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Thermally-Induced Structural Changes of Ultrathin Silicon-on-Insulator Structure

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1. Introduction

Ultrathin silicon-on-insulator (SOI) appears to be a key structure for CMOS LSIs and for Si future devices such as single-electron and a-few-electron dot devices [1]. However, if the top Si layer is thinner than several tens nm, the layered structure becomes unstable under critical annealing conditions. In fact, Si agglomeration occurs by thermal treatment in UHV, being commonly observed for SIMOX [2] and bonded SOI wafers [3].

Previously, we have reported thermal agglomeration (islanding) of top (100) Si in ultrathin bonded SOI and significant ordering of the islands [3]. However, mechanism of the island formation and the ordered alignment has not been clarified yet.

In this paper, after a brief review of the islanding phenomenon, we propose a strain-induced diffusion (SID) mechanism, as an extension of theoretical consideration by Ono *et al.* [2] to account not only for islanding but also ordering.

2. Agglomeration of Top Si Layer

A bonded SOI substrate with about 10-nm-thick (100) top Si was used. The sample was chemically cleaned and then loaded into a UHV chamber. In the UHV chamber, the sample was heated to elevated temperatures around ~900℃ for 10 s. After unloading the sample to the air, AFM and XPS observations were performed.

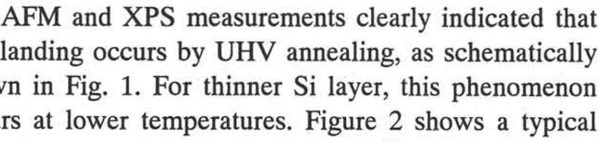

Fig. 1. Schematic view of the SOI sample before and after UHV annealing.

AFM and XPS measurements clearly indicated that Si islanding occurs by UHV annealing, as schematically shown in Fig. 1. For thinner Si layer, this phenomenon occurs at lower temperatures. Figure 2 shows a typical AFM image of the surface after 900℃ annealing. The AFM image indicates that the Si agglomeration accompanies square-shaped holes, whose sides run nearly in the <011> directions. In the holes, Si islands were formed with an ordered alignment mostly in the <013> directions. It is evident that the bottom surface of the hole is the buried oxide (BOX) surface. Furthermore, Si islands near the center of the hole are surrounded by facets of {111}, {113} and {100} planes.

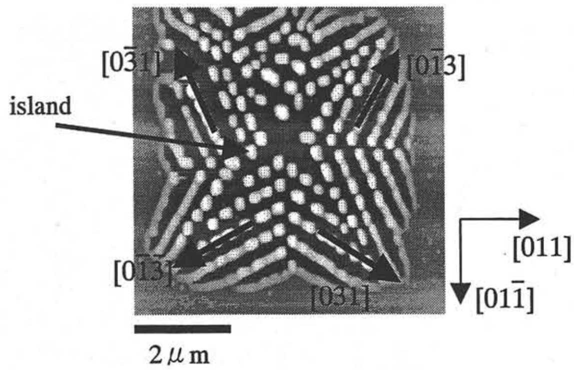

Fig. 2. AFM image of a 7-nm-thick (100)-bonded SOI surface after heating at 900℃ for 10 s in UHV.

3. Strain-Induced Diffusion (SID) Mechanism

In order to account for both islanding and ordering phenomena, we have applied "strain-induced diffusion (SID) mechanism", which was developed by Ono *et al.* [2] for hole opening of top Si layer in a SIMOX wafer. They ascribed the hole opening to enhanced local stress due to thickness fluctuation; the local enhanced stress causes an outgoing diffusion flux of surface Si atoms, resulting in local thickness reduction and thickness increase at the neighboring area. In this work, we have found that the SID mechanism can also account for island formation with almost a periodic spacing (a basis of ordering), in which hole and island formation successively occurs as propagation of a wave.

In the present work, we assume that a local area on the surface is accidentally thinner than the other area and the corresponding local stress is enhanced. Then, the surface flux of defects J can be given by

$$J = -a\left(x_0 D_d / kT\right)\nabla\sigma \qquad (1)$$

where a is the size of the surface atom, x_0 the equilibrium fraction of surface defect, D_d the diffusion coefficient of surface defect like vacancy, k the Boltzmann constant, and σ the stress. From above equation, the gradient of σ generates mass flow, therefore, the reduction rate in Si thickness $\dot{Z}$ can be expressed as

$$\dot{Z} = -\Omega\nabla \cdot J \qquad (2)$$

where Ω is the volume of a surface atom. The solution of eq. (2) has the form that Si thickness decreases near center of the stress. But, this thickness change automatically causes a thickness increase (protrusion formation) at the surrounding area because of mass balance. Therefore, this staggered change of Si thickness propagates outward from the center of the stress.

Figures 3(a)-3(d) show time-evolutional cross-sections, which are simplified as a one-dimensional system and Figs. 4(a) and 4(b) show experiments.

At the initial stage, as shown in Fig. 3(a), it is assumed that the local stress is enhanced in the thinner region (Region A). As a result, the Si atoms are exhausted by outdiffusion of Si to Region B, and BOX surface is exposed, as shown in Fig. 3(b). Now, the first hole is opened. Then, accumulation of Si atoms in Region B will generate a stress difference (a non-zero gradient of σ) between Region B and Region C. As a consequence, mass transport occurs again, so that the first islands are formed (Fig. 3(c)). In this way, many islands are successively formed, as shown in Fig. 3(d). Inter-island distance is expected to be almost uniform, since the distance is determined primarily by the Si (or vacancy) diffusion constant.

To confirm this, the AFM surface images (Fig. 4) were compared with the model. It can be recognized that Figs. 4(a) and 4(b) correspond to Figs. 3(b) and 3(c), respectively, when the comparison is focused only on one-dimensional <100> scheme. Wavy shape in the outer region, which is predicted by the model, is also observed.

Thus, island formation process and ordered alignment of Si islands can be basically explained by this simple mechanism. However, in order to explain the observed two-dimensional ordering, i.e., the ordered alignment in the <013> directions, it is necessary to take into account thermally stable facet surfaces such as {111}, {113}, and {100} planes. The facet formation effect must be closely related to the ordered alignment in the <013> directions. The mechanism in details will be further studied.

4. Conclusions

A mechanism based on the strain-induced diffusion has been qualitatively studied to explain the structural changes of ultrathin SOI. As a result, both of islanding and ordered alignment have been successfully explained. More precise modeling should include facet formation effects.

Acknowledgments

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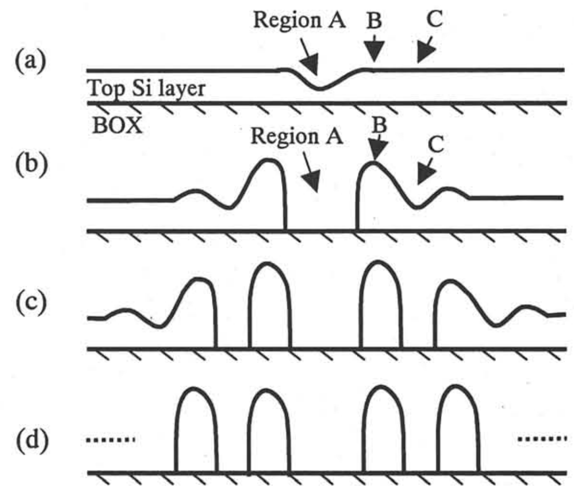

Fig. 3. Schematic illustrations of time-evolutional cross-sections based on SID mechanism.

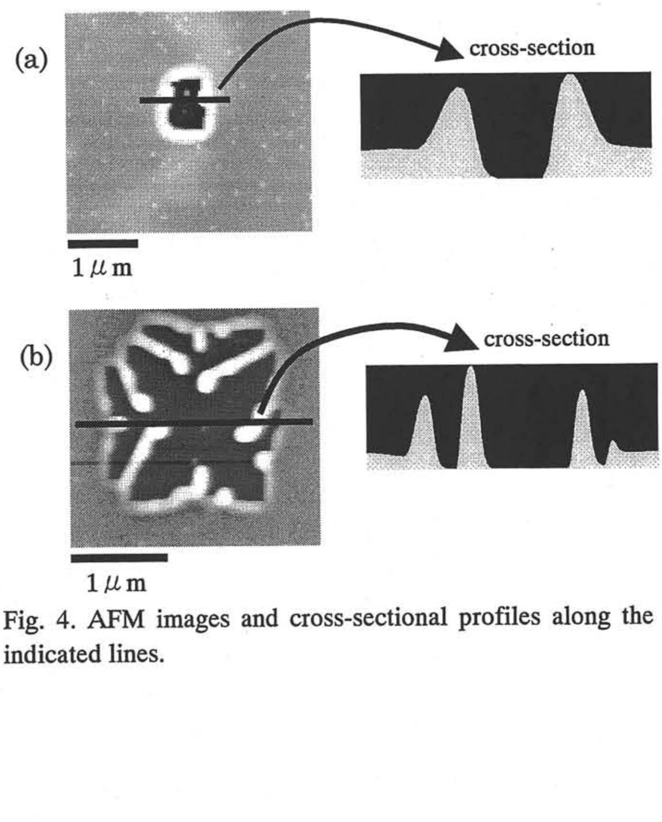

Fig. 4. AFM images and cross-sectional profiles along the indicated lines.