Pressure Dependence Mathematical Modeling of Microstructure Fabrication on Silicon by ArF Excimer Laser in SF6 Ambient Gas

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Abstract- Creation a self-organized microstructure on the silicon content surface by laser irradiation in halide ambient atmosphere is a well-known phenomenon. One of the most significant parameters on the process is the pressure of the ambient gas. Although there are many works about experimental validation of the pressure dependence of the process but theoretical investigation of the case does not have a lot reports. Here, A mathematical model based on fluid mechanics and Taylor series is suggested for describing the dependence of geometrical properties of the created self-organized micro-structure on silicon surface in the presence of SF6 ambient gas by the ArF excimer laser to the ambient gas pressure. Predicted results by the model have a good agreement with experimental ones.

Key Words: Microstructuring, Silicon, ArF laser, SF6, Newtonian fluid, Taylor series.

1. INTRODUCTION

Laser irradiation assisted solid surface modification has been reported for various materials such as metals, semiconductors and dielectrics [1, 2]. For the silicon content surfaces, the numerous laser pulses create a self-organized micro-structure [3-27]. The microstructure has some special properties may be utilized for solar cells, infrared photodetectors and the field emission devices. Nanosecond excimer laser pulses at SF6, Cl2 or O2 atmosphere generate a regular arrangement of micro-cones above the original silicon surface [3, 4, 8, 12, 23, 24]. At the laser fluences, 1-5J/cm2, when UV photoablation occurs the conical structures are formed [12]. A model developed previously [25] shows that the melting of silicon surface as well as the resonant of the surface waves are the main reasons for the formation of the self-organized regular micro-structures on the silicon surface. The results of previous researchers show that the self-organized regular micro-structures highly pressure dependent [23].

In this work we intend to predict the time of micro-cone re-solidification and the aspect ratio in terms of pressure for the self organized conical micro-structures formation on a silicon surface in presence of SF6 ambient gas using ArF excimer laser. A new model is developed based on the concept of Newtonian laminar fluid flow in an imaginary pipe used to predict the time of re-solidification as well as pressure dependence of aspect ratio. First, the time of re-solidification of molten silicon is predicted using the Newtonian laminar fluid flow model combined with the Taylor series expansion. Then the time of re-solidification predicted from our model is compared with the ones obtained previously [25]. Second, the aspect ratio in terms of pressure for the self organized conical micro-structures is predicted using the Newtonian laminar fluid flow model combined with the Newtonian binomial expansion. Then the aspect ratio predicted from our model is compared with the ones obtained under different SF6 pressures by conducting the experiments.

2. EXPERIMENTAL RESULTS AND SET-UP DESCRIPTIONS

Fig. 1 shows the experimental set up including gas dosing system, ArF excimer laser (Lambda Physik LPX-200, 193 nm), irradiation chamber (~100 cm3). The microstructure morphology was studied by scanning electron microscope (XLI30 Philips).

Table 1 shows the mean heights, the mean base diameters and the aspect ratios of the micro-cones in the SF6 ambient gas under various pressures. Figure 3 shows the aspect ratios versus the SF6 ambient gas pressures. Using the least square analysis a straight line with negative slope is fitted to the data depicted from table 1. The value of this negative slope is -0.004.

Table 1: The mean heights, the mean base diameters and the aspect ratios of the micro-cones in the SF6 ambient gas under various pressures

<table>
<thead>
<tr>
<th>SF6 gas pressures (mbar)</th>
<th>Micro-cone mean heights (L) (µm)</th>
<th>Micro-cone mean diameters (r0) (µm)</th>
<th>Micro-cone aspect ratio (L/r0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>99</td>
<td>4.81</td>
<td>20.57</td>
</tr>
<tr>
<td>500</td>
<td>101</td>
<td>4.97</td>
<td>20.29</td>
</tr>
<tr>
<td>800</td>
<td>103</td>
<td>4.64</td>
<td>22.16</td>
</tr>
<tr>
<td>1000</td>
<td>105</td>
<td>6.20</td>
<td>16.93</td>
</tr>
<tr>
<td>1500</td>
<td>105</td>
<td>6.56</td>
<td>16.00</td>
</tr>
<tr>
<td>1700</td>
<td>104</td>
<td>6.33</td>
<td>16.42</td>
</tr>
</tbody>
</table>

3. THEORITICAL BACKGROUND AND THE MODEL DISCUSSION

The time of re-solidification of micro-cones are predicted now using the Newtonian laminar fluid flow model combined with the Taylor series expansion. Assuming that the SF6 ambient gas pressures, P6, and the molten silicon pressure,
\[ P_{n} + \frac{\partial P_n}{\partial x} \Delta x + \frac{1}{2!} \frac{\partial^2 P_n}{\partial x^2} (\Delta x)^2 + \ldots \]  

Using a first order approximation Eq.1 is rewritten as:

\[ P_{SF6} = P_n + \frac{\partial P_n}{\partial x} \Delta x \]  

Now rearranging Eq. 2 in terms of aspect ratio,

\[ \frac{\partial P_n}{\partial x} \Delta x = \frac{\partial P_n}{\partial (L/r_0)} (L/r_0) \]

and using the experimental results for the negative slope:

\[ P_{SF6} = P_n - (1/0.004)(L/r_0) \]  

\[ \Delta P = \frac{4\sigma' L^2}{r_0} \]

Where \( \sigma' = \sigma/T \)

Fig. 1: Schematic diagram of experimental set-up.

Fig. 2: Gradual alteration of Silicon surface morphology in the ambient gas of SF6 irradiated by constant ArF laser fluence (4 KJcm-2) under the pressures of (a) vacuum, (b) 400 mbar, (c) 800 mbar, (d) 1000 mbar and (e) 1700 mbar.

Eq.3 shows a linear relationship between the aspect ratio and \( P_{SF6} \). Using the concept of Newtonian fluid flow in a circular tube, the mean velocity is defined as [28]:

\[ v_y = \frac{\Delta P}{4\sigma L}(r_0^2 - r^2) \]

Where \( v_y \) is the mean velocity in the y-direction, \( \Delta P \) is the pressure drop in the pipe, \( L \) is the length of the pipe, \( r_0 \) is the radius of the pipe, \( \sigma \) is the fluid viscosity and \( r \) is the radial distance measured from the pipe axis. Assuming the time of micro-cones re-solidification is \( T \) and the height of a micro-cone is \( L \) respectively. Then the velocity of micro-cones formations (\( V_{max} \)) is obtained by \( V_{max} = L/T \). The pressure drop for the maximum Newtonian fluid velocity in a circular pipe in terms of the micro-cones formations time is obtained from equation 1 using \( r=0 \) as:

\[ \Delta P = \frac{4\sigma' L^2}{r_0} \]

Fig. 3: The aspect ratios versus the SF6 ambient gas pressures.

The aspect ratios of the cones are obtained:

\[ \frac{L}{r_0} = \left( \frac{4\sigma'}{\sigma} \right)^{1/2} \left( P_{Si} - P_{SF6} \right)^{1/2} \]  

where \( P_{Si} \) is the molten silicon pressure (assumed to be constant) and \( P_{SF6} \) is the SF6 gas pressure. Combining Eq.s (3) and (6) one can evaluate the time of micro-cones re-solidification as:

\[ T = 0.016\sigma \left( \frac{L}{r_0} \right) \]

The aspect ratios of micro-cones are predicted now using the Newtonian laminar fluid flow model combined with the Newtonian binomial expansion. Expanding Eq.(6) using the Newtonian binomial expansion (\( P_{Si} > P_{SF6} \)):

\[ L/r_0 \approx -1/4(\sigma' P_{Si})^{1/2} P_{SF6} + 1/2(\sigma' P_{Si})^{1/2} \]  

Eq. (8) shows that the relationship between the aspect ratio and the SF6 pressure is a straight line with negative slope. Equating the negative slope of this straight line, \(-1/4(\sigma' P_{Si})^{1/2}\), to the negative slope obtained from the experimental results of Fig. 3, the value of \( \sigma' P_{Si} \) is obtained equal to 3844. We would like to compare the aspect ratio, \( L/r_0 \), obtained from the experiment with the aspect ratio obtained from the new model at zero pressure of the SF6 gas. The aspect ratio using the experimental results at zero SF6 pressure is obtained from Fig. 3 equal to 23. The aspect ratio using our new model at zero SF6 pressure by making use of \( \sigma' P_{Si} \) equal to 3844 is obtained to be equal to 31. The comparison between the aspect ratio obtained from the experimental results with the aspect ratio obtained using
our new model shows reasonable agreement. The aspect ratio for re-solidification is typically of order 10, therefore the time of re-solidification is obtained to be of order $10^4$ s. Here, we assume a value of 0.88 centipoises for $\sigma$ of molten silicon.

4. CONCLUSION

Here, a simple mathematical model based on Newtonian laminar fluid flow combined with the Newtonian binomial expansion was developed for the surface microstructuring on silicon surface by laser irradiation in the various pressures SF6 atmospheres. The model can predict the time of re-solidification of micro-cones as well as the aspect ratio of micro-cones. Comparison between the model results and the experimental data shows a good agreement. The re-solidification time for the molten micro-cones is $\sim 10^4$s.

REFERENCES

