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Dynamic Numerical Simulation of Melting and Resolidification Process in SOI Formation by Seeded Lateral Epitaxy

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Dynamic computer simulation of seeded lateral growth has been carried out, taking into account laser beam scanning and the melt/solidification process of the deposited poly-Si layer, to confirm the fundamental principles of seeded lateral growth. Crystal growth direction over the SiO_2 layer was found to change depending on the thickness of the layer, with sufficient lateral growth occuring with a thicker SiO_2 layer. Lateral crystal growth velocity was estimated to be about 50cm/s, which indicates the possibility of matching between beam scanning speed and growth velocity in obtaining large area SOI structures.

1. INTRODUCTION

Attracting great attention as a promising tool for achieving new device structures, single recrystallization of poly-Si films deposited on insulating substrates by high power laser beam irradiation has intensively been developed. In particular, seeded lateral epitaxy, which utilizes a single crystal substrate seed to define the crystal orientation of the recrystallized layer[1,2], has been acutely investigated.

However, the crystal regrowth process involves several critical parameters. These include laser irradiation conditions (laser irradiation power, beam scanning speed, etc.) and sample structures (poly-Si and insulator thicknesses, etc.). Furthermore, difficulties in optimizing these parameters sometimes lead to crystal imperfections in the grown layer, which makes the layer unsuitable for device realization.

Optimization of the above mentioned parameters by simulating the crystal regrowth process through calculation was performed to find a solution to these problems, and several papers have reported on calculation of the temperature profiles caused by laser irradiation [3,4]. However, "dynamic" calculation that deals with the moving laser beam and on-going melt and solidification of the deposited poly-Si layer has yet to be reported.

The present paper describes dynamic computer simulation of laser-induced seeded lateral epitaxy. It particularly, focuses on simulation of laser irradiation by a moving beam and on-going single crystal regrowth. Results of simulation which were carried out by varying underlying insulator thickness revealed the fundamental principle of seeded lateral epitaxy; that is, single crystal regrowth occurs through liquid epitaxial regrowth from the single crystal seeding region.

2. CALCULATION PROCEDURES

The two-dimensional heat conduction equation was numerically solved by the finite element method. All the energies absorbed by the poly-Si layer were assumed to be transferred into heat immediately. The main problems encountered in the calculations were;

(1) Physical constants, such as thermal conductivity, vary widely when the temperature of the poly-Si changes by over 1200 C due to laser irradiation.

(2) Since the process involves melting and resolidification, the value of specific heat becomes infinite due to latent heat absorption and release at the melting temperature.

For the former, empirical formula for the temperature dependence were applied. For the latter, specific heat (C) was treated in terms of enthalpy (H), which is the temperature integral of the specific heat ($C=\partial H/\partial T$). Although the value of enthalpy has a discontinuity at the melting temperature, it was approximated by three value change steps with finite gradients in the vicinity of that discontinuity.

The model of sample structure used in the simulation is shown in Fig.1. A SiO_2 layer whose thickness ranged from 150 to 600nm was assumed to be recessed into a Si substrate at the right half of the sample, with the entire surface of the sample assumed to be covered by a 300nm-thick poly-Si layer. The whole system was divided into finite elements, with the smallest (0.1μm in the lateral direction parallel to beam scanning and 0.05μm in the normal direction) near the SiO_2 edge. These elements were made to gradually increase in size with distance from the SiO_2 edge. This was done for detailed investigation of the thermal gradient near the edge. Also shown in the figure is the laser beam intensity profile (TEM_{00} mode) with a beam diameter of 100μm, which is defined at the $1/e^2$ point. Initial temperature of the sample was set at 500 C, and irradiation was assumed to start with the beam center positioned 45μm from the SiO_2 edge. The scale in the figure indicates the position of the beam center as a function irradiation time when the beam is scanned at 100cm/s.

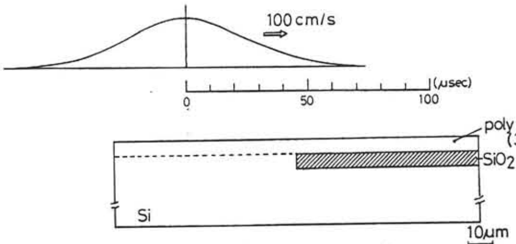


Fig.1 Simulated sample structure and beam intensity profile.

The calculations were carried out using a HITAC S-810 array processor, and the CPU time required for the case in which the laser beam scanning speed was set at 100cm/s was about 15min.

3. RESULTS AND DISCUSSIONS

3.1 Temperature rise in the poly-Si layer

Laser irradiation power dependence of temperature rise at the poly-Si surface over both Si and SiO_2 substrates 1μm from the SiO_2 edge are shown in Fig.2 as a function of irradiation time. That for scanning speed dependence is similarly shown in Fig.3. No significant difference in temperature rise was noted in either region in the early stage of irradiation. However, as the beam center approached, the surface temperature of the poly-Si layer over the SiO_2 became higher than

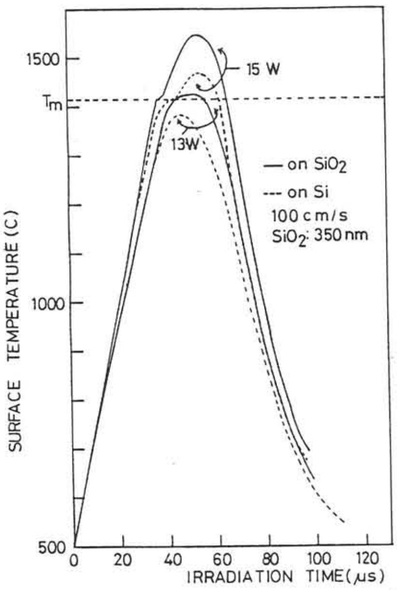


Fig.2 Laser induced surface temperature rise on poly-Si.—laser irradiation power dependence.

that over the Si. Near the melting point, a kink in temperature rise due to latent heat absorption was observed. After reaching maximum, the surface temperature began to decrease leading to solidification. It is significant that, in the solidification process, the previously noted kink in temperature profile is not seen. This

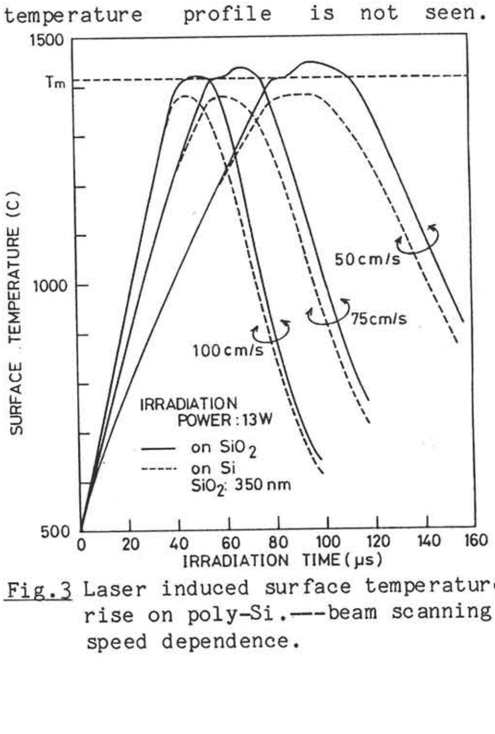


Fig.3 Laser induced surface temperature rise on poly-Si.—beam scanning speed dependence.

indicates the existence of large thermal flux toward the Si substrate.

The irradiation conditions for the calculation shown in Fig.2 were: laser power, 13 and 15W; beam scanning speed, 100cm/s. In the case of 13W irradiation, laser power was only enough to slightly melt the surface of the poly-Si layer on the SiO_2 substrate. However, when the power was raised to 15W, melting occured both over the SiO_2 and Si substrates. It can be seen that increasing laser irradiation power increased both maximum temperature and melting period.

On the other hand, as shown in Fig.3, where the laser power was fixed at 13W and the beam scanning speed was varied from 50 to 100cm/s, the change in scanning speed caused a major change in the melting period but not in the maximum temperature. This result coincides well with the experimental results[5], which indicates that optimum laser irradiation condition depends largely on laser power rather than on scanning speed, especially in the high scanning speed range.

Since the laser energy absorbed by the poly-Si layer doubles when the beam scanning speed is changed from 100cm/s to 50cm/s, the surface temperature could be expected to show a more notable change. The fact that it did not again indicates the existence of high thermal flux toward the Si substrate.

3.2 Movement of the liquid/solid interface in seeded lateral growth

Movement of the liquid/solid interface during melting and resolidification are shown in Figs.4 and 5. The laser irradiation conditions are: laser power, 14.5W; and scanning speed, 100cm/s for both figures. The thickness of the underlying SiO_2 layer is 150nm in Fig.4 and 600nm in Fig.5. The interface was plotted as a function of the distance from the SiO_2 edge to the center of the laser beam.

As the laser beam moved towards the SiO_2 edge, melting of the poly-Si started, first over the SiO_2 substrate away from the SiO_2 edge and then gradually moved toward the seeding region, as shown in Figs.4(a) and 5(a). The liquid/solid interface crossed the poly-Si/Si interface and

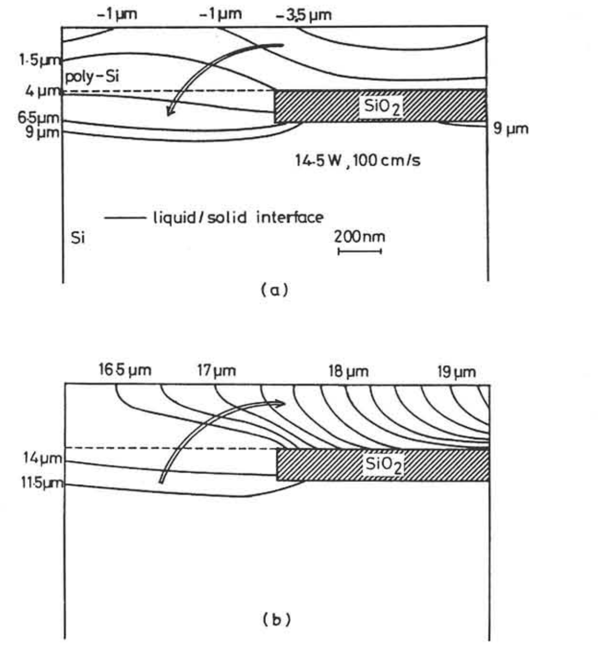
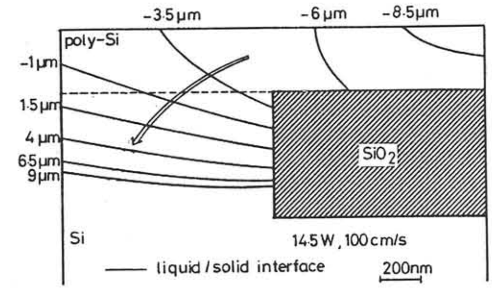


Fig.4 Movement of the liquid/solid interface in (a) melting and (b) solidification as a function of the distance from the SiO_2 edge to the center of the laser beam for thin (150nm) SiO_2 layer.

proceeded into the single crystal region. After the beam center passed over the SiO_2 edge, the movement stopped and then began to reverse itself, that is solidification. As shown in the figures, solidification occured from the seeding region and then extended toward the SOI region to accomplish seeded lateral growth. Under the simple assumption that epitaxial growth takes place when the liquid/solid interface proceeds into the single crystal substrate, these results indicate that epitaxial growth can be accomplished with melting of a seeding region of less than 1μm, because the melting proceeds opposite to the beam scanning direction.

The roles of the underlying SiO_2 layer as a thermal insulator can be clearly understood by comparing these two figures. With the thin (150nm) SiO_2 layer shown in Fig.4, temperature rise is not as high as with the thick (600nm) SiO_2 layer shown in Fig.5 due to the inability of the SiO_2 to stop thermal flux movement toward the Si substrate. In this case, the liquid/solid interface appears both on the Si substrate near to beam center and on the SiO_2 substrate.

Moreover, as melting proceeds, the Si sub-



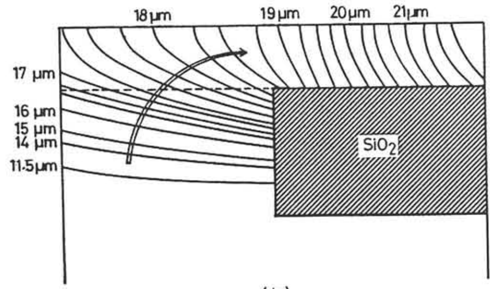


Fig.5 Movement of the liquid/solid interface in (a) melting and (b) solidification as a function of the distance from the SiO_2 edge to the center of the laser beam for thick (600nm) SiO_2 layer.

strate under the SiO_2 layer begins to melt. This melting starts in the region away from the SiO_2 edge. In the vicinity of the SiO_2 edge, thermal energy absorbed by the poly-Si layer over the SiO_2 substrate flows down to the back surface of the sample mainly through the seeding region. However, as it gets farther from the SiO_2 edge thermal flux flows mainly through the SiO_2 layer causing melting from the above location.

In the case of the thick SiO_2 layer, melting occurs only from the SOI layer and the molten zone on Si substrate is beyond the boundary of the figure. Also, the interface proceeds faster than the thin SiO_2 case due to the larger thermal flux flowing from the SOI region. The maximum melting depth at the left edge of both figures differs by 180nm, even though the irradiation conditions are the same in both calculations.

Single crystal regrowth is mainly defined by movement of the liquid/solid interface during solidification, because the crystal growth proceeds normal to the interface. In Fig.5(b), the interface over the SiO_2 substrate is almost normal to the surface, which means that crystal orientation information obtained at the seeding area should be transmitted to the SOI region. However, in the case of the thin SiO_2 layer (Fig.4(b)), the interface becomes parallel to the surface as it moves away from the SiO_2 edge. When this happens, crystal growth normal to the surface, starting from the region in contact with the SiO_2 layer, occurs and the molten poly-Si layer is regrown into a large grain poly-Si layer. Thus, in this case, seeded lateral epitaxial growth is limited. Moreover, it is possible that a single crystal layer would be obtained only in the surface region, with large grain poly-Si in the deeper region.

Crystal growth speed, which was estimated from Fig.5(b), was about 50cm/s, which coincides well in magnitude with the beam scanning speed of 100cm/s. This indicates the possibility of matching between beam scanning speed and growth velocity in obtaining large area SOI structures.

4. CONCLUSIONS

Dynamic computer simulation of seeded lateral growth accomplished by moving-laser-beam irradiation, has been carried out numerically. The results indicate the fundamental principle of single crystal regrowth, although melting was found to first proceed opposite to the beam scan. By extending this, the method should become a powerful tool for optimizing laser irradiation parameters and device structures in the near future, because coming 3-dimensional LSI's are supposed to have more complicated structure systems consisting of several different materials.

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