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The Effects of Shadowing and Diffusion on Surface Morphology in Thin-Film Growth

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Abstract

Recent experiments on vapor deposited CF_2 thin-films have shown a power-law distribution P(□h) for nearest neighbor sites height-differences (□h) where P(□h) ~ (□h)$^{-□}$, and □ ≈ 4.6. In order to understand this we have studied the effects of shadowing and diffusion on thin-film growth by sputter deposition using four distinct models in two and three dimensions. Our simulations indicate that both shadowing and sideways growth (overhangs) are necessary to observe a power-law distribution of the height-difference. For the case of “cosine” distribution we found that in two dimensions □ ≈ 2.6 and in three dimensions □ ≈ 3.1. We also observed shadowing and sideways growth lead to a porous film and anomalous scaling of the height-difference correlation function.

I. **Introduction**

How does shadowing affect surface morphology? What are the roles of surface diffusion, and sideways growth in controlling surface morphology in vapor deposition? Based upon previous work done by Dr. Jacques Amar and his associates [1], in which they defined □,□, and n for some of the same simulations we have incorporated into this project, we, however, will investigate the height-difference distribution for several computer simulations of sputter deposition.

Sputter deposition is an important process, which is used industrially□to deposit thin-films. The morphology of the film can play an important role in affecting its behavior.□As a result there has been a great deal of interest in modeling the dependence of the surface and thin-film morphology and microstructure□on growth conditions. In sputter deposition, the atoms are deposited from a range of angles. A distribution of angles leads to shadowing of lower levels by higher. Fig. 1 shows a representation of sputter deposition where the particles are approaching the substrate from an angle □ which measured from the substrate normal.

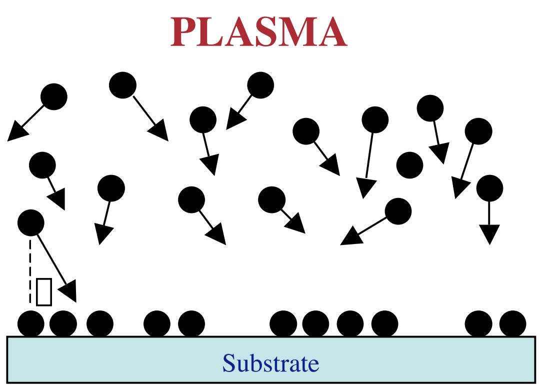

Fig. 1: Diagram of Sputter Deposition

In order to quantitatively characterize the surface morphology the height profile h(r) must be determined (see Fig. 2).□Once this is done one may calculate the r.m.s. surface roughness w(t),the ht-ht correlation function $G_2(r)$,and the lateral correlation length □(t). Typically 3 exponents are determined, □,□, and n.□For example, the dependence of the surface width on film thickness or time t, is typically described by a power-law in which

$$w(t) = < [h(r,t) - h_{av}(t)]^2 >_r{}^{1/2} \sim t^{\square} \qquad (1)$$

where □ is the growth exponent. In addition $G_2(r)$, and □(t) have power law behavior which is typically described by

$$G_2(r) = < | h(r) - h(0) |^2 >_0 \sim r^{2□} \qquad (2)$$

and

$$□(t) \sim t^n \qquad (3)$$

where n is the coarsening exponent and □ is the roughness exponent.

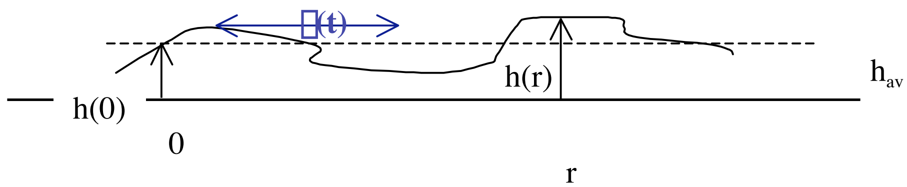

Fig. 2: Diagram of how exponents measured

Recent experiments on vapor deposition of CaF_2 on glass, carried out by D.R. Luhman and R.B. Hallock, have produced a porous film with unusually large exponents of □ ≈ 0.88, □ ≈ 0.75 and n ≈ 0.85 [2]. In addition to these large exponents the researchers also studied the distribution of height-differences (□h) where:

$$P_□(□h) \sim (□h)^{-□} \sim (□h)^{-(□+1)} \qquad (4)$$

and results indicated an □ ≈ 4.6. The height-difference is measured at distance □ away and done so for all i in the system (see Fig.3) .The authors, Luhman and Hallock, suggest that this behavior is due to power-law noise, which they explain by use of the KPZ equation with power-law noise. What we are trying to understand is what mechanism could produce power-law height fluctuations.

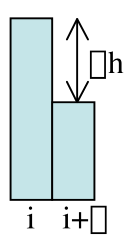

Fig. 3: Diagram of $P_□(□h)$

In order to try to understand this we have studied four different models in two and three dimensions. The first model we studied□□s the ballistic deposition model [3] [4] as shown in Fig. 4, which was originally developed as a model of sedimentation. In this model (see Fig.

4(a)) particles "rain down" one-at-a-time on the substrate from random positions above the substrate, and stick to the first particle they encounter. Since particles can "stick" on the side this leads to sideways growth. In order to simulate the effects of shadowing, we have also considered a modification of this model in which particles are deposited with a "cosine" distribution, which is equivalent to a uniform deposition flux for angles theta between $-\pi/2$ and $+\pi/2$ (where θ is the angle with the substrate normal) as shown in Fig. 4(b). While both of these models have sideways growth, in order to understand the effects of diffusion on the surface morphology, we have also considered a version of this model ("sliding model", see Fig. 4(c)) in which after contacting the side of a column, a particle "diffuses" immediately to a low-energy "kink" site at the bottom of the column. Finally, we have also studied a fourth model (diffusion limited aggregation), which corresponds to "extreme shadowing". In this model particles diffuse to the surface and stick irreversibly, and are even less likely to penetrate below a local maximum.

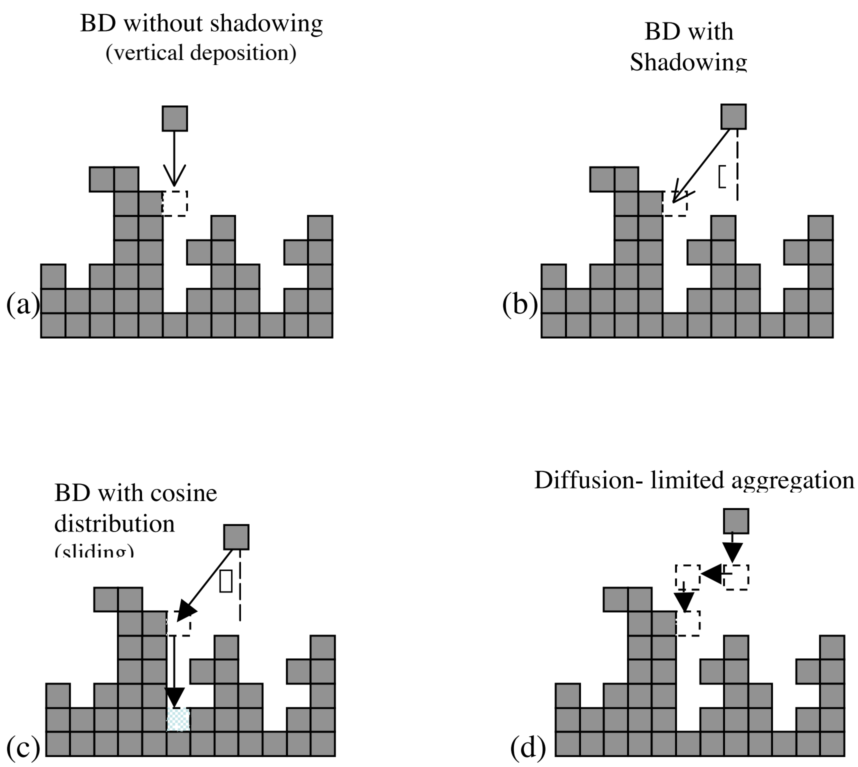

Fig. 4: Diagram of Simulations used

While in previous work the exponents were studied, in order to understand the new experimental results we have studied the height-difference distribution $P_{□}(\Delta h)$. In particular we measured the $P_{□}(\Delta h)$ for different values of □ = 1, 2, 4, 8 and for different film thicknesses. Fig. 5 shows numerical results for α, β, and n in the 2D models for the vertical deposition (Fig. 5(a)) and “cosine” distribution (Fig. 5(b)). Jianguo Yu and Jacques G. Amar established these results back in 2002 [1].

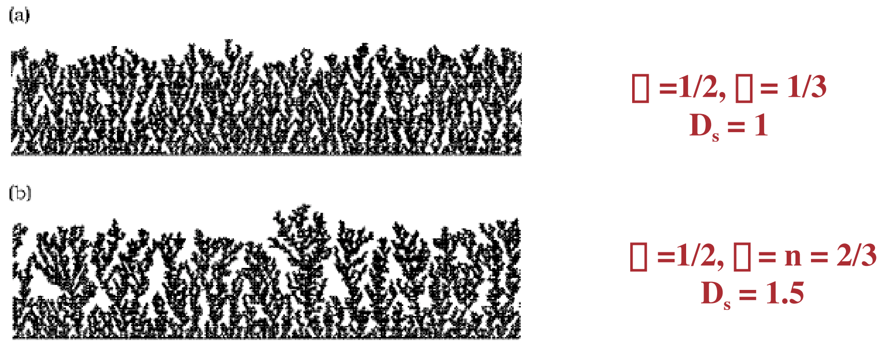

Fig. 5: Surface Morphology of (a) vertical deposition (b) cosine distribution deposition

II. Results

II.A. 2D

Fig. 6 shows our results for the two-dimensional simulations. As shown the cosine and DLA exhibit over a decade of power-law behavior, where the extrapolated values of □ are 2.6 for cosine and 1.7 for DLA. Comparatively the vertical (no shadowing) and the "slide" (no sideways growth) show no power-law behavior. Fig. 7 shows more detailed results for the dependence of the height-difference distribution on film thickness and distance delta for the cosine model. As shown with an increase in thickness there is an extension of the power-law distribution (Fig. 7 left). In addition, with an increase in the distance □ at which the height-difference is measured there is also an increase in the exponent □. And Fig. 8 shows similar results for the DLA model.□ Interestingly for DLA pure-power-law and □ = D_f. Our 2D results indicate that both shadowing and sideways are necessary to have power-law distribution of height-difference. We now present our 3D results.

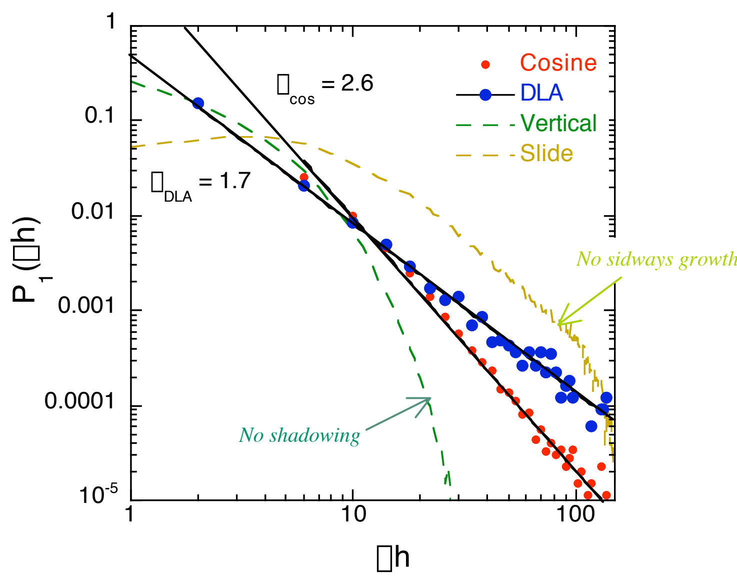

Fig. 6: Height-Difference Distribution P_1(□h) (2D)

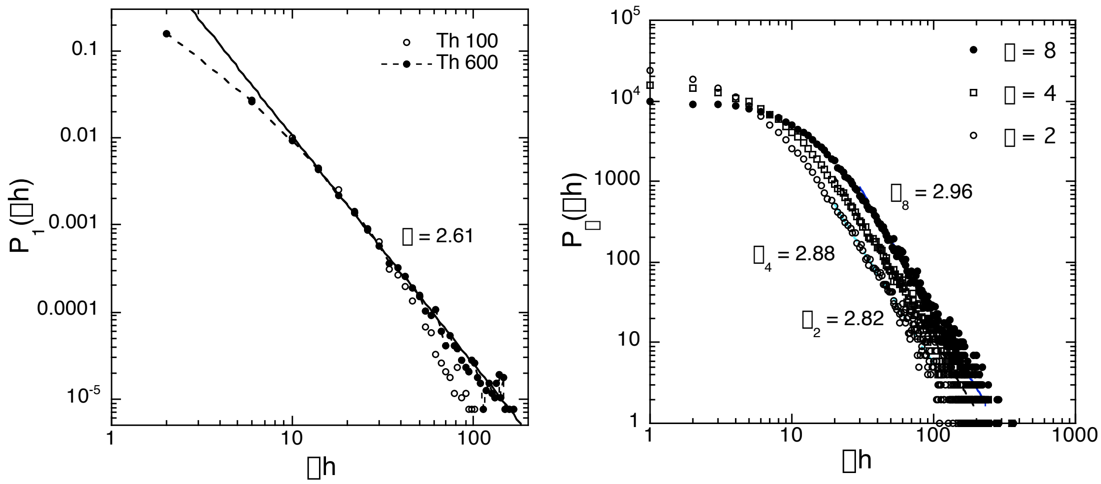

Fig. 7: BD with Cos Distribution in 2D (L = 131k Th 600)

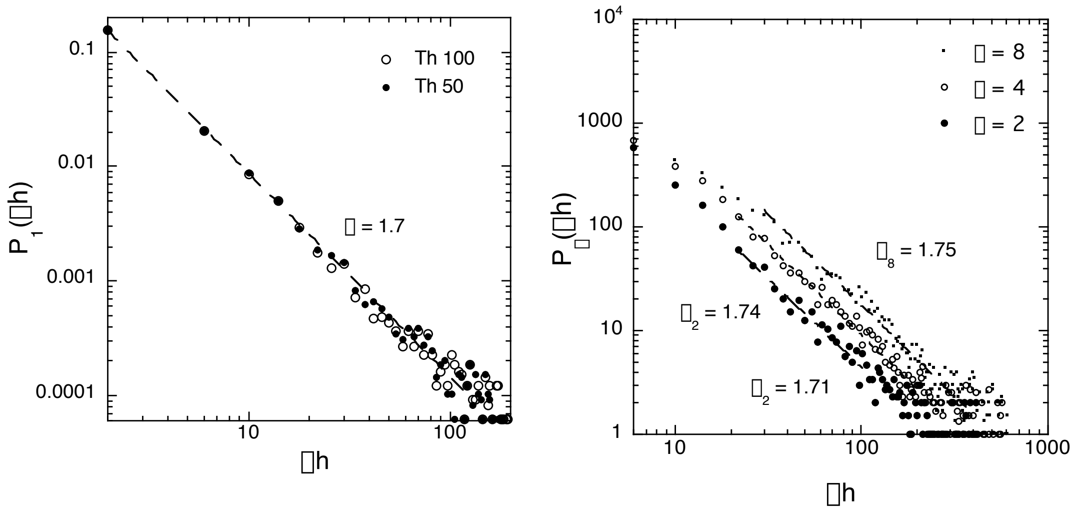

Fig. 8: Diffusion-Limited Aggregation (DLA) [2D] (L = 16k Th 100)

II.B 3D

Fig. 9 shows our results for the three-dimensional simulations. As in two-dimensions the three-dimensional cases exhibit the same trend in which no power law is observed in the cases of vertical and sliding and significant power-law behavior for the cosine and DLA. As an example Fig. 10 shows results for growth and coarsening exponents n and b as well as the roughness exponent □ for the cosine model.□As can be seen good fits, larger than normal due to shadowing, but still somewhat smaller than experiment. In particular □ seems to be still increasing. In addition to cosine the □,□□, and n for the slide, vertical and DLA were also plotted and measured in like manner, these values are given in Table I.

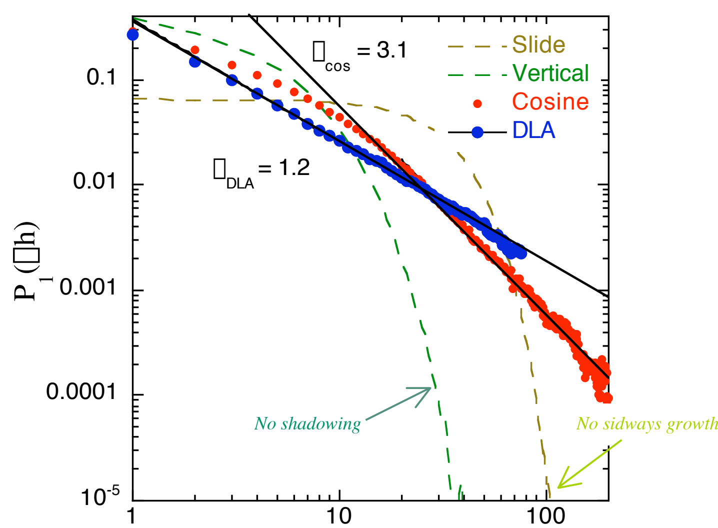

Fig. 9: Height-Difference Distribution P_1(□h) (3D)

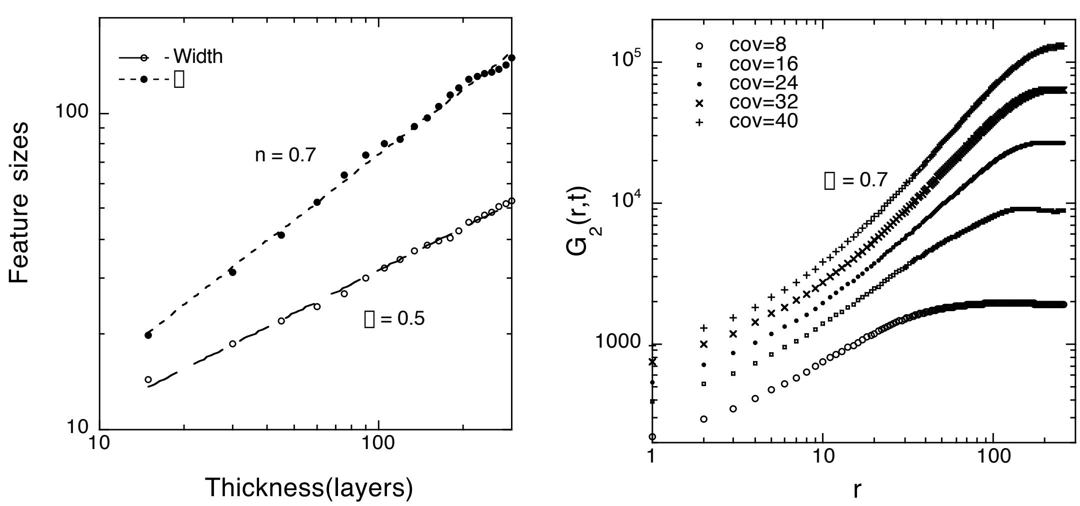

Fig. 10: BD with Cos Distribution in 3D (L = 1k Th 40)

Table I

	n	□	□	□
Expt.	0.85	0.88	0.75	4.6
3D BD (cos)	0.7	0.7	0.5	3.1
3D BD (slide)	0.65	0.5	1.0	*no pwr law*
3D BD (vert)	0.2	0.2	0.1	*no pwr law*
3D DLA	0.7	0.3	0.7	1.2
2D BD (cos)	0.7	0.5	0.6	2.6
2D BD (slide)	0.67	0.5	1.0	*no pwr law*
2D BD (vert)	0.56	0.35	0.30	*no pwr law*
2D DLA	1.2	0.4	1.4	1.7

III. Conclusions/Discussion

Our results indicate that shadowing and sideways growth (overhangs) are necessary to observe power-law height fluctuations. This is a new mechanism for producing power-law noise. Comparatively, in the absence of shadowing and sideways growth no power-law height fluctuations are observed in 3D. Table I shows a summary of our results. As can be seen our values are lower than those observed in the experiment; we expect that the experiment lies somewhere in between the cosine, in which there are both shadowing and sideways growth, and the sliding, in which there is shadowing and fast surface diffusion. For example if an average is taken of the □ for cosine and sliding a value of 0.75 is returned, which is comparative to that of the experiments result for □. It is also important to note that simulations with shadowing and sideways growth lead to a porous film and anomalous scaling of the height-difference correlation function, which is consistent with the experiment. It is also possible that deviations from the simple power-law observed in experiment could be due to competition between shadowing and sideways growth with surface diffusion ("sliding").

Some of the future work to be conducted on this matter is further study into the height-difference distribution $P_{□}$(□h) for a model with limited surface diffusion, as well as for a model with finite vapor density (vapor diffusion length). Also further investigation on the dependence of $P_{□}$(□h) on distance □ could be studied. Finally, analysis of $P_{□}$(□h) for sputter deposited CdS film whose surface profile was previously measured via AFM by University of Toledo REU student Ryan Snyder.

References

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