Effect of Mechanical Stress on Characteristics of Silicon Thermal Oxides

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The characteristics of oxides grown on silicon wafers under external mechanical stress were studied. It was found that the SiO₂ films grown under external compressive stress had a decreased etching rate. From capacitance–voltage (*C*–*V*) measurements, it was observed that a tensile sample had a reduced interface state density, while that of a compressive sample was increased. [DOI: 10.1143/JJAP.41.81]

KEYWORDS: oxides, mechanical stress, interface state density

As silicon technology continues to be promoted and the feature size of devices is continuously scaled down to the deep sub-quarter-micrometer regime, the trend of scaling and integration has brought attention to the fundamental and physical limits of devices. Therefore, the issue of reliability of mechanical stress becomes critical since the devices have become much more complex in terms of geometry and process steps. Many defects and failures of integrated circuits can be traced ultimately to mechanical stress that occurs at various process steps.¹⁾ Mechanical stress generally occurs due to the deposition of different kinds of films such as SiO₂, poly-Si, Si₃N₄ and metal electrodes. The structure of devices at sharp corners and interconnect edges exhibits high stress as well. Mechanical stress causes not only the dislocation of the silicon substrate, cracking or failure of thin films, but also the degradation of electrical characteristics. It has been proposed that compressive and tensile stresses from temperature nonuniformity or mechanically applied forces may affect oxidation kinetics and rates,^{2–4)} and there is still interest in studying the mechanical stress effect on the electrical characteristics of devices further. In this work, we report the stress effects based on etching rate and interface trap density data.

P-type, (100)-oriented, 3-inch silicon wafers with a resistivity of 1–10 Ω·cm were used in this experiment. After standard cleaning followed by HF (H₂O : HF = 50 : 1) dip and DI water rinse, the wafers were oxidized many times in a furnace with a dilute oxygen flow (O₂ : N₂ = 1 : 1) at 900–950°C, at 1 atm. The wafers were placed vertically on a quartz boat. A small slice of quartz about 20 g was placed across the middle of two adjacent wafers so that the two adjacent wafers sustained compressive and tensile stress, respectively, as shown in the inset of Fig. 1. After oxidation, the oxide thickness was measured using an automatic-scanning ellipsometer with an accuracy of ±5 Å. No post-oxidation annealing was carried out on the grown oxides. MOS capacitors 150 μm × 150 μm were fabricated by photolithography and wet etching. Evaporated aluminum films were used as gate electrodes and also as back ohmic contacts after back oxide removal. No post-metallization annealing was carried out on the samples for electrical measurements in this work.

The SiO₂ films of our samples were repeatedly dipped in 1% dilute HF solution and the thickness of the remaining oxides was measured using an automatic-scanning ellipsometer at 5 mm pitch. Figure 1 shows the etching results of

Fig. 1. Etching results and average etching rates of bulk and strained-layer oxides for compressive, tensile, and reference samples. The inset showed the experimental setup.

oxide thickness versus etching time for the above three samples. It is noted that each value of oxide thickness in the figures is taken as the average thickness of measured points by the ellipsometer over a central 2 cm² area of silicon wafers. From the figures, one can see the decreased etching rates of three samples when the oxide thickness is less than approximately 20 Å. The etching rates of bulk oxides and the strained layer are also calculated, as shown in this figure. From Fig. 1, we can see that all three samples have a strained-layer oxide near the Si–SiO₂ interface.^{5,6)} The etching rates of the bulk oxides of the three samples are nearly equal to 18–19 Å/min. However, the etching rate of strained layers for the compressive sample is different from the others, i.e., the etching rate of the compressive sample is slightly lower than that of the reference or tensile sample. This can possibly be explained by the following. Because there is an approximate 125% volume expansion from Si to SiO₂ during thermal oxidation,^{7–13)} all the SiO₂ films grown on silicon substrates are observed in a state of compressive stress, except when the oxidation temperature is as high as about 1100°C.^{14,15)} When the silicon substrate is oxidized under tensile stress, the SiO₂ film grows downward freely, and is observed to have a high oxidation rate. The SiO₂ film on a tensile Si substrate is likely to have the same strained-layer structure as that of the reference sample since it is grown without constraint, as shown by our etching results. However, when SiO₂ film is grown on a silicon substrate

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under compressive stress, the mismatch of lattice constants between SiO_2 and Si will be enhanced. Therefore, it is possible to form more Si dangling bonds at the Si/ SiO_2 interface to create a Si-rich suboxide layer. Thus, the etch rate of such oxides should be decreased.

The interface state density is the most important factor determining the quality of SiO_2 films. High-quality SiO_2 films must have low interface state density for use as gate dielectric material. Midgap interface trap density (D_{itm}) and flat-band voltage (V_{fb}) were extracted from the high- and low-frequency capacitance–voltage (C – V) curves. A mechanism based on experimental results was proposed by Ma and Hook^{16,17} in which interface trap generation could be explained by the broken bond model. The broken bond model suggests that a strained Si–O or Si–Si bond broken by capturing an incident carrier tends to propagate toward the Si– SiO_2 interface due to the gradient of bond strain, which is found to be present within an interfacial region of about 3 nm. This will finally result in interface-trap generation. Since larger strains exist at the Si– SiO_2 interface for thicker oxides, more traps are generated at the Si– SiO_2 interface. Ma¹⁶ observed that D_{itm} increases with oxide thickness. Our control samples with different thickness are also in agreement with the experiments and model proposed by Ma.¹⁶ Figure 2 compares the D_{itm} for oxides grown under different stress conditions. The inset of Fig. 2 shows the low-frequency C – V curves for gate oxides grown on silicon substrates with compressive, tensile, and no stress. The C – V curves are measured on devices within a central 1.5 cm^2 area of silicon wafers. It is naturally expected that D_{itm} increases with oxide thickness. However, in our work, the $80 \text{ \AA}$ oxides of the compressive sample have higher D_{itm} than the $87 \text{ \AA}$ oxides of the reference sample (with no applied stress),

Fig. 2. Comparison of D_{itm} for oxides grown under applied compressive, tensile, and no stress. The inset shows the low-frequency capacitance (C – V) curves for oxides grown on silicon substrates under different stresses.

while the $106 \text{ \AA}$ oxides of the tensile sample have lower D_{itm} than those of the reference sample. Clearly, the results of Ma and those of our control samples are different. This can be explained by the fact that the D_{itm} is affected by the stress applied on the Si substrates. It is believed that our experimental results are in complete contrast to the well-accepted broken bond model; the difference in D_{itm} is mainly caused by the applied mechanical stress. Based on the physical model of the Si– SiO_2 interface and the discussions in our previous studies, it is suggested that a tensile stress on the silicon surface will enlarge the atom spacing of silicon and the oxygen atoms become more easily diffused and connect more easily to the dangling bonds. However, a compressive stress will shorten the atom spacing of silicon and leave a greater numbers of dangling bonds at the Si– SiO_2 interface during oxidation. Therefore, it is reasonable to consider that the D_{itm} of a tensile sample is lower than that of a compressive one.

Silicon oxidation with externally applied mechanical stress is useful in studying stress-related problems. In this work, the effects of externally applied mechanical stresses on the characteristics of silicon thermal oxides have been investigated. This is important in the investigation of oxide quality under stress especially for next generation silicon technology.

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