

Investigation of the formation of nanostructures on silicon thin films by excimer laser irradiation

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Abstract. We present a theoretical study and experimental results on the formation of conical nano-tips on silicon thin films as a result of single-pulse excimer laser irradiation. The fabricated structures have heights of about 1 μm and apical radii of curvature of several tens of nanometers. An individual cone is formed when a mono-crystalline silicon film on an insulator substrate is irradiated in air environment with a single 25ns pulse from a KrF excimer laser, homogenized and shaped to a circular spot with diameter of several micrometers. Atomic force microscopy was used to study these structures. A simplified analytical model for the formation of these structures is proposed. We also present computer simulations of heat transfer in Si films that results from irradiation with a single laser pulse, shaped to a circular spot.

1. Introduction

Recently [1], we reported conditions for controllable, direct laser fabrication of sharp conical tips with heights of about 1 μm , base diameter of about 1.5 μm and apical radius of curvature of several tens of nanometers (referred to as nano-tips). An individual cone is formed when a single-crystal silicon film on an insulator substrate is irradiated in air environment with a single pulse from a KrF excimer laser, homogenized and shaped to a circular spot several microns in diameter. Simple and low-cost techniques for fabrication of such micro- and nano-tips of silicon and other materials, as well as large, high-density arrays of such tips, are desirable in a number of technological applications. The technique that we are presenting has so far shown the capability of producing Si nano-tips (and dense arrays of such tips) with heights in the range of 0.2 to 2 μm and apical radius of curvature of several tens of nanometers. Atomic force microscopy (AFM) and scanning electron microscopy (SEM) were used to study the structures [1, 2]. We have also studied the nano-structuring that resulted from irradiation with a narrow line beam shape (width of several microns) [3].

In this work we investigate scenarios leading to the appearance and growth of the above-mentioned conical tips as a result of the predominantly lateral propagation of a solidification front into the liquid phase of the laser-melted silicon film.

2. Phenomenological model of silicon nano-tip formation

The proposed quasi-static model assumes predominantly lateral heat transfer in irradiated layers of Si film on SiO_2 substrate. To assure such a scenario we need to satisfy the condition $R_o \geq (\sigma\tau)^{1/2} > H_{film}$,

where R_0 is the laser spot radius, σ is the thermal diffusivity and τ is the duration of the laser pulse (figure 1). Since fused silica is not an ideal thermal insulator, for predominantly lateral heat flow we also need a condition $Q_{lateral} > Q_{substr}$ to be satisfied, where $Q_{lateral}$ and Q_{substr} are the radial heat flow along the film and the vertical heat flow into the substrate, respectively. Since $Q_{lateral} = 2\pi R_0 H_{film} k_{Si} \partial T / \partial r$, (k is the thermal conductivity) and $Q_{substr} = \pi (R_0)^2 k_{SiO_2} \partial T / \partial z$, one obtains $R_{spot} < H_{film} k_{Si} / k_{SiO_2}$ (assuming that gradients are of the same order). We can combine the two conditions into: $H_{film} < (\sigma\tau)^{1/2} \leq R_0 < H_{film} k_{Si} / k_{SiO_2}$.

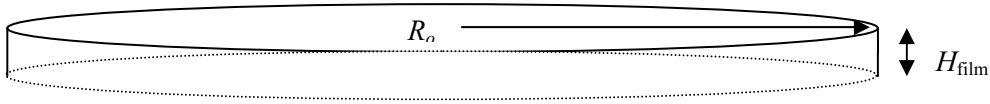


Figure 1: Irradiated spot with radius R_0 that is much bigger than film thickness.

Because of the difference in liquid/solid densities the wafer surface will become elevated at the liquid spot surface. For simplicity we assume the liquid/solid interface is horizontal below. Since the heat transfer is predominantly lateral, at the time of solidification the liquid/solid interface moves toward the center of irradiated spot and the interface surface will become almost vertical. This interface is represented by the conical surface showed in figure 2(a) and defined by the cross-section AOO_1A_1 . Figure 2(b) illustrates how the cross-section changes when the radius of melt decreases by value dR . The melted Si is located between two circles of radii R and $r = R - H \tan \beta = A_1O_1$. Since the thermal conductivity σ_{SiO_2} is about 100 times less than σ_{Si} , it is reasonable to assume that the temperature near the Si/SiO₂ (point O_1) is only slightly lower than the temperature on the Si surface (point O) and the angle β between the isothermal surface and the vertical line is small. Below, subscripts _L and _S denote liquid and solid state accordingly. By using $V_{cone} = 1/3\pi R^2 H$ and upon implementing an appropriate algebraic transformation one can obtain

$$V_L = \pi R^2 H - \pi R H^2 \tan \beta + \pi H^3 (\tan \beta)^2 / 3 \tag{1}$$

for the volume of the melt. From this equation we have the differential change of melt volume dV_L with change in radius dR :

$$dV_L(R) = V_L(R + dR) - V_L(R) = \pi H dR (2R - H \tan \beta) = -dV_S(R) \times (R + dR) \tag{2}$$

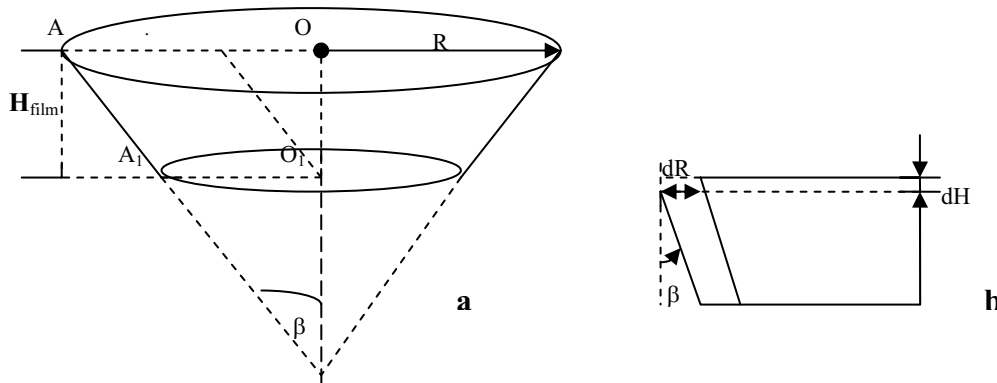


Figure 2: The melt is restricted by a part of the conical surface with a cross-section AOO_1A_1 (a) Small changes in cross-section AOO_1A_1 (b)

The density of solid Si is lower than that of liquid Si and therefore the re-solidified Si occupies larger volume than melted Si. Thus the solid/liquid interface, which is moving towards the center, pushes the surface level of the remaining liquid Si upwards. Therefore we can write the change of melt volume as $dV_L(dH) = \pi R^2 dH$. The mass conservation equation for this process (in first order by dR and dH) is given by:

$$(\rho_L - \rho_S)\pi H dR(2R - H \tan \beta) + \rho_L \pi R^2 dH = 0 \quad (3a)$$

Hence,

$$dH / dR = -(\rho_L - \rho_S) / \rho_L (2R - H \tan \beta) H / R^2 \quad (3b)$$

Let's designate $(\rho_L - \rho_S) / \rho_L = \mu$ (equals 0.08 for liquid and mono-crystalline Si) and $y=H/R$. Then we obtain $dH / dR = y + R dy / dR$ and equation (3b) transforms to

$$\frac{dy}{y[1 + \mu(2 - y \times \tan \beta)]} = -\frac{dR}{R} \quad (4)$$

After integrating (4) it is not difficult to obtain the expression

$$\frac{H}{H_o} \left(1 - \frac{H\mu \times \tan \beta}{(1 + 2\mu)R} \right) = \left(\frac{R_o}{R} \right)^{2\mu} \quad (5)$$

In (5), H_o is the initial height of liquid layer and R_o is the irradiated spot radius. This equation is valid until the distance AO_1 becomes equal to zero (figure 2b). At this point, one obtains $R = R_{cr} = H_{cr} \tan \beta$ and the solidification process is almost complete. Substituting R_{cr} in (5) one obtains an expression for H_{cr} :

$$H_{cr} = R_o \left(\frac{H_o(1 + 2\mu)}{R_o(1 + \mu)(\tan \beta)^{2\mu}} \right)^{\frac{1}{2\mu+1}} \quad (6)$$

Algebraic equation (5) can be solved numerically to find H as a function of R .

In the frame of this model ($\beta=\text{const}$), for $R < R_{cr}$ the remaining liquid can only move up. One obtains a height of $H(R) = H_{cr} + (R_{cr} - R)\mu / \tan \beta$ which yields a maximum height of

$$H(0) = H_{cr}(1 + \mu) \quad (7)$$

Calculated spike heights for different angles β along with values of H_{cr} and R_{cr} are listed in the Table 1.

Table 1: Heights of spike for 0.2 micron silicon film for radius of irradiated spot $R_o=2.8$ microns and different values of angle β according to expressions (6) and (7).

Angle β , deg	R_{cr} , μm	H_{cr} , μm	$H(0)$, μm
2.5	0.019346	0.446340	0.478538
5	0.035222	0.402584	0.434791
10	0.064446	0.365490	0.394729
15	0.092440	0.344991	0.372591

Solving equation (5) against H one can obtain the dependence for $H(R)$

$$H = \frac{H_o(1 - \sqrt{1 - 2A(R_o/R)^{2\mu+1}})}{AR_o/R} \quad \text{where } A = \frac{2\mu \tan \beta H_o}{(1 + 2\mu)R_o} \quad (8)$$

The dependence of $H(R)$ for $0 < R < 0.5 \mu\text{m}$ according to equation (8) with $\beta=2.5^\circ$ is shown on figure 3.

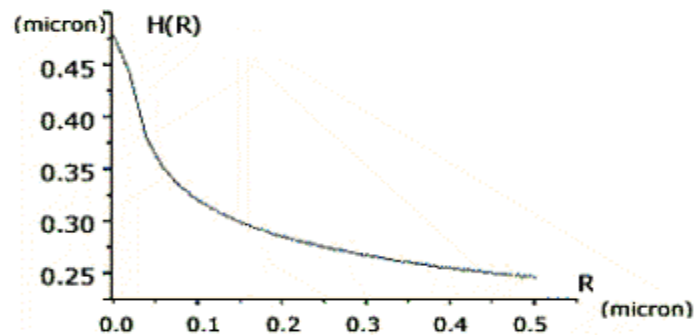


Figure 3: The calculated tip profile yielding a conical structure with $\beta=2.5^\circ$

3. Experimental results and discussion

Details of experiment along with AFM images of nano-tips obtained on silicon films with different thickness are reported in [1], [2] and [3]. Figure 4 shows an AFM image of a spike formed on 0.2 micron thick silicon film after UV (248nm) irradiation with single 25 ns, $2.8\mu\text{m}$ spot radius pulse of fluence of 1.5 J/cm^2 . The experimental height of $1\mu\text{m}$ for that fluence is in a reasonable good agreement with the calculated height of the tip of approximately $0.5\mu\text{m}$ (Figure 3). This small difference might be the result of the assumption that $\beta=\text{const}$ (instead of $\beta=\beta(R)$), and of the model being static. To support our assumption about liquid/solid border that angles away slightly from a vertical line, we performed computer simulations of heat transfer in the Si/SiO₂ structure (0.2 microns Si film on thick SiO₂ substrate). It was shown that at the time of re-solidification there is still a small temperature difference between the silicon top surface and the Si/SiO₂ interface. The detailed results of computer simulations will be published elsewhere.

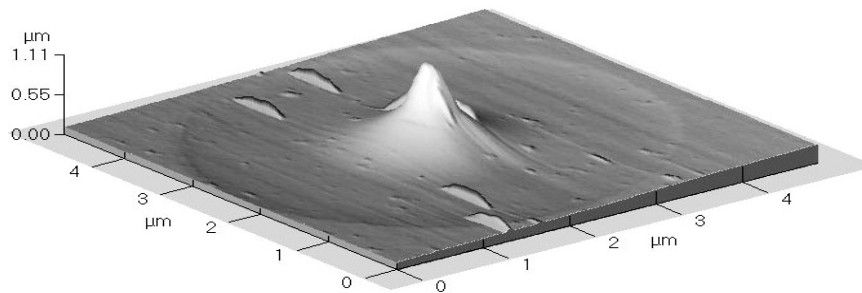


Figure 4: AFM image of tip fabricated with a single pulse of fluence 1.5 J/cm^2

4. Conclusions

The simplified analytical model of the complex problem of the formation of nano-tips has produced encouragingly good results that are in a reasonably good agreement with the experiment. Further experimental and theoretical work is in progress to investigate the nature of nano-tips and to provide better quantitative agreement between the model and experiments.

References

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