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Roughness of CdTe thin films grown on glass by hot wall epitaxy

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Abstract
CdTe films were grown on glass substrates using the hot wall epitaxy (HWE) technique. The samples were polycrystalline with a preferential (111) orientation. Scanning electron micrographs reveal a grain size between 0.1 and 0.5 µm. The surface morphology of the samples was studied by measuring the roughness profile using a stylus profiler. The roughness as a function of growth time and scale size were investigated to determine the growth and roughness exponents, β and α, respectively. From the results we can conclude that the growth surface has a self-affine character with a roughness exponent α equal to 0.69 ± 0.03 and almost independent of growth time. The growth exponent β was equal to 0.38 ± 0.06. These values agree with that determined previously for CdTe(111) films grown on GaAs(100).

1. Introduction
CdTe is recognized as a very attractive material for the fabrication of low cost and highly efficient electronic devices such as solar cells, gamma and x-ray room-temperature nuclear detectors and electro-optic modulators [1–3]. As an example, polycrystalline CdTe/CdS solar cells have achieved a very high conversion efficiency of 16% [4]. The growth techniques most used to produce CdTe thin films have been metal-organic vapour phase epitaxy, electrodeposition and closed space sublimation [5–7]. Independent of growth procedure, it has been shown that grain size and surface morphology are one of the most important aspects affecting the efficiency of these devices [8]. Therefore, understanding the growth dynamics and the process of surface morphology evolution is a key factor to further develop the applications of these materials.

Investigation of surface morphology in conjunction with dynamic scaling theory is an important tool for addressing the growth properties of thin films [9]. A parameter of easy physical interpretation used to characterize the surface morphology of a sample is its roughness, which can be considered as an inheritance of the growth process. It is defined as the root mean square value of the fluctuations of surface height h(x, ε) over a length scale ε along the x direction.
More explicitly, the roughness $w(\varepsilon)$ can be calculated by equation (1):

$$w(\varepsilon) = \left\langle \frac{1}{\varepsilon} \sum_{i=1}^{\varepsilon} h(x_i)^2 - \left(\frac{1}{\varepsilon} \sum_{i=1}^{\varepsilon} h(x_i)\right)^2 \right\rangle_j^{1/2},$$

where the brackets $\langle \cdots \rangle_j$ denote an average over the window position $j$ [10].

For a self-affine surface, the roughness $w$ over a range $\varepsilon$ satisfies the scaling law $w \sim \varepsilon^\alpha$, where $\alpha$ is known as the roughness (Hurst) exponent, and provides a quantitative measurement of the roughness of the growing surface. It is also assumed that the roughness $w$ changes with growth time $(t)$ as $w \sim t^\beta$, where $\beta$ is known as the growth exponent that characterizes the time-dependent dynamics of the roughening process. The determination of these exponents can be used to identify the main growth mechanisms involved in the film growth and help to better understand the deposition process [9].

Usually, the critical exponents, $\alpha$ and $\beta$, are obtained from surface images measured by atomic force microscopy (AFM) [11], which is very precise but is limited to areas of a few microns and has a limited number of points (512 or 1024). In this work we have used a stylus profiler with vertical resolution of 10 Å and lateral resolution of 10 nm to measure the rough profile. Such an instrument is cheaper than an AFM, can scan profiles with up to 25 mm and up to 50 000 points and can, therefore, be used to investigate larger samples with much higher roughness, which are not accessible to an AFM, but can also be used with our samples.

We have investigated a series of CdTe films deposited on glass substrates by hot wall epitaxy (HWE) with varying growth times. The samples were further characterized using x-ray diffraction, scanning electron microscopy, AFM and optical transmission. Details of the sample structural and optical properties will be published elsewhere.

2. Experimental details

The samples were deposited on glass substrates using the HWE technique. HWE is a very simple growth technique, used for the growth of compounds which evaporate congruently [12]. It has already proved to produce very high quality CdTe epitaxial layers in different substrate materials [13, 14]. The growth system used, which has been described previously [15], is maintained at a pressure of less than $1 \times 10^{-6}$ Torr during the growth and can control the growth rate from 0.01 to 5 Å s$^{-1}$. In this work, the source furnace, containing polycrystalline CdTe (99.999% pure), was maintained at 530 °C and the substrate temperature was 150 °C, resulting in a growth rate equal to 1.4 Å s$^{-1}$. The glass substrates were degreased, dipped in a 2% HF solution for 2 min, and thoroughly rinsed in deionized water just before their introduction in the growth system. The deposition times used varied from 30 to 450 min, resulting in film thickness between 0.4 and 6 μm, as determined by the stylus profiler.

Figure 1 shows key features of the structural characterization of the grown layers. Figure 1 shows the x-ray diffraction pattern of sample CdTe03 with 1.7 μm, measured using Cu Kα radiation. Although grown on glass substrates, the films obtained were highly oriented. As can be seen, only the {111} reflections are observed. All samples, independent of growth time, showed a similar pattern. In the inset one can see a scanning electron micrograph of the same sample, which reveals a mean grain size of about 0.2 μm. Optical transmission measurements, not shown here, showed the typical absorption of bulk CdTe, with an energy gap of about 1.5 eV at room temperature.

The height profiles $h(x)$ were measured using a stylus profiler (XP1—Ambios). The scanning length used in all measurements was 300 μm with a stylus force of $1 \times 10^{-2}$ N. Each
Roughness of CdTe thin films grown on glass by hot wall epitaxy

Figure 1. Diffraction pattern of sample CdTe03 (1.7 µm thick, growth time of 120 min), showing only \{111\} reflections. The inset shows a scanning electron micrograph, which reveals a mean grain size of about 0.2 µm.

Figure 2. A typical scan profile obtained for sample CdTe04 (growth time of 300 min).

sample was measured in four different locations and each location was measured at least three times. A typical profile is shown in figure 2.

3. Results and discussion

From the height profile \( h(x) \) we evaluated the roughness \( w \) of the profile using equation (1). The \( \log(w) \) versus \( \log(\varepsilon) \) plot shows a broad straight part extending over at least one decade. The slope of the line fitted to this straight part allows us to evaluate the roughness exponent. These results indicate that the CdTe surface morphology has a self-affine character.
Figure 3. Roughness as a function of window length for samples CdTe05 (growth time of 30 min) and CdTe03 (growth time of 120 min). The roughness exponents, determined from these plots, are 0.67 and 0.63, respectively.

Figure 4. Roughness exponent as a function of growth time for all samples studied. The value of $\alpha$ is approximately independent of growth time.

Figure 3 shows the scaling plot of the roughness as a function of scale length for samples with two different growth times. Since all profiles were taken in the same conditions (scan length and velocity), $\varepsilon$ is given here in number of pixels of the digitalized image.
Figure 5. Roughness for a 1000 points window length (a) and global roughness (b) as a function of growth time. The growth exponent is the same in both cases, but the error is smaller when using the first procedure.

The final value of the exponent $\alpha$ for each sample is obtained taking the average of the values determined from the twelve different profiles for that sample. In figure 4 we show the effect of growth time in the mean value of $\alpha$. As can be seen, within the experimental uncertainty, the roughness exponent is independent of the growth time, yielding an average value of $\alpha = 0.69 \pm 0.03$. This result indicates that the self-affine character of the CdTe surface morphology does not depend on the growth time. This value is approximately the same as has been measured previously for CdTe(111) layers grown on GaAs(100) by metal-organic chemical vapour deposition after the transition to a 3D growth regime [16].

For the determination of the growth exponent $\beta$, we have used two different methods. In the first one, we calculated the sample’s global roughness, $w(L)$, using equation (1) with $\ell$ equal to $L$, the total scanning length. In the second, the roughness of a given sample was taken from the graph of the roughness as a function of length window, described previously, at a fixed window. The window selected was the same for all profiles and equal to 1000 points. In both methods, the final value of $\beta$ for a given sample was again calculated taking the average for all profiles. Of course, the absolute roughness, $w$, measured using these procedures were not the same, but the value of $\beta$ is almost the same. This can be seen in figure 5, which shows the plots of the roughness as a function of growth time, determined using both processes. The
growth exponents are 0.38 and 0.39, determined using the roughness at a fixed window and the
global roughness procedure, respectively, but the last yields a larger error. Again, this value
of $\beta$ is the same, within the experimental error, as the one that has been reported for CdTe on
GaAs [16].

4. Conclusions

In this work we have investigated the surface morphology of CdTe films grown on glass by
HWE, using the formalism of the dynamic scaling theory to characterize the growth process.
Our results show the self-affine character of the growth surface with an average value of $\alpha$ equal
to 0.69 ± 0.03. Furthermore, we have shown that, for the range investigated, the roughness
exponent does not depend on growth time. We have also calculated the growth exponent $\beta$
and the value obtained was 0.38 ± 0.06, when considering the procedure that gives the smaller
error.

These values of $\alpha$ and $\beta$ are very close to, and within the experimental error of, those
reported in [16], for CdTe grown on GaAs by metal-organic chemical vapour epitaxy. Although
it is probably too premature to get a final conclusion, one should notice that the same critical
exponents despite the use of a different substrate, at a different temperature and another growth
technique, could indicate that the growth dynamic is the same in both cases, and is probably
a characteristic of CdTe. If true, this would be very important when comparing the properties
of thin films produced by different techniques.

It is also important to notice that all these results were obtained using a stylus profilometer,
and although our results do not permit us to say that it gives the same results as an AFM, we have
certainly shown that valuable information can be obtained by this not so glamorous technique.

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