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# Epitaxial bridging with nanocluster assisted film growth under the mesoplasma condition

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**Abstract**

**The feasibility of thick epitaxial film growth over porous substrate has been attempted by the nanocluster assisted epitaxial film growth under mesoplasma condition. Molecular dynamics simulation has suggested that the epitaxial lateral growth hanging over the pore groove is realized if liquid-like nanoclusters become the deposition precursor having high-sticking capabilities.**

## 1. Introduction

Thick epitaxial films have been longed for a variety of devices, including single crystalline Si solar cells and bulk template for wide bandgap materials. As one of the unique approaches to attain epitaxial film deposition at fast rate and at relatively low temperature simultaneously, mesoplasma has been proposed [1]. Under the mesoplasma condition, liquid-like nanoclusters form as actual deposition precursors during rapid condensation ahead of the substrate, and a strong correlation between the nanocluster size and the film microstructure is revealed [2]. Molecular dynamics simulation has further identified that loosely-bound nanocluster deforms upon impingement on a substrate surface and the constituent atoms rearrange their positions according to the lattice underneath [3]. Such a spontaneous and instantaneous atom rearrangement is not limited on a flat substrate surface and it occurs also on uneven surface, which facilitates thick epitaxial film growth through multiple nanocluster impingement [4].

To produce such thick epitaxial films economically, these films are to be deposited on a porous template and lifted-off at the pore layer for free standing. Considering a lift-off layer transfer with mesoplasma deposition, highly sticking but deformable nanocluster precursors would be favorable to grow laterally over the pores from the step coverage point of view. In this work, therefore, the groove coverage dynamics during deposition is numerically analyzed and the requirements for epitaxial overgrowth on porous surface are discussed.

## 2. Experimental

*Monte-Carlo groove coverage simulation (MC)*

Since MD simulation of a cluster impingement on a groove at large scale is not practical, the Monte-Carlo simulation has been employed to obtain the tendency of the groove coverage with nanoclusters. The groove width is fixed to be 15 times of the building block size as the coverage shape is not affected by a few elements but still controlled by the impingement of multiple building blocks [5]. Other simulation conditions are the same with the conventional coverage simulation [6].

*Molecular dynamics simulation (MD)*

Restricted to a smaller length scale, atomistic characteristics during cluster impingement is simulated using MD. Nanoclusters used is created in advance following the procedure reported elsewhere [3]. In brief, 83 Si atoms are first heated up to 1.78 Tm (Tm is the Si melting point of Tersoff potential **[7]**) to be at random positions (vapor). They are subsequently cooled down to 0.79 Tm at which nanocluster nucleates. The resultant nanocluster is loosely-bound with average diameter of 1.5 nm. This nanocluster is injected to substrate from random positions in random angles at an average interval of 180 ps. In most cases, the preceding atom sticks before the next atom injection. On a Si(100) substrate, a trench groove with 50 nm wide is created. The calculation cell wall except trench is set to be the periodic boundary condition. Other conditions are the same with the previous report **[4]**.

## 3. Results and discussion

*Lateral projection over a groove*

The degree of the lateral projection over a groove is evaluated with MC by the step coverage (Sc) that is a relative thickness of a film deposited on the side wall at the groove top to that at the groove bottom. In the mesoplasma CVD, as the actual deposition precursor nanoclusters are 2-3 nm in diameter [2], the sticking coefficient upon impingement at a groove is assumed to be unity. Also, the relative size of the groove entrance to that of the mean free path (MFP) of incoming nanocluster should affect the deposition dynamics. Assuming that precursors are distributed uniformly, MFP of a cluster is calculated roughly to be 81mm, while that for atomic Si is 90 $\mu$m [1]. If the model groove is 1 $\mu$m opening, Knudsen number should become 90 at the smallest, which is reasonably assumed to be infinity. Under these conditions, Sc is estimated as a function of aspect ratio (AR) of a groove, as shown in Fig.1(a). In the case of Kn = $\infty$, Sc reaches approximately 0.35 at AR = 1. If the deposition precursors are more collisional, Sc decreases more significantly down to 0.06 at Kn = 0.2. These results suggest that the sticking coefficient of 1 influences largely the film coverage compared with Kn. The lateral projection, the reciprocal of Sc, is then plotted in Fig.1 (b). For AR = 1, the projection degree becomes 2.9. This means that when the lateral projection length at the entrance reaches the half of the groove width, i.e. 0.5L, the bottom of the groove is filled only 0.17L. That is, 0.66L wide space still remains as pore at the bottom of the groove. In the case of a model groove of Kn = 100 and AR =1, the groove opening ranging from 1 $\mu$m to 100 $\mu$m and the groove depth as deep as 1 to 100 $\mu$m could be served as a lift-off template and facilitate the lateral overgrowth leaving pore underneath.

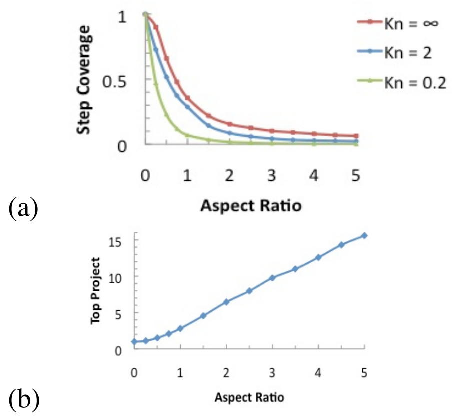


Fig. 1(a) MC estimated variation of the step coverage with aspect ratio of a groove (sticking coefficient = 1) and (b) the projection degree change with aspect ratio.

*Lateral epitaxial overgrowth*

Fast rate epitaxial growth is made possible under mesoplasma condition owing to the instantaneous and spontaneous rearrangement of the cluster constituent atoms upon impingement on substrate. Such an epitaxial atom rearrangement can be expected at the atomistic length scale during also deposition over the groove as discussed above. Figure 2 shows the time evolution of the deposited nanoclusters impinging onto a groove at a Si(100) surface. At the initial stage of the deposition (t = 1100 ps), nanoclusters attach preferentially at the groove entrance as is expected by the MC calculation. However, the shape of the deposits is not uniform and it tends to grow both vertically and laterally. At the very close to the groove wall, the atoms are seen to align epitaxially while the surface of the nanoclusters are still random structure. With additional cluster impingement, the deposits grow from both walls and merge together at the central part of the groove. Again, it is noted that the merged part shows random atom alignment initially but it changes to the epitaxial ordered structure as time proceeds.

The time variation of the individual atom potential is compared in Fig.3 for different regions within the deposits.

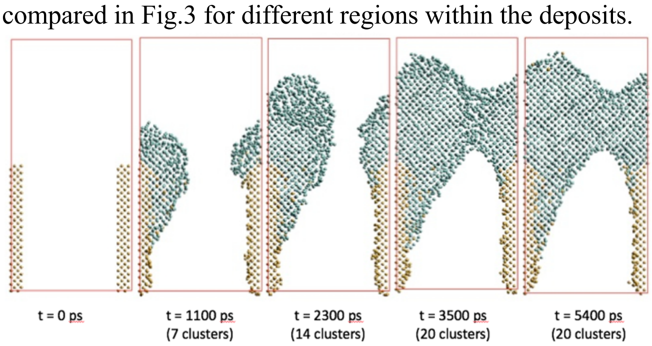


Fig. 2 Snapshots of MD calculation during multiple impingement of Si nanoclusters onto grooved Si wafer at 0.89 Tm.

As a general tendency, the atom potential is high at the time of impingement, but it decays with time to a certain constant value. At the position closer to the merge point, the atom potential at the impingement becomes small and the corresponding stable value seems to be slightly high. This might be associated with the distance from the well-defined groove wall and also with the impingement on uneven surfaces. Nevertheless, it is important to note that even the groove with AR = 1, nanoclusters create an epitaxial bridge over the groove leaving enough volume of pore underneath.

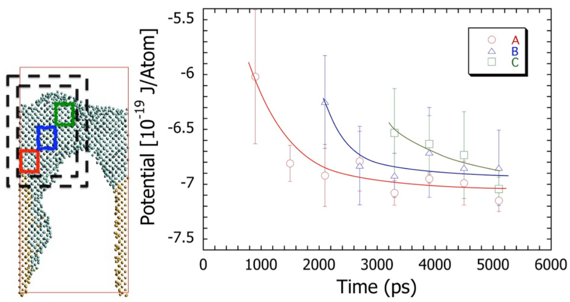


Fig. 3 Snapshots of MD calculation during multiple impingement of Si nanoclusters onto grooved Si wafer.

*Epitaxial thick films on porous template*

Silicon film deposition has been attempted on a porous substrate under a typical epitaxial condition. The porous surface is created by a standard anodizing [8] and the groove opening size is typically ranging from 100 nm to 1500 nm and the depth is roughly several 100 nm. [1]. According to the MC and MD model above, these pore are within the dimension that lateral epitaxial overgrowth is possible. In fact, on this porous surface, 10 $\mu$m thick epitaxial film with has been deposited and this layer is lifted off with ease at the porous layer [8]. Considering the lateral growth velocity of 2000 nm/sec on $SiO_2$ mask estimated experimentally [9], epitaxial bridging on 1 $\mu$m wide pore can be completed in 0.25 sec.

## 4. Conclusions

Epitaxial thick film deposition is possible on a porous substrate under mesoplasma condition. Owing to highly sticking but deformable nanocluster characteristics, epitaxial films grow laterally over a pore leaving a pore space underneath. Such epitaxial bridging is expected even the pore size as large as several $\mu$m wide and even shallow groove with AR~1.

## References


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