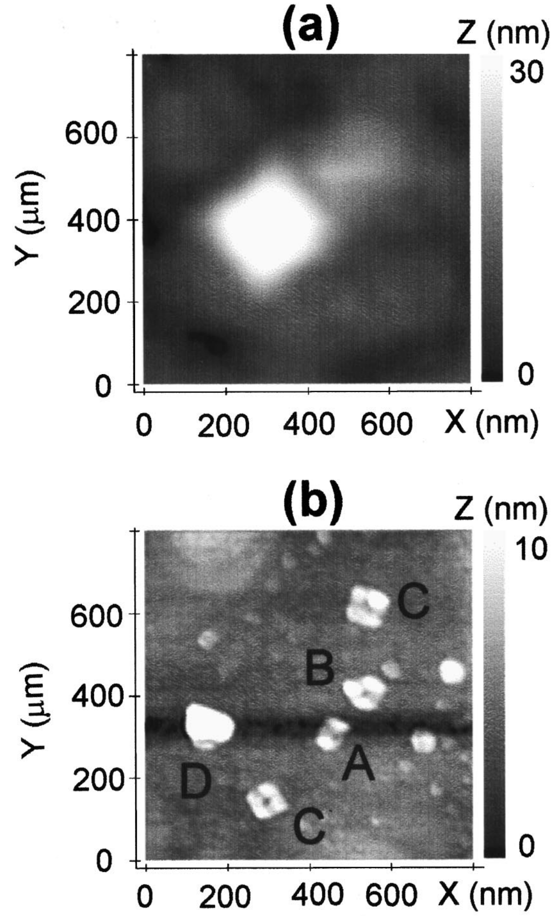

FIG. 4. AFM images (top view) of the Si substrate surface after BOX removal for the structures implanted with 0.39×10^{18} O^+ cm^{-2} and annealed at (a) 1310 and (b) 1350 °C for 8 h. Axis orientation: $x\|[100]$, $y\|[010]$, $z\|[001]$.

in the buried oxide and surrounding silicon. If not all of the implanted oxygen has yet been collected in the BOX, additional precipitation of SiO_2 ribbons occurs locking Si islands into the SiO_2 and blocking Si outdiffusion. The pressure driven oxide precipitation constitutes a mechanism with a positive feedback with respect to the implanted O^+ dose, thus explaining the results shown in Fig. 2(a).

Evidence of the role of the internal pressure postulated in our model comes from two approaches: First, the sharp increase in the density of Si inclusions in the BOX for increasing D should correspond to a decrease in the density of dislocations in the top Si layer. Indeed, this behavior has been observed: in the samples annealed at 1350 °C for 8 h the density of dislocations detected by the selective etching technique decreases from 2×10^7 to 2×10^5 cm^{-2} as the O^+ dose increases from 0.39 to 0.45×10^{18} cm^{-2}.[10] Second, the application of external pressure, known to influence oxygen precipitation in silicon,[11] may affect the incorporation of Si islands into the BOX. This very effect is reported elsewhere:[12] the application of a capping layer during PIA leads to substantial improvement of the BOX insulating properties and reduces the density of Si clusters in the oxide. The AFM analysis of the samples studied in Ref. 12 indicates that the primary structural effect of the capping layer consists of a reduction in the density and height of inhomogeneities as revealed by HF etching of the BOX. Thus, the redistribution of internal strain in the silicon favorably affects the incorporation of Si island in the BOX and may improve the quality of SIMOX structures.

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