# Simulating Thin Films: The Effects of a Rotating Substrate on Surface Morphology in Oblique Incidence Epitaxial Growth


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The effects of substrate rotation during deposition on the surface morphology and roughness in oblique-incidence epitaxial growth are studied via kinetic Monte Carlo simulations, and compared with previous results obtained without rotation. In general, two main effects are observed. At high deposition angles, θ, rotation leads to a drastic change in the surface morphology. In particular, it leads to isotropic mounds and pyramids rather than the strongly anisotropic structures observed in the absence of rotation. At large angles, very regular pyramids are observed. Rotation also leads to a reduced surface roughness, although the surface roughness tends to increase with rotation rate Ω. An explanation for these effects is given in terms of the effects of rotation rate on shadowing and coalescence. Some interesting effects at low rotation rate (less than 1 rev/ML) are also discussed. Our results are also compared with the case of deposition with fixed deposition angle but random azimuthal angle.


## INTRODUCTION

Thin film simulations have previously been studied with various different parameters. Recent projects looked at deposition at normal incidence as well as oblique incidence epitaxial growth [1]. The latter looked at the effects of shadowing on surface morphology. They examined four different angles: 70°, 80°, 85°, and 88°. At 70°, the particles form into mounds. The mounds are anisotropic, irregularly shaped, and arranged close to each other almost into rows. At 80°, the surface is organized into ripples. The ripples are lumpy in some places and not straight. At 85°, there is a mixture of ripples and pyramids. These forms are like the ripples, but more block shaped with pyramids found randomly dispersed through out. At 88°, the ripples and pyramids are replaced by rods. These rods are not smashed together like the mounds, ripples, and pyramids found at lower deposition angles. There are some gaps where the rods have shadowed the spots around them. In addition to the morphology, the surface roughness was studied. It was found to be a power law, $w \propto t^{\beta}$, where $w$ is the surface roughness, $t$ is the thickness of the film, and β, is the growth exponent.

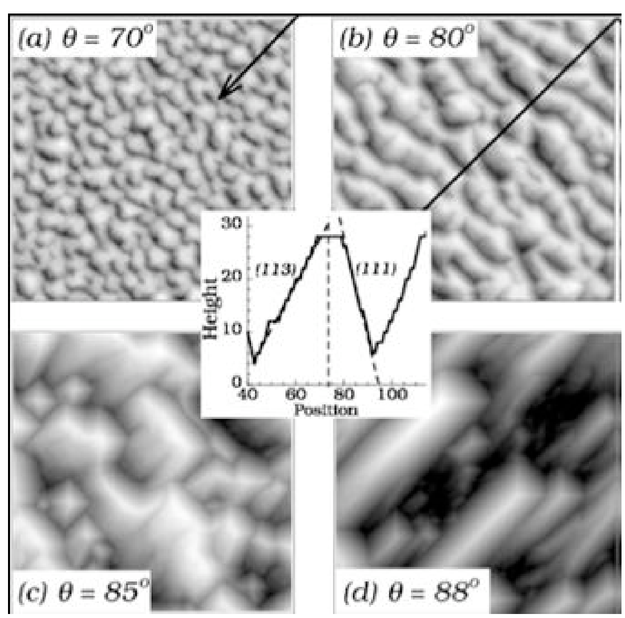

FIG. 1 Examples of the morphology found with oblique incidence epitaxial growth without rotation. (512x512 portion of $L$= 2048 system, at $t$= 50 ML.) Arrow indicates deposition direction. [1]

The results from the oblique incidence growth brought about questions of what happens if the substrate rotates during deposition. We wanted to determine how the rotation rate and deposition angle affect the surface morphology.

To figure this out, we used a FORTRAN77 program that collects data about the surface roughness, information to make picture, and a variety of other information. From here, we take the roughness data and use KaleidaGraph to graph the surface roughness versus thickness and surface roughness versus rotation rate. We take the picture files and use a program in C to make sgi files and the use Quick Time Pro to make a movie of the growth. The movie is very useful in the respect that we can look at how the structures form.

The work done this summer looked at oblique incidence epitaxial growth with a rotating substrate. The deposition was a simple model of molecular dynamics without long range attraction.

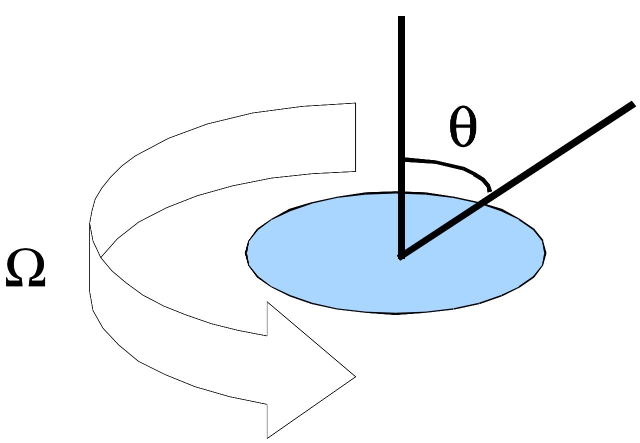


FIG. 2 Image description of the substrate.

## DATA AND ANALYSIS

This summer we looked at the deposition angles 70°, 80°, 85°, and 88°. There was a significant difference between the morphology with and without rotation. By looking at the pictures, we can tell that the greatest difference is the fact that rotation drastically alters the morphology. It changes anisotropy into isotropy for the pyramids seen in large deposition angles. It also converts ripples to irregular pyramids/mounds and rods to regular pyramids.

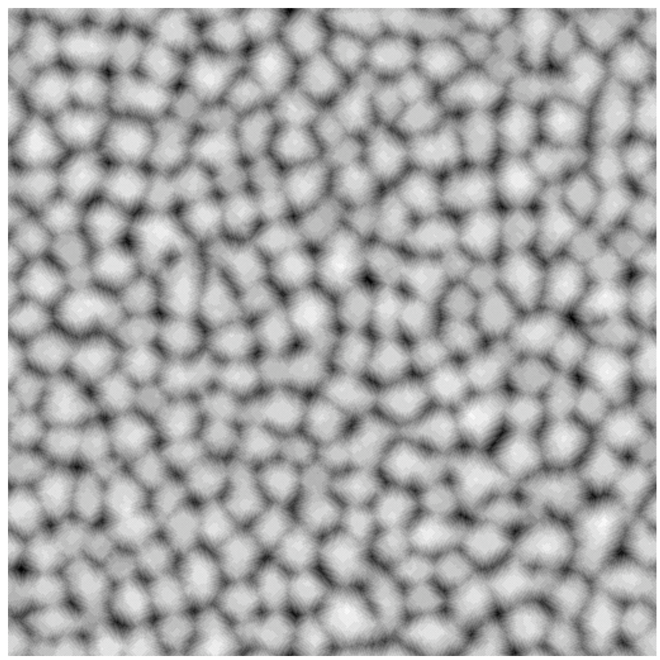

FIG. 3 L=512, t=50ML, $\theta$=70°, $\Omega$= 1/4 rev/ML

The picture of 70° shows mounds. Everything is pushed together and there is little space in between. However, the mounds are neither square nor exactly round. This makes them not as isotropic as the morphology seen in other deposition angles. There is not much change in the size, shape, and amount of mounds when the rotation rate is changed.

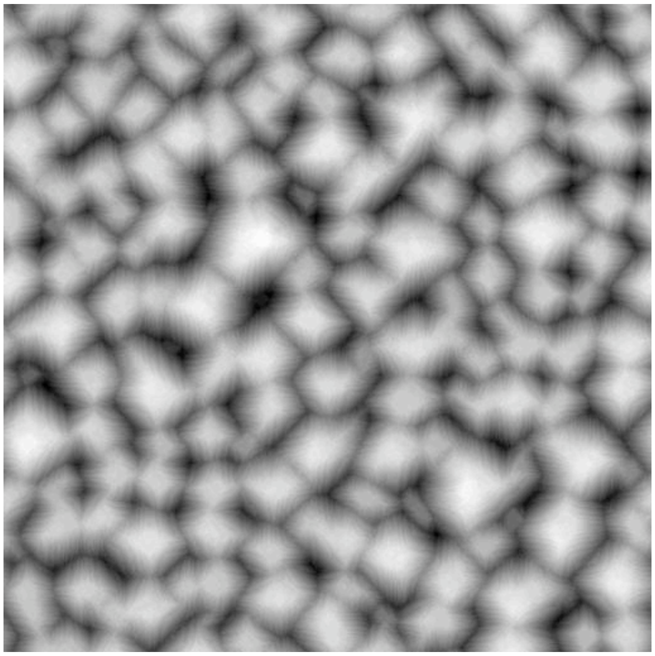

FIG. 4 L=512, t=50ML, θ=80°, Ω=1/5 rev/ML

The picture of 80° shows a combination of mounds and pyramids. Everything is much more isotropic but not as ordered like in ripples or rows. However, there are no gaps or open spaces between the mounds/pyramids.

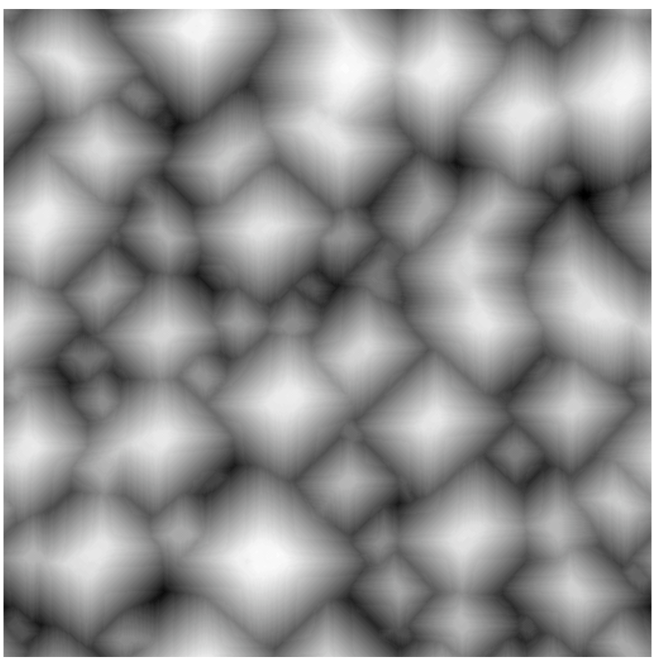

FIG. 5 L=512, t=50ML, θ=85°, Ω= 1/3 rev/ML

The picture of 85° shows many pyramids that are smashed into each other like the mound/pyramids seen at 80°. Everything is much more isotropic.

For some rotation rates the tops of the pyramids are flat or there is a divot.

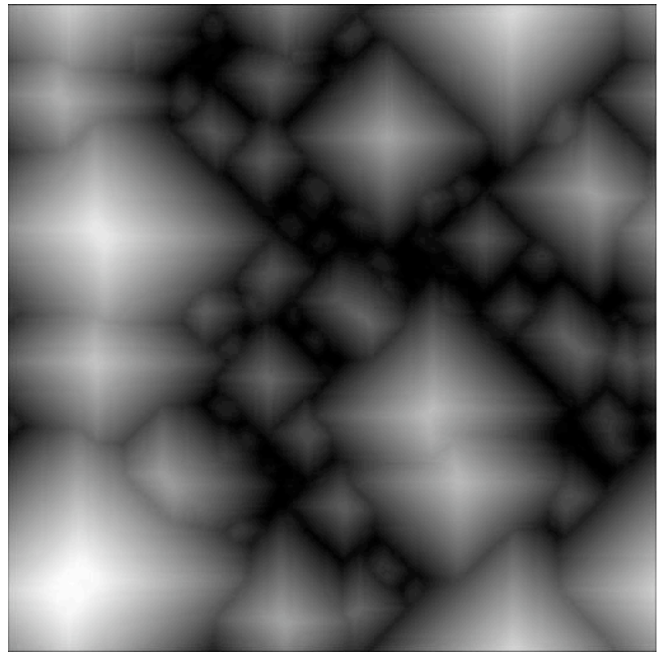

FIG. 6 L=512, t=50ML, θ=88°, Ω=1/2 rev/ML

The picture of 88° shows incredibly isotropic pyramids. Depending on the rate of rotation, the spaces between the large pyramids increases and decreases as do the number of tiny pyramids.

To analyze the data, we also plot the surface roughness versus the rotation rate. From this graph we can see which of the rotation rates has the least roughness and it helps to see if there is an ideal rotation rate for a given deposition angle.

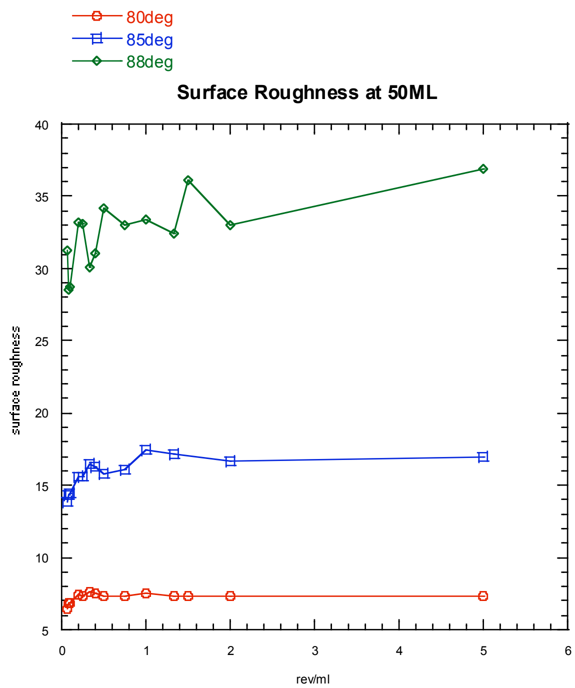


FIG. 7 Surface roughness at 50ML for all simulated rotation rates, except no rotation and random deposition.

We can also determine the rotation rate in which saturation occurs. By looking at the plot above we can see that at 80°, there is not a great difference depending on the rotation rate. At 85°, there is a little more deviation in the surface roughness at 50ML. Then by looking at 88°, we can see even more that there is a great dependence rotation rate as well at the deposition angle for surface roughness.

## ACKNOWLEDGMENTS

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## RESOURCES

[1]Y. Shim and J. G. Amar, Phys. Rev. Let. **98,** 046103 (2007).