

Flattening of micro-structured Si surfaces by hydrogen annealing

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Abstract

We report atomic scale flattening of surfaces of microstructures formed on Si wafers by furnace annealing. To avoid thermal deformation of the fabricated structures, advantage was taken of hydrogen annealing, which enables us to decrease the relaxation rate of Si surfaces due to surface hydrogenation. We examined cross-sectional shape and sidewall morphology of 3 μm deep trenches on Si(0 0 1) substrates after annealing at 1000 °C under various H₂ pressures of 40–760 Torr. We successfully formed Si trenches with flat surfaces composed of terraces and steps while preserving the designed trench profile by increasing H₂ pressure to 760 Torr.

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1. Introduction

Fabrication techniques of precisely shape-controlled microstructures are desired for developments of a wide range of devices; for example, semiconductor devices, micro-electro-mechanical systems (MEMS), photonic crystals, and various nano-devices. Especially with silicon devices, various types of three-dimensional devices, such as trench metal-oxide-semiconductor field effect transistors (MOSFET) [1] and fin-FET [2] have attracted increasing interest. With the downscaling of microstructures, an atomic level flatness for their surfaces is required. Thermal annealing shows promise for obtaining atomically flat surfaces. It is well known that Si wafer surfaces are atomically flattened and terrace-and-step structures are formed by annealing at above 1000 °C under UHV conditions or under various gas atmospheres [3–6]. However, when high temperature annealing is applied to a micro-structured Si substrate, the fabricated microstructures decay or are significantly deformed by thermal relaxation because they are thermodynamically unstable [7–14]. This problem is more serious for smaller structures, since the thermal relaxation times become shorter.

In this study we report a method that enables surfaces of microstructures formed on Si substrates at an atomic scale to be thermally flattened without structural deformation. Recently, we reported our investigations into the shape transformation of micron-sized deep trenches fabricated on Si(0 0 1) substrates by furnace annealing in various gas ambients [10–14]. When a Si trench is annealed at sufficiently high temperatures above 1000 °C, the trench shape is largely deformed, though terrace-and-step structures appear on the surface. Moreover, it has been shown that, as annealed in H₂ gas ambient, the rate of shape transformation decreases with increasing H₂ pressure [12]. We consider that the effect from H₂ pressure originates from the hydrogenation of the Si surface, since there is both experimental [15] and theoretical [16–18] evidence that the surface diffusion of Si adatoms is suppressed on H-terminated Si surfaces. In this work, aided by the advantage of H₂ annealing, which enabled us to control the surface diffusion, we have successfully flattened a surface while preserving the designed shape of the microstructure.

2. Experimental procedure

In the experiment we used phosphorus-doped n-type CZ Si(1 0 0) substrates (2.0–3.0 $\Omega\text{ cm}$), on which micron-sized trenches along the [1–10] direction were fabricated by

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anisotropic reactive ion etching (RIE) with a SiO_2 mask. The width, depth, and length of the trenches are $0.7\ \mu\text{m}$, $3.0\ \mu\text{m}$, and $3.0\ \text{mm}$, respectively. The trenches formed by reactive ion etching slightly taper from the top to the bottom, and the sidewall surface deviates by about 1° from the $\{1\ 1\ 0\}$ plane. After trench etching, the oxide mask was removed by dipping in HF solution, and the surface was cleaned by the standard RCA cleaning procedure. Samples were then annealed at 1000°C in H_2 gas ambient at pressures of 40–760 Torr using a ramp furnace. We evaluated the trench profiles by scanning electron microscopy (SEM), cleaving samples normal to the trench direction. We also observed the morphology of the trench sidewall by atomic force microscopy (AFM), by cleaving the sample at the center of the trench along the trench direction.

3. Results and discussion

Fig. 1 shows a typical cross-sectional profile and sidewall morphology of as-etched trenches. The ion-etched surfaces are rough with ditches introduced by anisotropic RIE; the root-mean-square (RMS) roughness and peak-to-valley height measured from the AFM image are 1.7 and 10 nm, respectively.

Fig. 2 shows typical results of H_2 annealing at 1000°C under reduced pressure conditions of 40 (Fig. 2(a and b)) and 100 Torr (Fig. 2(c)). From the SEM images showing the cross-sectional shapes of the trenches, we can see that the trench corners are rounded by H_2 annealing. The AFM images show the surface morphologies of the sidewalls of the trenches. These AFM images were obtained at mid regions of the sidewalls of the $3\ \mu\text{m}$ deep trenches. The left and right hand sides on the images correspond to the bottom and the top corner sides, respectively. On all sidewall surfaces after H_2 annealing, the rough sidewall morphology on as-etched trenches as shown in Fig. 1 are

completely removed after H_2 annealing, and structures composed of atomic steps and $(1\ 1\ 0)$ terraces are observed. However, we can see that a large corrugation appears on the sidewall after annealing. On the sidewall surface treated in 40 Torr H_2 for 30 s, large $(1\ 1\ 0)$ regions with curved single steps are formed near the top and bottom of the trench. After 3 min annealing in 40 Torr H_2 , the corrugation becomes larger, and a groove structure is formed (Fig. 2(b)). Previously we have shown that, during 1000°C annealing in 40 Torr H_2 , such structural changes occur on the sidewall surfaces spontaneously, involved in rounding of the trench corners [14]. The formation of the corrugated structures on the trench sidewalls is due to the large surface atom currents induced by the relaxation of the trench corner. Both SEM and AFM images for 3 min annealing in 100 Torr H_2 shown in Fig. 2(c) are closer to the results by annealing for 30 s in 40 Torr H_2 (Fig. 2(a)) than those for 3 min in 40 Torr H_2 (Fig. 2(b)). This result shows that the rate of shape evolution decreases under higher H_2 pressures.

Fig. 3 shows the structure of the trench as H_2 pressure during annealing increases up to 760 Torr. The annealing duration is 3 min. Comparing the cross-section SEM image shown in Fig. 3 with that of the as-etched trench (Fig. 1(a)), shape deformation cannot be distinguished within the spatial resolution of the SEM. On the AFM image of the sidewall after 760 Torr H_2 annealing, no surface corrugation can be found, as seen in Fig. 2. Fig. 4 shows a magnified AFM image of the sidewall surface after annealing in 760 Torr H_2 , clearly showing the formation of a structure composed of steps and terraces. The steps ascend from the top towards bottom of the trench. Most steps are single layer high, and the average separation between steps is estimated to be about 20 nm. Since this step separation corresponds to about 1° deviation from $(1\ 1\ 0)$, the observed step configuration is consistent with the slightly tapering profile

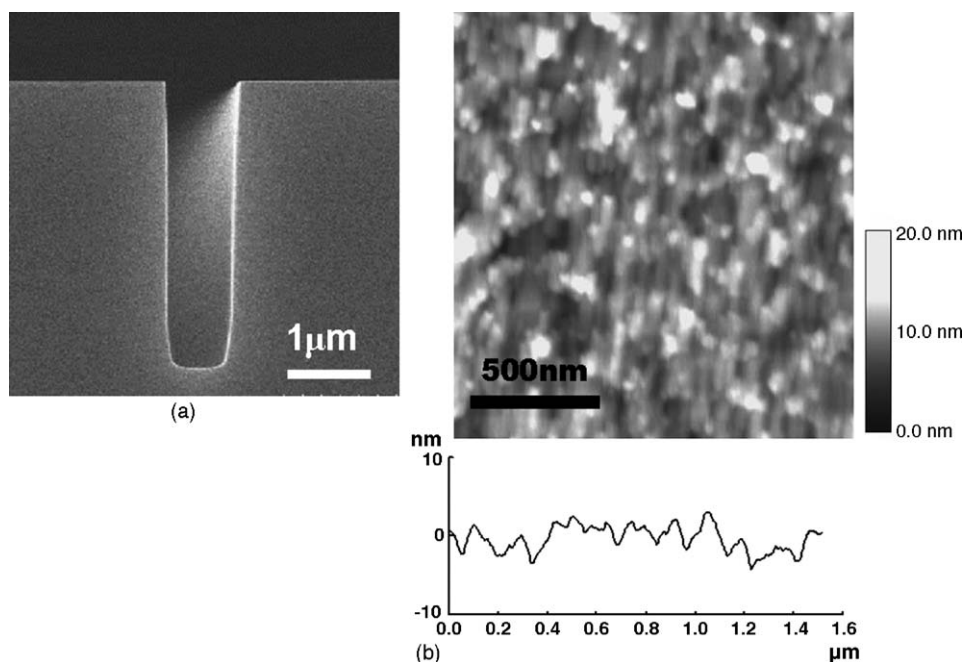


Fig. 1. Structure of a trench fabricated on a $\text{Si}(0\ 0\ 1)$ substrate by reactive-ion etching. (a) A SEM image showing the cross-sectional trench profile. (b) An AFM image of the sidewall surface and the horizontal AFM cross-section.

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