"Novel Mechanisms on the Growth Morphology of Films"

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ABSTRACT

Random surface roughness very often can occur during the growth or etching of films under non-equilibrium conditions. Several competing mechanisms such as noise, surface diffusion, and shadowing all play a role in the evolution of surface roughness. However, recent results obtained in many growth and etching processes exhibit an unusual tendency: the morphology is very rough where it is expected to be smooth and vice versa. The origin, we believe, is due to the fact that during the deposition and etching processes the atoms very often do not stick to the surface upon their first strikes. Atoms actually bounce around before all settle on surface sites. This non-unity sticking probability can lead to a very rough surface during etching and a very smooth surface during sputter or chemical vapor deposition that cannot be explained by the conventional mechanisms.

INTRODUCTION

It is common knowledge that during either deposition or etching of a film the surface (growth or etch front), very often tends to become rough under a wide variety of processing conditions. With the recent development of modern characterization tools including real space imaging and diffraction techniques, the growth front roughness evolution can be studied quantitatively [1]. Large amounts of data have been reported in the literature. However, quantitative understanding of the roughening phenomena is far from complete. The conventional models [2,3,4] that include noise, surface diffusion, and shadowing effects cannot explain much of the roughening data obtained by common deposition and etching methods such as sputter deposition, chemical vapor deposition (CVD), and plasma etching. In this work we shall show, in addition to surface diffusion and shadowing, that non-unity sticking coefficient can play a very important role in understanding many roughening phenomena.

EXPERIMENTAL SURVEY

Figure 1 shows four commonly employed deposition techniques: thermal evaporation, sputter deposition, chemical vapor deposition, and oblique angle deposition. Included also in Fig. 1 is a graph showing the incident flux distribution for various deposition techniques. The θ is defined as the angle between the surface normal and the direction of the incidence beam of atoms. Every often the deposition is performed at sufficiently low temperature and the surface diffusion is not strong enough to completely smoothen the growth front. Any fluctuations at the growth front would therefore cause some initial non-uniformity or roughness across the surface.

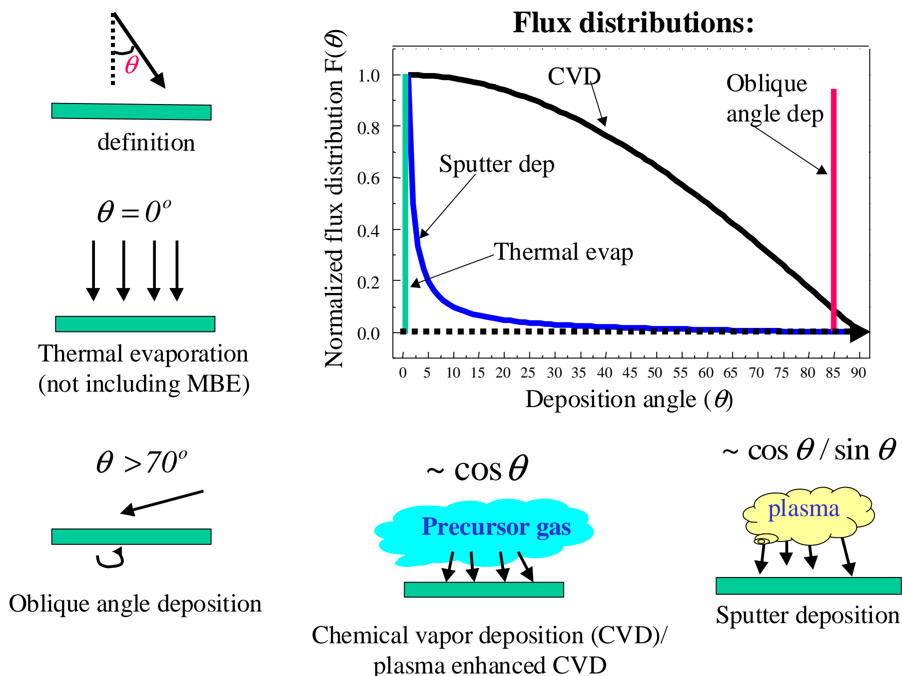

Fig. 1. Schematic diagrams showing the geometries of several commonly employed deposition techniques. The inset is a plot of the incident flux distribution of the atoms arriving at the substrate in different deposition techniques.

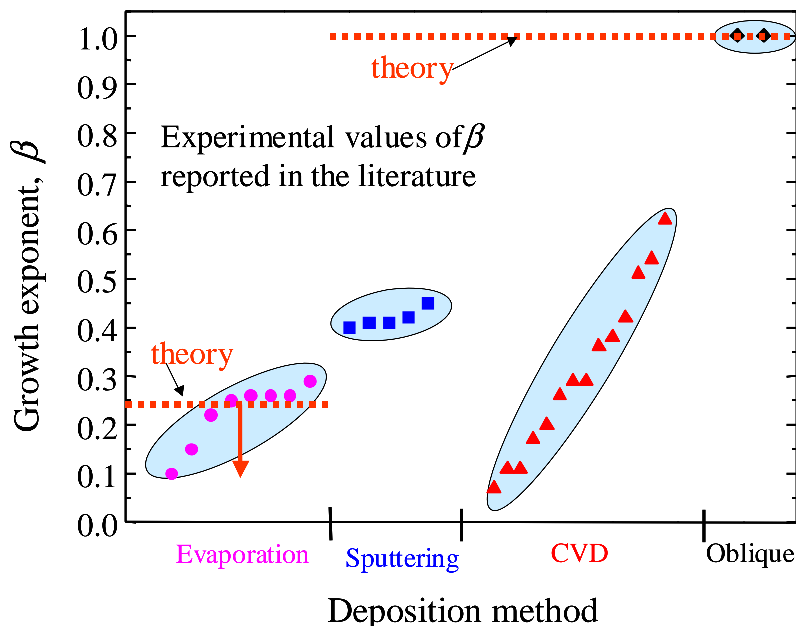

Fig. 2. A survey of experimentally obtained values of growth exponent β reported in the literature for different deposition techniques.

There are at least three important parameters required to quantify the roughness of a surface, the root-mean-square roughness (RMS), lateral correlation length, and the roughness exponent (describing how wiggly the local surface is) [1]. But in this report we shall only concentrate on the RMS roughness, which is defined as $\omega(t) = \sqrt{[h(r,t) - \langle h \rangle]^2}$, where $h(r,t)$ is the height of the surface at a position r and time t, and $\langle h \rangle$ is the average height at the surface. In most of the growth phenomena, the RMS grows as a function of time in a power law form [2], $\omega \sim t^{\beta}$, where β is the "growth exponent" ranging between 0 and 1. $\beta = 0$ for a smooth growth front and $\beta = 1$ for a very rough growth front (the RMS could be as large as the film thickness). Figure 2 shows a collection of experimental β values reported in the literature [5]. Theoretical predictions (all based on unity sticking coefficient) basically fall into two categories. One involves various surface smoothing effects, such as surface diffusion, which lead to $\beta \leq 0.25$ [2,3,4]. The other category involves the shadowing effect (which always occurs in sputtering and CVD) during growth which would lead to $\beta = 1$ [6]. With shadowing, any surface smoothing effects cannot reduce the value of β to less than one.

MONTE CARLO SIMULATIONS

In Fig. 2, a large number of data points are left unexplained. In particular, the sputtering data appears to be crowded around 0.4 to 0.5. Obviously the anticipated value of 1 was not realized in realistic experiments. Figure 3 (left) shows such a surface. It is a sputter deposited Si/Si at room temperature [7]. ω is ~3.2 nm for a film of about 3µm thick. The measure β value is ~0.41. To explain this discrepancy, we performed a series of Monte Carlo simulations that include the possibility of varying the sticking coefficient s_o for different diffusion rate *D/F* for the case of sputtering (flux $\sim \cos\theta/\sin\theta$). *D/F* is defined as the number of surface atoms participating in the jump per incident atom. The details of the basic processes used in the code are given in Ref 7. We took into account surface diffusion, shadowing, and re-emission effects (non-unity sticking coefficient) in our simulations. We assume that when an atom first strikes the surface at point A at the surface (see the inset in Fig. 4), it has a sticking coefficient of s_o. When the atom bounces from the position A to strike the surface at position B, the sticking coefficient is unity. The results are plotted in Fig. 4.

Figure 4 shows that varying the sticking coefficient can change qualitatively the behavior of β while surface diffusion can result only in quantitative change in β. At small sticking coefficient, surface diffusion has little effect and the surface always tends to be smooth (small β). Also, surface diffusion has little effect at high sticking coefficient and surface tends to be rough (β ~1). Some changes of β are seen for intermediate values of the sticking coefficient due to surface diffusion. But the shadowing and non-unity sticking coefficient are shown to have a larger effect on the growth exponent than surface diffusion.

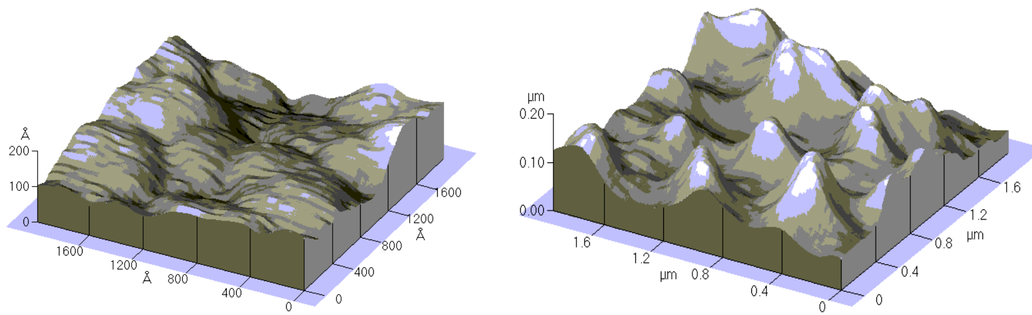

Fig. 3. Left: an AFM image of sputter deposited Si on Si. The film is about 3µm thick with a RMS roughness of ~3.2 nm. Right: an AFM image of a Si surface etched in a plasma environment. 3µm Si thick has been removed and the surface has a RMS roughness of 36 nm. Note the difference in the scales for the two images.

For sputter deposition it is known that very often the sticking coefficient s_o is not unity due to the energetic of the depositing particles, which can be 1 - 10 eV. For example, sputtered Si atoms may have a sticking coefficient around 0.5 - 0.7 [7]. Upon the first strike, the re-emitted atoms will have a lower energy due to the loss of energy during the first impact and the sticking coefficient of the second impact will be large (assumed to be 1). This can give a growth exponent β around 0.4 - 0.5 that was observed experimentally (Fig. 2). Although Fig. 4 is plotted for sputter deposition where the incidence flux is ~$\cos\theta/\sin\theta$, qualitative behavior of the growth exponent should also apply to the case of CVD where the incidence flux ~$\cos\theta$ [8]. For CVD, the precursors usually do not stick to the surface upon the first strike. In fact, the sticking coefficient depends on the chemistry and the substrate temperature and has a wide range of values. It is not surprising that the growth exponent reported in the literature (Fig. 2) exhibits a wide range of values.

ETCH FRONT ROUGHENING

For an etching process, the etchants arrive and react with the surface atoms to form volatile species. The volatile species would leave the surface and leave vacancies on the surface. For plasma etching the incidence flux is a cosine function. If the sticking coefficient is unity, then as time evolves, the shadowing would lead to a smoothing of the surface to give β ~0. The effect is just the opposite of the growth case. During the etching, the top of the hills gets removed and the valleys are not exposed to the etching flux. Thus for a large sticking coefficient, the etching leads to the smoothing of the growth front.

However, if the sticking is not unity, as in many etching cases using etchants such as CF_4, the etchant can reach the valleys of the surface. Therefore the atoms at the valleys can be removed and the valleys get deeper to form a rougher surface (large β) [9,10]. Figure 3 (right) shows such a surface. It is a plasma etched Si surface. The surface RMS roughness ω is ~36 nm after etching of 3µm deep. The measured value of β is ~1. The simulated results of the growth exponent as a function of the sticking coefficient are shown in Fig. 5. In this simulation the surface diffusion is not included. Just like in the case of

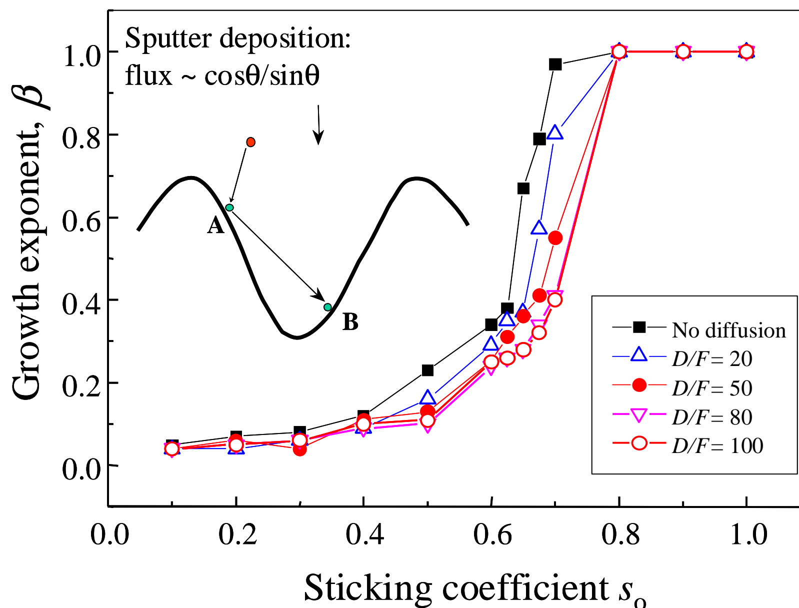

Fig. 4. Monte Carlo simulated β value as a function of sticking coefficient s_o for sputter deposition. We assume that the sticking coefficient of the second strike at the surface for the re-emitted atom is 1.

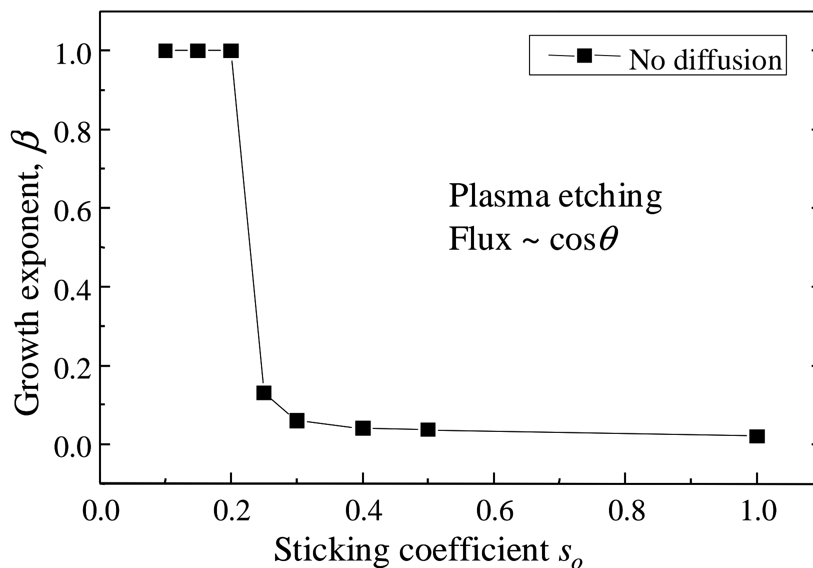

Fig. 5. Monte Carlo simulated growth exponent β as a function of the sticking coefficient for plasma etching of a surface. Diffusion is not considered in this simulation. Diffusion will not change the qualitative nature of the result.

deposition, we expect the surface diffusion would not change the curve qualitatively. The simulation results would explain why $\beta \sim 1$ in several Si etching experiments.

CONCLUSION REMARKS

In conclusion, we have shown that the sticking coefficient plays a decisive role in the interpretation of surface roughness evolution of commonly employed deposition and etching techniques. In particular, the relatively smooth morphology obtained in sputter deposition and chemical vapor deposition can be explained by a non-unity sticking coefficient upon the first impacts of the incident atoms on the surface. On the other hand the very rough surface generated by plasma etching can be explained by a similar mechanism, that is the non-unity sticking coefficient during the first impacts of the etchants on the etch front.

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