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 µm. 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 \( \beta \) 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 about
mechanism of these films from magnetron sputter deposition. We hope to
develop ideas on how to grow a more efficient solar cell. These results
used to guide future computer simulations of the thin-film deposition.

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 cantilever:
cantilever to bend, and a position-sensitive photodetector (PSPD) mea-
deflection of the laser beam as the sample is moved under the tip. The
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 direction.
As the tip of the AFM is brought closer to the surface, the ato-
van der Waals forces. This attraction increases until the atoms of the
tip are brought so close together that their electron clouds begin to repel
 electrostatically. This repulsion weakens the van der Waals force as
separation continues to decrease. The total force goes to zero when the
reach a couple of angstroms apart, about the length of a chemical bond;
force becomes positive (repulsive), the tip and sample are in contact
electrostatic force balances any force that tries to push the tip an
When the cantilever pushes the tip against the sample, the cantilever:
forcing the tip and sample atoms closer together. Due to this elect:
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;
resolution.

II. Analysis

The surface morphology of the CdS thin films was quantitatively
the height-difference correlation function \( G(2r) \) and the height-height correlation function \( G(r) \) where \( r \) is the distance from a selected point in the film to the origin:

\[
G(r) = \langle (h(r) - h(0))^2 \rangle
\]

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 function is represented by the expression \( <(h(0) - <h>)(h(r) - <h>)> \) where \(<h>\) is the height of the sample.

At small length scales, one expects \( G_2(r) \) to increase as \( r^\alpha \), where \( \alpha \) is the roughness exponent. However, at larger length scales, \( G_2(r) \) saturates. The value at which \( G_2(r) \) saturates would be expected to increase with thicker samples since the height difference at larger length scales. The distance \( r \) from the origin at which \( G_2(r) \) saturates should increase with thickness as well since the grains coarsen as the film thickness increases. Normally, the value of \( G_2(r) \) at small distances from the origin would not be expected to change with increasing film thickness. However, if the value of \( G_2(r) \) for small \( r \) increases with film thickness, this would indicate increasing slopes.

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

The square root of \( G(r) \) at \( r = 0 \) is the root mean square (rms) fluctuation sometimes known as the width. The width is expected to vary as \( \sqrt{<h>^b} \) where \( b \) is the growth exponent.

The \( r_c \) value varies as \( <h>^n \) where \( n \) is the coarsening exponent, and indicates how fast the lateral size of the grains are growing with film thickness. The rms width (Fig. 4) was also plotted as a function of film thickness to provide information about the angle at which the grains of CdS we...
A computer program was written to calculate \( G(r) \) from the AFM height function of distance from an origin. For each sample, the values for \( r_c \), \( \alpha \), and \( \beta \) were calculated. The width values for each sample were used to measure \( x \), \( \alpha \), and \( \beta \), respectively.

**Results**

Figure 1 shows the correlation function \( G(r) \) for a typical sample thickness for this plot was 2000 Å. The curve crosses the x-axis at the \( r_c \) value of approximately 500 angstroms.

![Graph showing \( G(r) \) curve](image)
Figure 2 shows the $G_2(r)$ curves for all samples grown on BSG glass. It is seen (except for the 5000 Å sample) that the 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 variation in growth. The samples from 500–2000 Å all show an increase in the initial value for $G_2(r)$ at initial $r$ values for the thinner samples (50 – 300 Å). The slope of the grains is increasing. The samples from 500–2000 Å all show an increase in the initial value for $G_2(r)$ at initial $r$ values around 0.6 indicate that the angles at which the grains are choosing to grow is still very random. The samples with 500, 1000, and 10000 Å give values of 0.7 (close to 1) indicating the grains are still preferred angle at which to grow.

Figure 3 displays the width as a function of film thickness. The data indicate a value for the growth exponent $\beta$ of about 0.82. This indicates a possible instability because the rms width is growing almost as fast as the height. Figure 3 does show that the samples are becoming rougher for increased thickness, and the roughness is growing much faster than expected.
Figure 3. The root-mean square width of $G(r)$ with $r = 0$ for sample thickness $e$.

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 $f_1$, was 0.82.

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

$n=0.69$
and 300 Å, have very high values given their thickness. This is probably due to the initial roughness of the raw BSG glass. An AFM scan of the raw BSG sample showed an rms width value of about 50 Å which on Figure 3 would place it in the class of thicker samples with heights measuring thousands of angstroms. The coarsening exponent $n$ is somewhat similar to the value of 0.82 from Figure 3. The similarities in the two numbers indicate the grains of thicker are finding preferred angles at which to grow.

Figure 5 displays how the variable width/r$_c$ as a function of film thickness varies. The thinner films show that the rms width is increasing faster than the thicker samples. For thicker samples there is evidence of a saturation indicating, as mentioned before, that the grains are finding preferred angles at which to grow.

![Figure 5. width/r$_c$ as a function of sample thickness](image)

Figure 6 shows how the width of samples of CdS deposited on boro-silicate glass compared to the width of CdS samples deposited on microscope glass. A sample taken on the microscope glass presented a growth exponent $\beta$ of 1.1 for thicknesses 1000, 4750, and 9200 angstroms. It is unlikely that the results will continue if more samples deposited on microscope glass were analyzed. The results do lend evidence to the initial roughness of the surface not the rms width. A more complete study may provide different findings, but these results grew similarly 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 ($\alpha = 0.9$) and a growth exponent ($\beta = 0.3$) were measured to conclude that the growth was consistent with linear diffusion dynamics. Krim [2] studied scaling behaviors of vapor-deposited silver onto quartz temperature and found similar results for the roughness growth exponents ($\beta = 0.29$). Zeng and Vidali [3] measured similar values for growth (roughness exponent $\beta = 0.3$) for growth of Pb on Cu(100) using helium beam at 150 K.

Our results differ from those presented above. Our roughness exponent smaller, and it indicated that our samples needed to be grown higher to saturate and approach a preferred angle of growth. The lower value of $\alpha$ in our experiments may be due to the higher growth temperature of 250 C used in these experiments. It should be mentioned that the magnetron-sputtering process involves 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 deposited films, which may explain the lower roughness observed in our experiments.

The $\alpha$ and $\beta$ values displayed in Figure 4 are very high for the thin sample. A possible explanation for this fact is the initial roughness, which presents data that shows the rms width of CdS deposited on microscope glass.
surface, growing similarly to CdS on BSG. A more complete study of the glass and measurement of \( r_c \) values could provide insight into why high \( r_c \) values were found for thin samples.

Probably the most interesting result is the value of 0.82. The experiments mentioned above attained growth exponent values of 0.3. The possible 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 such a way to allow the CdS to be deposited on the surface at a wide range of angles toward the surface at these wide angles may be blocked by peaks on the previously deposited. This allows the peaks to grow higher and the CdS will still be deposited in the valleys if it is a suitable angle, but the large value seems to indicate that shadowing is taking place.

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 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\textsubscript{2} coated glass which is currently the substrate used for CdS/CdTe solar cells.

References