Oxidation Simulation of Silicon Nanostructures on Silicon-on-Insulator Substrates

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Oxidation of silicon nanostructures fabricated on SOI substrates (pattern-dependent oxidation = PADOX) is a key process in the fabrication of silicon single-electron transistors (SETs) [1]. The characteristic features of PADOX are mainly determined by the oxidation-induced strain and by the oxidation from below due to oxygen diffusion through the buried oxide, which pushes the silicon on the oxide upward [2]. However, commercial oxidation simulators cannot reproduce the upward movement of the silicon. In this paper, we present a two-dimensional simulation of PADOX of silicon nanostructures fabricated on SOI substrates.

In order to take into account the features of PADOX, a transition region in which silicon is converted to oxide is set up at the silicon/oxide interface (Fig. 1) [3]. The strain due to oxidation-induced volume expansion is applied to the transition region as a dilational strain, and this expansion pushes the silicon on the oxide upward. The transition region method has been used for the simulation of LOCOS [4]; however, it has not been applied to PADOX. According to the expansion, strain development are solved and stress-strain are analyzed. The calculation flow is shown in Fig. 2. In addition, the silicon oxide and the transition layer are treated as viscoelastic solids, and the stress-induced reductions of oxidation reaction, oxygen self-diffusion in the oxide, and oxide viscosity are taken into account.

The shapes of silicon and oxide after dry oxidation at 1000 and 1100 °C were simulated and compared with the cross-sectional TEM images (Fig. 3: 1100 °C). The initial silicon line has a width of 50 nm and a height of 30 nm with an oxide mask. The shapes of the silicon and oxide after oxidation were satisfactorily reproduced, which suggests that the oxidation-induced strain is properly taken into account in the simulation. The oxidation-induced strain and stress obtained from the simulation are compression in the silicon and in the oxide near the interface, and are of the orders of 1 % and 1×10^{10} dyne/cm^2, respectively, both at 1000 °C for 80 min and at 1100 °C for 40 min. This compressive stress reduces the oxide viscosity by a few orders of magnitude, and this reduction may play an important role in PADOX. In addition, the compressive strain of 1 % in the silicon wire region reduces the bandgap by about 0.1 eV, and this reduction is critical for the formation of the potential barrier responsible for SET operation [5]. The compressive strain obtained in the present simulation is consistent with that predicted from SET operation. Therefore, the present simulation will be helpful in designing SET structures.

In conclusion, we successfully simulated PADOX on SOI substrates, especially for the upward movement of the silicon. The simulation results suggest that the stress-induced reduction of oxide viscosity plays an important role in PADOX. In addition, the oxidation-induced strain obtained from the simulation is consistent with that obtained from the analysis of SET operation.

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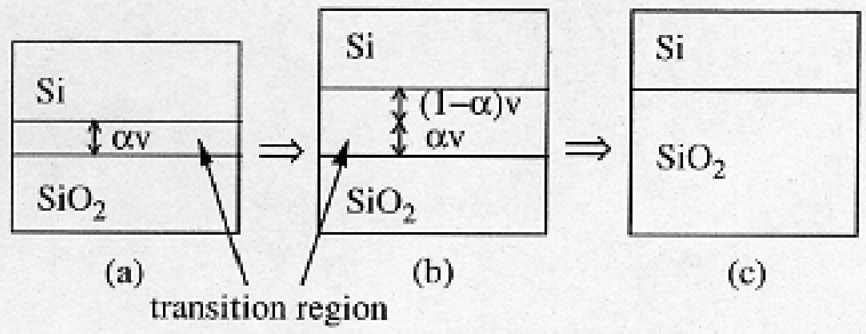

Fig. 1. A transition region is set up so that silicon is pushed upward. (a) Creating the transition region according to oxidant concentration obtained from the oxidant diffusion equation. (b) Volume expansion of the transition region. (c) The transition region is converted into oxide. Here, v is the total amount of oxidation obtained from the oxidant concentration and α is the volume ratio of consumed silicon.

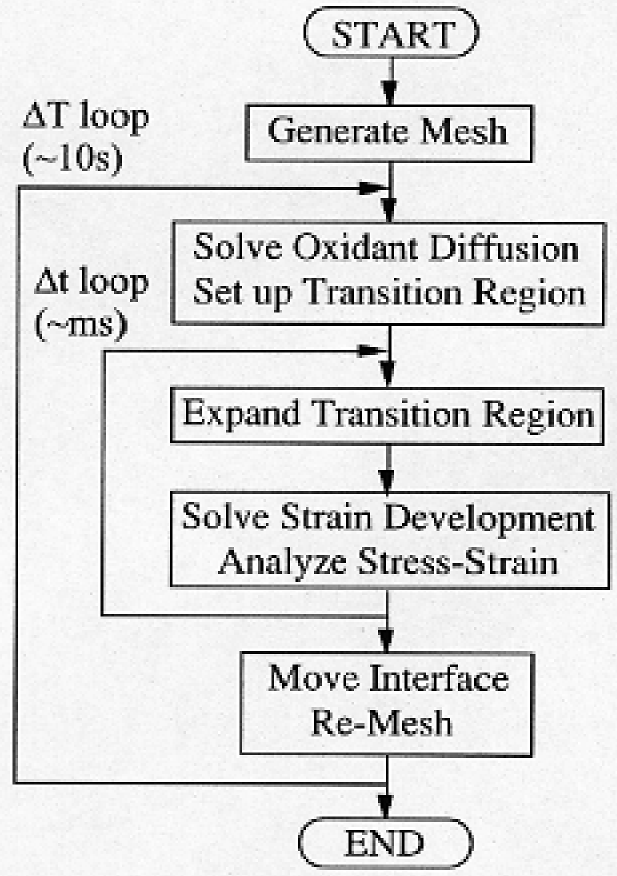

Fig. 2. Calculation flow.

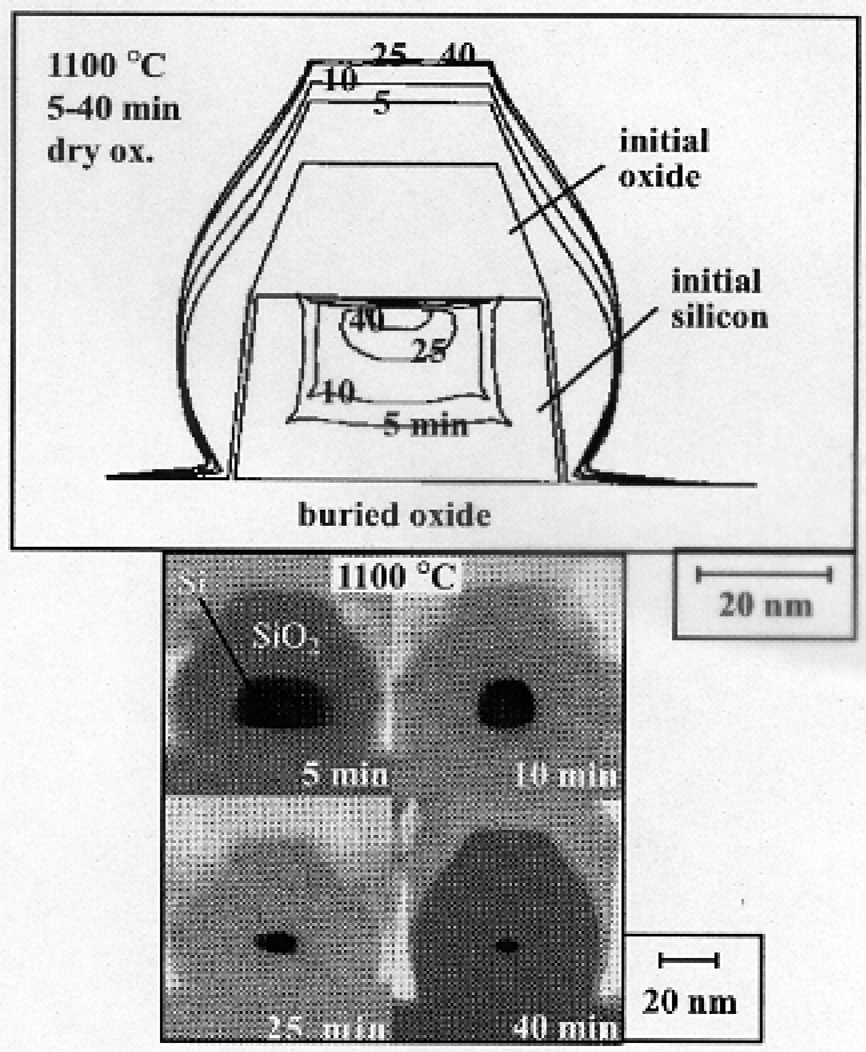

Fig. 3. Simulated shapes (above) and cross-sectional TEM images (below) of silicon lines after dry oxidation at 1100°C.