University of Toledo REU Program
Summer 1998

Atomic Force Microscopy Analysis of Microstructure Evolution and Morphology of Magnetron-Sputtered CdS Thin Films

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ABSTRACT

Using atomic force microscopy, the surface morphology and microstructure of magnetron-sputtered CdS thin-films grown at 250 C on glass substrates were studied as a function of film-thickness with thicknesses ranging from 50 A to 1 μ. For each thickness, the height-height difference and product correlation functions G(r) and $G_2(r)$ were used to calculate the surface width and typical grain size r_c. From these results, values for the growth exponent $\beta = 0.82$, surface roughness exponent $\alpha = 0.5 - 0.7$ and coarsening exponent $n = 0.7$ were calculated. For small and intermediate thicknesses, anomalous scaling of the height-difference correlation function was observed, indicating an increase of the average grain angle with thickness as well as a large distribution of grain-angles. However, at large thicknesses the average grain angle was found to saturate while the grain angle distribution narrowed. The large value of β as well as the rapid increase in the average grain angle at small and intermediate thicknesses indicate the existence of an instability during the sputter deposition process. We conjecture that this instability is due to "shadowing" which occurs as a result of scattering of incoming Cd and S atoms by the Ar plasma during the deposition process and leads to a range of incident angles for deposition. Such instability can lead to grooves between the grains and "pinholes" which can destroy a completed CdS/CdTe solar cell. We suggest some methods to eliminate shadowing during the deposition process and thus eliminate the instability.

I. Introduction

In this work, we studied the kinetics of growth for CdS on boro-
magnetron sputtering at 250°C. CdS is a n-type material used in creating the
in a solar cell. It was our objective in this study to learn more abo
mechanism of these films from magnetron sputter deposition. We hope t
to develop ideas on how to grow a more efficient solar cell. These re
used to guide future computer simulations of the thin-film depositior

Atomic force microscopy (AFM) was used to collect height informa
CdS films, and the data collected allowed us to study the morphology
various thicknesses. AFM was developed from the Scanning Tunneling M
it uses a small cantilever (about 0.1 mm long) with a small tip. The
underneath the cantilever, and the cantilever is scanned line by line
the sample with the tip in direct contact with the sample surface. A
scanner head of the AFM is directed at a mirror that must be adjusted
beam directly over the tip. The forces between the tip and the canti
cantilever to bend, and a position—sensitive photodetector (PSPD) mea
deflection of the laser beam as the sample is moved under the tip. Th
displacements of light as small as 10 angstroms. The ratio of the pat
cantilever and the detector to the length of the cantilever itself re
amplification. This allows sub-angstrom resolution in the vertical di
capability of the AFM to carry out small scan sizes allows for a comp
the horizontal direction.

As the tip of the AFM is brought closer to the surface, the atom
van der Waals forces. This attraction increases until the atoms of th
are brought so close together that their electron clouds begin to rep
electrostatically. This repulsion weakens the van der Waals force as
separation continues to decrease. The total force goes to zero when t
reach a couple of angstroms apart, about the length of a chemical bon
force becomes positive (repulsive), the tip and sample are in contact
electrostatic force balances any force that tries to push the tip and
When the cantilever pushes the tip against the sample, the cantilever
forcing the tip and sample atoms closer together. Due to this electr
care must be taken to ensure that the tip does remain in contact with
repulsive force can occasionally force the tip away from the sample r
resolution.

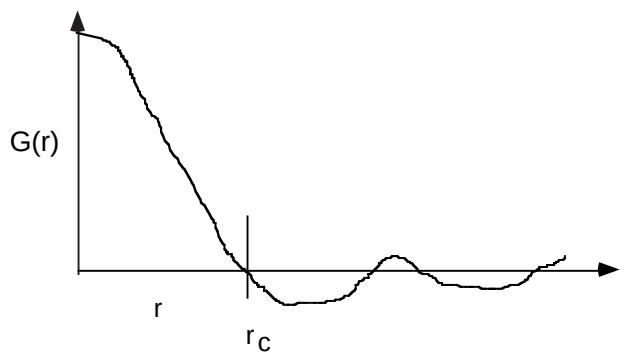
II. Analysis

The surface morphology of the CdS thin films was quantitatively
the height-difference correlation function $C_2(r)$ and the height-height correlation f
G(r) where r is the distance from a selected origin in nanometers. G
$C_2(r) = \langle (h(r) - h(0))^2 \rangle$
where h(r) is the height of the film a distance r from the origin in
the height of the film at the origin. The value for the difference in

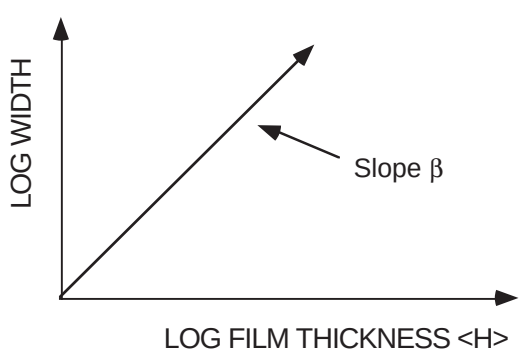
averaged over the entire surface. The height-height correlation funct represented by the expression <(h(0) - <h>)(h(r) - <h>))> where <h> i height of the sample.

At small length scales, one expects $G_2(r) \propto r^{2\alpha}$ where α is the roughness exponent. However, at larger length scales $G_2(r)$ saturates. The value at whi $G_2(r)$ saturates would be expected to increase with thicker samples si height difference at larger length scales. The distance r from the or saturation occurs should increase with thickness as well since the gr coarsen as the film thickness increases. Normally, the value of $G_2(r)$ at very small distances from the origin would not be expected to change with increa However, if the value for $G_2(r)$ for small r increases with film thickness, thi grains with increasing slopes.

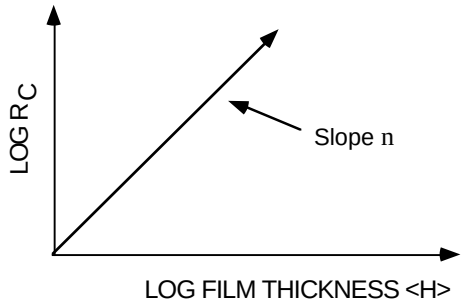
The G(r) graph shown below shows that the G(r) curve crosses th value r_c which is approximately the lateral size of the grains.



The square root of G(r) at r = 0 is the root mean square (rms) fluctu sometimes known as the width. The width is expected to vary as $\langle h \rangle^{\beta}$ where β is the growth exponent.



The r_c value varies as $\langle h \rangle^n$ where n is the coarsening exponent, and its v indicates how fast the lateral size of the grains are growing with in thickness. The rms width ($G_2(r_c)$) was also plotted as a function of f to provide information about the angle at which the grains of CdS wer



A computer program was written to calculate G(r) from the AFM height, sample width, value and for r as a function of distance from an origin. For each sample, r_c and w_c were calculated. The width values for each sample were used to measure α and β, respectively

Results

Figure 1 shows the correlation function G(r) for a typical sample. The thickness for this plot was 2000 Angstroms, and the r_c value, where the curve crosses the x-axis is approximately 500 angstroms.

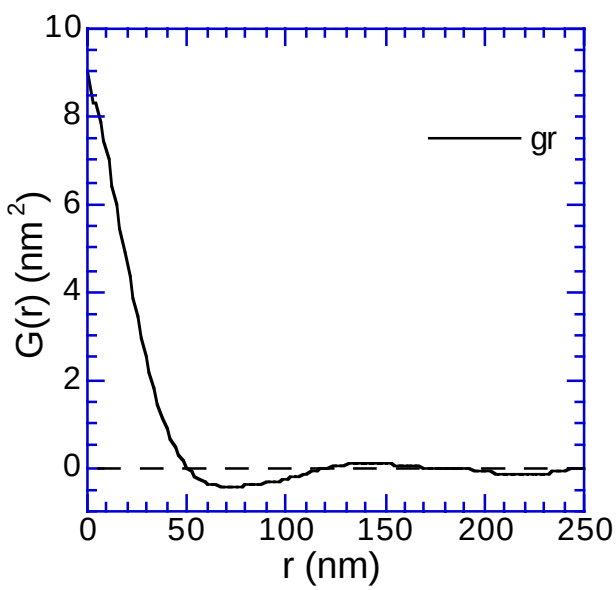


Figure 1. G(r) curve for a 2000 A sample of CdS on BSG

Figure 2 shows the $G_2(r)$ curves for all samples grown on BSG glass. A seen (except for the 5000 A sample) the $G_2(r)$ value at which each sample begins to saturate increases with sample thickness. The increase in $G_2(r)$ for thicker samples is expected since the surface should become rougher due to more variatio increase in $G_2(r)$ at initial r values for the thinner samples (50 – 300 A slope of the grains is increasing. The samples from 500-2000 A all sh initial value for $G_2(r)$, but the α values around 0.6 indicate that the angles at w grains are choosing to grow is still very random. The samples with t and 10000A give α values of 0.7 (close to 1) indicating the grains are st preferred angle at which to grow.

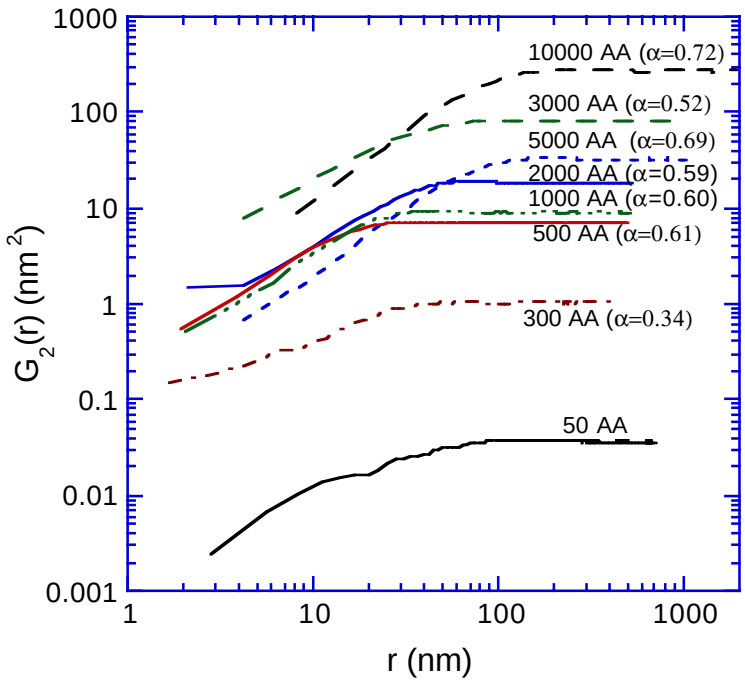


Figure2. The $G_2(r)$ curves for sample thicknesses from 50 to 10000 A

Figure 3 displays the width as a function of film thickness. The indicates a value for the growth exponent β of about 0.82. This indicates a possibl instability because the rms width is growing almost as fast as the he Figure 3 does show that the samples are becoming rougher for increas the roughness is growing much faster than expected.

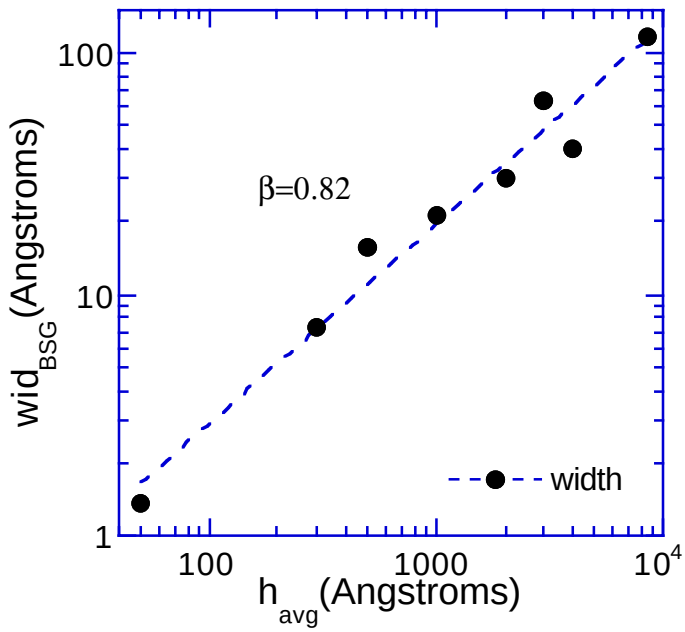


Figure 3. The root-mean square width of G(r) with r = 0 for sample thickness

Figure 4 shows how the value of r_c varies as a function of film thickness. The coarsening exponent calculated with a fit to the last 6 data points was 0.69. The first two data points on Figure 4, corresponding to f

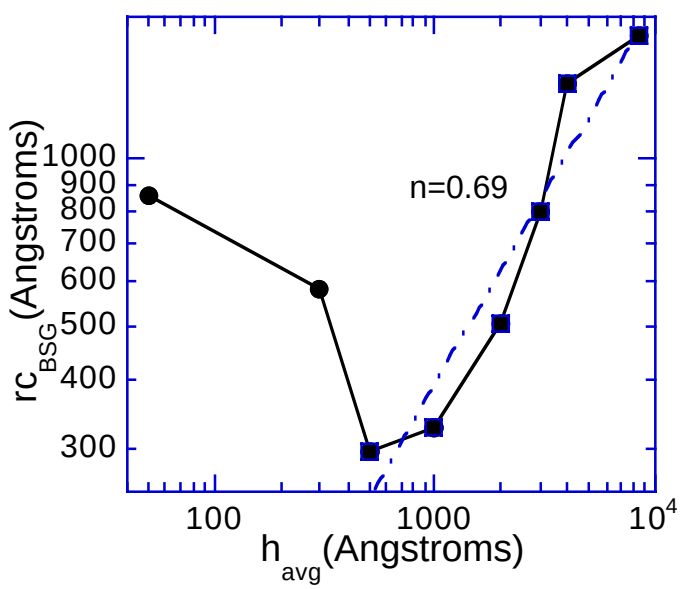


Figure 4. r_c as a function of sample thickness with a power law fit to the data to measure the coarsening exponent n

and 300 A, have very large γ values given their thickness. This is probably d
initial roughness of the raw BSG glass. An AFM scan of the raw BSG s
an rms width value of about 50 A which on Figure 3 would place it in
thicker samples with heights measuring thousands of angstroms. The va
coarsening exponent n is somewhat similar to the β value of 0.82 from Figure 3. The
similarities in the two numbers indicate the grains of thicker are f
at which to grow.

Figure 5 displays how the value of width/r_c varies as a function of film thickne
The thinner films show that the rms width is increasing faster than r
samples there is evidence of a saturation indicating, as mentioned be
sample are finding preferred angles at which to grow.

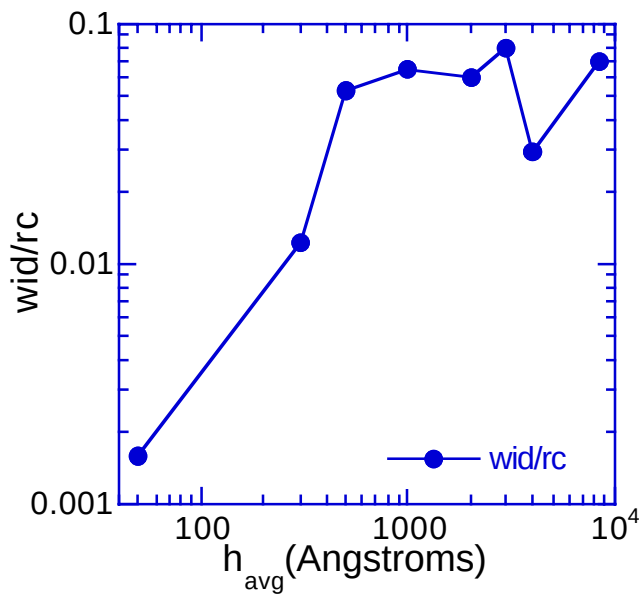


Figure 5 . width/r_c as a function of sample thickness

Figure 6 shows how the width of samples of CdS deposited on bor
compared to the width of CdS samples deposited on microscope glass.
taken on the microscope glass presented a growth exponent β of 1.1 fo
thicknesses 1000, 4750, and 9200 angstroms. It is unlikely that the
continue if more samples deposited on microscope glass were analyzed
results do lend evidence to the initial roughness of the surface not
the rms width. A more complete study may provide different findings,
grew similarly on BSG glass and microscope glass.

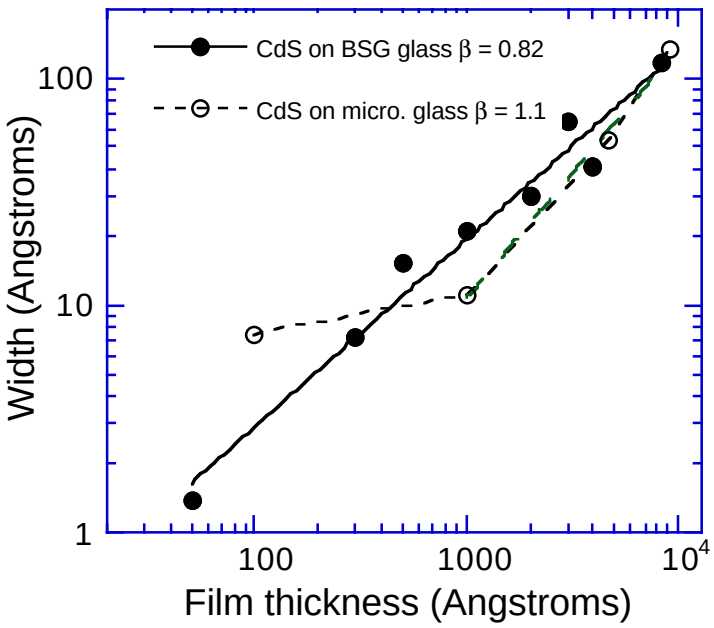


Figure 6. Comparison of rms width as a function of film thickness for CdSdeposited on BSG glass and microscope glass

Conclusions

There have been great efforts devoted to understanding the kinetic roughening of growing surfaces with various techniques. Jeffries, Zuo, and Craig [1] studied the growth of Pt sputter deposited on glass at room temperature for film thicknesses of 15-140 nm. A roughness exponent (α =0.9) and a growth exponent (β =0.3) were measured to conclude that the growth was consistent with linear diffusion dynamic Krim [2] studied scaling behaviors of vapor-deposited silver onto qua temperature and found similar results for the roughness (α = 0.82) and growth exponents (β = 0.29). Zeng and Vidali [3] measured similar values for growth (roughness exponents (β = 0.3) for growth of Pb on Cu(100) using helium beam at 150 K.

Our results differ from those presented above. Our roughness exp smaller, and it indicated that our samples needed to be grown higher saturate and approach a preferred angle of growth. The lower value of experiments may be due to the higher growth temperature of 250 C used experiments. It should be mentioned that the magnetron-sputtering pro these samples involved Ar ions hitting a target and knocking off Cd and S atoms. The ejected CdS then travels through an Ar plasma before being deposited Collisions with the Ar plasma most likely lead to a wide range of dep better understanding of how the Ar plasma interacts with the CdS cou understanding our results.

The r_c values displayed in Figure 4 are very high for the thin sar 300 A. A possible explanation for this fact is the initial roughness presents data that shows the rms width of CdS deposited on microscope

surface, growing similarly to CdS on BSG. A more complete study of t
glass and measurement of r_c values could provide insight into why high r
found for thin samples.

Probably the most interesting result is the β value of 0.82. The experiments mentioned above attained growth exponent values of 0.3. The possible the large value in our experiment an effect called shadowing. When Cd knocked off the target by Ar ions, they travel through the Ar plasma deposited on the surface. This Ar plasma interacts with the CdS in su allow the CdS to be deposited on the surface at a wide range of angle toward the surface at these wide angles may be blocked by peaks on th previously deposited. This allows the peaks to grow higher and the rn fast as a result . CdS will still be deposited in the valleys if it a suitable angle, but the large β seems to indicate that shadowing is taking

This rough surface may affect the efficiency of the solar cell. pinholes inhibiting the function of the pn junction in a CdS/CdTe so way to correct for this shadowing effect is to rotate the substrate a deposited. Changing the conditions of the Ar plasma such as voltage, field strength, etc. may also correct this effect.

These experimental results certainly provide many exciting areas to be studied. Computer simulations can be done to try and model the plasma to come to a better understanding of how it interacts with the CdS. More AFM work can be done with microscope glass as the substrate and with SnO_2 coated glass which is currently the substrate used for CdS/CdTe solar cells.

References

[1] J.H. Jeffries, J.-K. Zuo, and M.M. Craig, Phys. Rev. Lett. 76, 4931 (1996).
[2] G. Palasantzas and J. Krim, Phys. Rev. Lett. 73, 3564 (1994).
[3] H. Zeng and G. Vidali, Phys. Rev. Lett. 74, 582 (1995).