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Computer Simulation of Thin Film Growth via Sputter Deposition

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Abstract

This report looks at properties of surfaces produced by sputter deposition simulations of film growth. In this research, we present computer-simulated results directed at understanding the surface morphology of thin film growth. The columnar growth model includes surface diffusion and trajectories of atoms sputtered form a target onto a substrate. From results obtained using the height-height correlation function, the surface width and column width was calculated. Inclusion of the cosine angular distribution gave results similar to those obtained experimentally. The coarsening exponent, n = 1 and the growing exponent, $\beta = 1$. Experimentally, the results for $\beta = 1$ and n = .73. The model mimicked the growth of thin film at intermediate temperature. In this report, a background summary of the meaning of sputter deposition will be given along with the results and discussion of the simulations carried out.

Introduction

Sputter deposition is an industrial process used for growing thin film and coating of solar cells.

In sputter deposition, atoms are knocked form a target by Argon ions in plasma and then scattered by the Argon gas before deposition onto the substrate. In fig.1, the target is attached to the cathode and the substrate is attached to the anode. A D.C. voltage is applied, and when the applied voltage reaches the ionization energy of the Argon gas, electrons collide with the Argon atom, ionizing it and creating plasma. The positively charged Argon ion quickly accelerates towards the cathode knocking out atoms that then travel towards the anode and depositing on to the substrate.

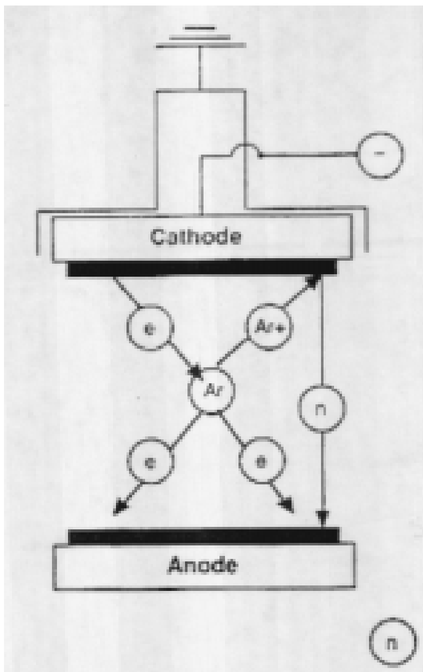

Fig. 1 A schematic of the sputter deposition process

In sputter deposition, the atoms are deposited on the surface from a wide range of angles. A large distribution of angles leads to shadowing of lower levels by higher levels. This is known as the shadow instability or the shadowing effect. There are two distributions of the angles: cosine angular distribution corresponding to atoms directly falling vertically as they come of the target and uniform angular distribution having a wide range angles. For simulation purposes, the cosine angular distribution fits the experimental results better than uniform angular distribution.

There are essentially three growth modes in sputter deposition. The first, zone I, is at low temperature. In this growth mode, atoms stick to surface and do not diffuse. This gives a “porous”columnar structure. In zone II, at intermediate temperature, atoms can diffuse to lower energy sites but not fast enough to smooth the surface. This is essentially the surface morphology in which we are studying. At the third growth mode, zone III, the temperature is high enough where atom diffusion is large and grains can form and grow both vertically and laterally with only a small amount of shadowing.

In order to study the surface morphology of the columnar growth model, a mathematical method was obtained to determine the surface width and column width of the structures. In this model, the height-height correlation function was used for calculations. In this, equation($G(r) = <(h(0) - hav)(h(r) - hav)>$), the product of the two fluctuations was determined a distant r away from the origin. From these results, exponential values associated with surface and column width were obtained.

Method

A computer simulation of ballistic film deposition consists of particles falling vertically in straight lines onto random points on a substrate. A modified version of the ballistic deposition model was written in C to produce a model sputtered deposited with a range of angles. For the simple model, atoms deposit one at a time on a one-dimensional surface to produce a two dimensional film. In the simple two-dimension model, if an atom hits the side to a 'column' it diffuses to the bottom where it remains. If the atom lands on top of a 'column, it can 'diffuse' one column to the left or one column to the right depending on which column is lower. If the columns are of equal height, the atom remains where it dropped. Because atom diffusion is not a fast process the shadowing effect leads to dense columnar structure. The computer code was further modified for a two dimensional surface to produce a three dimensional film. In this version, atoms can diffuse more than one time.

Results

Films were analyzed for several different system sizes. The range of system size was 100 to 131K. The program was modified several times to obtain results for both the cosine angular distribution as well as the uniform angular distribution. For the cosine distribution program, the growth exponent beta associated with the surface width was calculated to be 1. The coarsening exponent p (rc ~<h>^p) was calculated at .7 (fig.2a). These results are close to experimental values with beta = 1 and p = .73. For the case of the uniform angular distribution, beta was found to equal1 however p was equaled .87 (fig2b). By comparing these results with experimental results, it was concluded that the cosine angular distribution best fits the experimental process of growing films produces by sputter deposition.

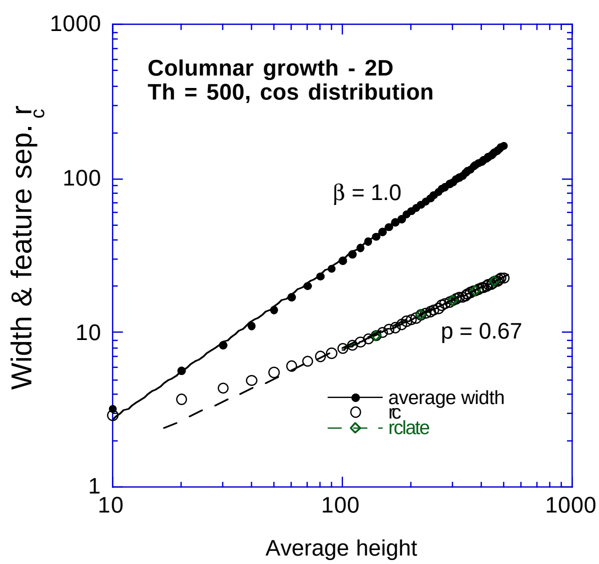

Fig.2a Results obtained with cosine distribution

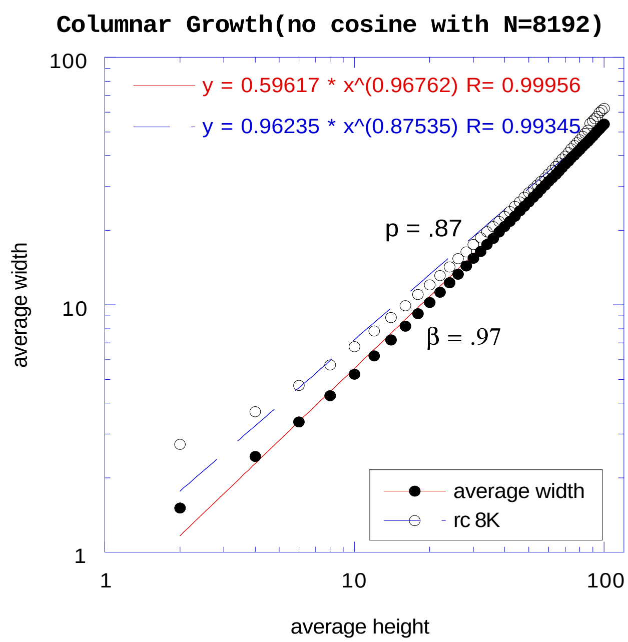

Fig.2b Results obtained with uniform distribution

It is interesting to not that for the case of the uniform angular distribution,, a wide distribution of column heights was quickly formed and one column height quickly dominated the system. Since it is known that a larger argon pressure can lead to a range of angles close to a uniform distribution, these results indicate that to grow good quality film by sputter deposition, the agron gas should not be too high. It was interesting to compare our results with those obtained by others using a continuum model for which a uniform angular distribution was assumed. While these results were almost certainly limited by the small size of the system, they also indicate an effective coarsening exponent smaller than the experimental value.

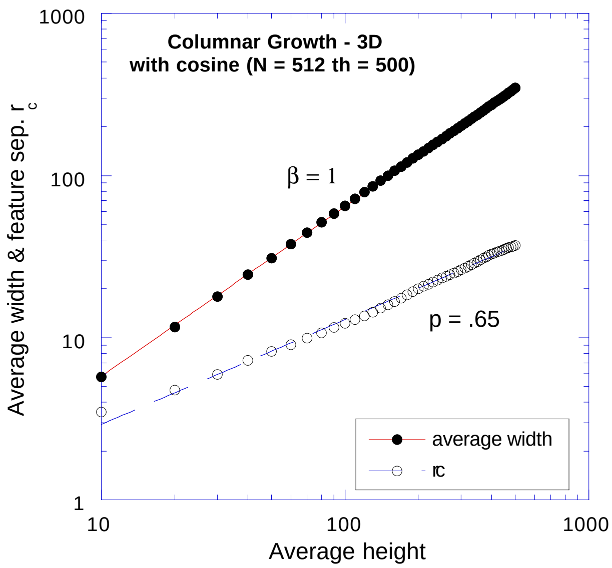

Fig.3a Values for β and rc in three dimension with cosine

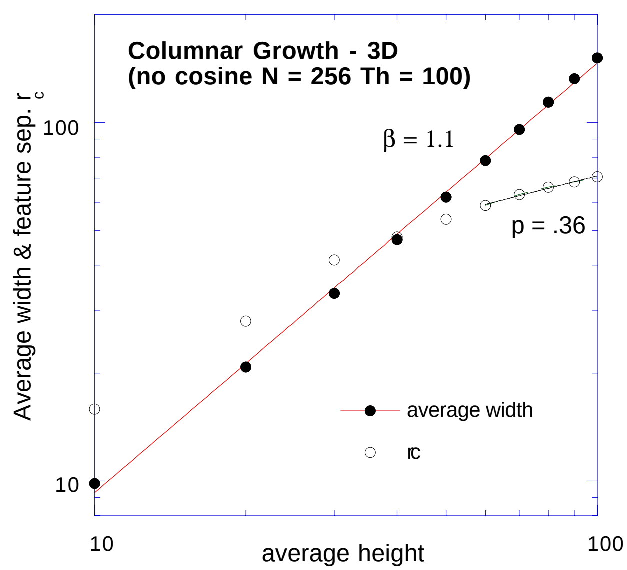

Fig.3b Values for β and rc in three dimension without cosine

Conclusion

In conclusion, simulations of two-dimensional and three-dimensional discrete models of columnar growth were carried out and the data was analyzed. It was found that there was good agreement with experimental values using the cosine angular distribution in the program. From the simulations, it was seen that uniform angular distribution lead to anomalously large shadowing where one column dominated the entire system.

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