

The Surface Morphology of CdTe Thin Films Obtained by Open Evaporation in Vacuum

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The different thicknesses CdTe thin films were obtained by method of open evaporation in vacuum on glass and silicon (100) substrates. The surface of films was investigated by AFM analysis. Applying the two-dimensional discrete Fourier transform and autocorrelation function, for the first time the patterns of the structure of the surface of cadmium telluride thin films formed during the vapor phase of condensation are studied. A periodic object grid is discovered. The grid period is related to the mismatch between lattice parameters of substrate and condensate.

Keywords: Cadmium Telluride, Thin films, The open evaporation in vacuum method, Autocorrelation function, Fourier transformation.

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1. INTRODUCTION

CdTe crystallizes in the zinc blende structure with a lattice parameter $a = 6.481 \text{ \AA}$ and melts at temperature 1074°C . The width of the bandgap of this semiconductor is 1.45 eV, which corresponds to the maximum of the solar radiation spectrum. Therefore, the solar photoelectric elements with base layer of cadmium telluride have a high efficiency [1]. Also, it should be noted the set of basic physical and chemical parameters for good practical use, such as high optical absorption coefficient, low concentration of own charge carriers, good mechanical and thermal characteristics. Thus, *p*-type conductivity cadmium telluride is the optimal material for the creation of highly efficient solar photoelectric applications. And the close values for both of its lattice parameter and chemical composition with HgCdTe, make CdTe an ideal substrate material for the growth of IR detectors [2-4].

A significant increase of the efficiency of photovoltaic converters from 16.0% [5] to 22.1% [6] has been shown in the last 20 years. Along with this, the important commercial task is to reduce the cost of such envelopes. Polycrystalline CdTe films with micrometer grain sizes today are among the best in terms of the quality of absorption layers of photocells in the ratio of "efficiency-cost" [7]. Applied properties of such layers are determined, mainly, by the structure of the surface, which can be accurately predicted by technological methods.

Now, there are a large number of methods for obtaining CdTe thin layers. There are the "hot wall" method for epitaxial growth [8-11], organometallic chemical deposition of vapor (MOCVD) [12, 13], molecular beam epitaxy (MBE) [14, 15]. One of the most promising methods is open evaporation in vacuum [16, 17]. This method makes it possible to receive the high purity films during a well-controlled process thanks to the constructive features of the evaporator.

At this time, the research for cadmium telluride as a component of solar cells is in the active phase of study [18, 19]. However, a large number of unsolved physical and technological problems are becoming an

obstacle to obtaining quality functional CdTe films with controlled properties. Therefore, it is important to study the surface morphology of the CdTe thin films [20-26]. The problems of forming of the film surface are due to the complexity of the processes of evaporation and the transfer of matter in the vapor phase, and also of the condensation of steam on the substrate.

The most interesting substrate materials for growing CdTe thin films for solar cells are silicon (Si) and glass.

In the case of silicon, which is transparent in the optical spectrum of the CdTe region, a discrepancy between the lattice parameter is significant (up to 20%): 5.43 Å for Si and 6.48 Å for CdTe [24].

In [25] the surface condensates CdTe deposited on Si (211), (111) and (100) orientations are considered. Sufficiently perfect surface structures obtained by the method of MOCVD, which is quite expensive from commercial point of view. In [24] the process of forming CdTe on Si (211) and (111) was considered. If the first type of substrate it received larger grain sizes, then on the second – a more perfect structure of the finite material. In [26] deposited films of CdTe on glass substrates have been investigated. The structure and photovoltaic properties of the obtained material were investigated at the change of the complex of technological parameters. However, only nanoscale thicknesses films were considered in the paper that deposited from the gas phase at room temperature.

In this paper, the results of the study of nanoscale objects formed on the surface of CdTe deposited on polycrystalline silicon or amorphous glass substrates are presented. A model of discrete Fourier transforms [27] was proposed for describing the characteristics of the nanocondensates obtained on the basis of the AFM images analysis of the cadmium telluride surface.

2. EXPERIMENT

Researched films were prepared by deposition of pre-synthesized CdTe material by the method of open evaporation in vacuum under silicon (100) and glass substrates. The substrate was pre-purified by chemical etching. The temperature of the evaporator was

$T_E = 820$ K, and the temperature of the substrates $T_S = 470$ K. The thickness of the films was determined by time of deposition and varied in the range of 120-300 sec. and measured by Bruker Dektak XT profilometer [10, 11, 28].

Surface morphology was investigated by atomic force microscopy (AFM) in periodic contact mode (AFM CSM Instrument). Measurements were carried out in the central part of the samples using the serial silicon probes Veeco MNSL-10 with a nominal radius of curvature of the tip up to 10 nm. The surface morphology and profilograms were studied as results of ASM images analyses. The size of nanocrystals in the lateral direction is determined by their height and roughness in software package Gwyddion.

The symmetry and frequency of surface structures of the original image allow establishing by two-dimensional Fourier transforms and auto-correlation function. The Fourier spectrum is ideally suited for detecting periodic or quasiperiodic of the two-dimensional structures in the image. Textures easily differ in the spectrum in the form of impulses with high intensity.

The Fourier coefficients $S(k, l)$, forming the two-dimensional frequency spectrum of the image $s(n, m)$, were determined by the direct Fourier transform formula:

$$S(k, l) = \sum \sum s(n, m) \exp(-j2\pi(kn + lm) / N),$$

where N is the number of image points.

A two-dimensional auto-correlation function $C(k, l)$ was calculated by the formula

$$C(k, l) = \left(\sum \sum s(n, m) \cdot s(k + n, l + m) \right)^{1/2} N.$$

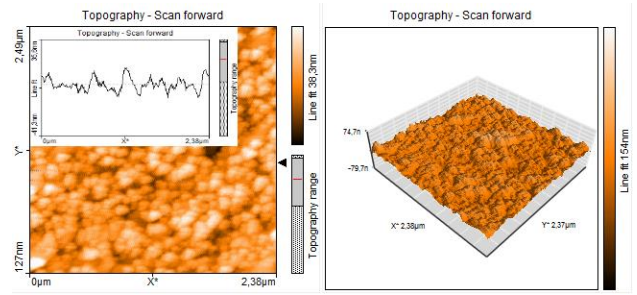
The 2D- and 3D- auto-correlation images as well as Fourier transforms were obtained in the graphical programs Microsoft Excell and Origin.

3. RESULTS AND DISSCUS

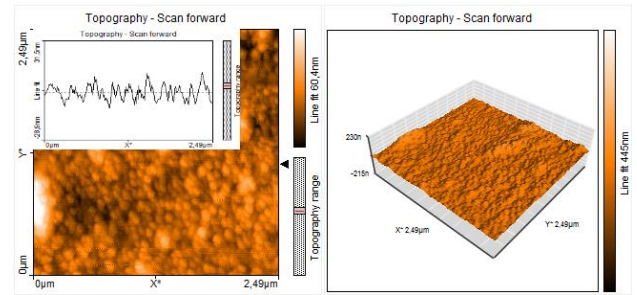
The AFM images of CdTe films of different thickness deposited on the glass substrates shows in Fig. 1. We can see that the surface of film with larger thickness contains nanobjects, whose size is an order of magnitude larger than the size of nanobjects on the surface of film of smaller thickness. Note, that the size of nanobjects on the surface of films deposited on silicon almost unchanged remain (Fig. 2) with change in film thickness. The increase of film thickness in 3-4 times does not significantly increase the characteristics of the heights of the surface. In table 1 shows the processing of AFM relief. From which it is also seen that the surface parameters are more sensitive to film thickness than to the substrate material.

Consider the more detailed distributions of N objects at altitudes h on the film surface (Fig. 3). As can be seen, the distributions are normal. This means that the most probable height of the relief is just about 25 nm for films deposited on silicon substrates and is 35 nm for films deposited on glass substrates.

We used auto-correlation images (Fig. 4) in order to establish periodicity in the location of nanobjects on

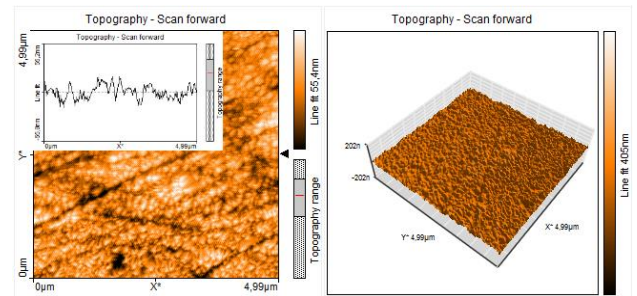


a

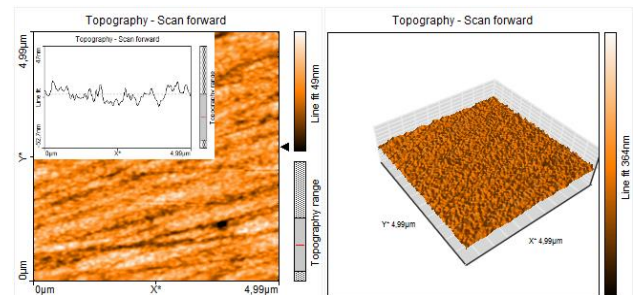


b

Fig. 1 – AFM images of the CdTe films, deposited on glass with thick (a) and thin (b) thickness (No 7 and No 9, see table 1). The size of the observed surface is 2.5 x 2.5 micron²



a



b

Fig. 2 – AFM images of the CdTe films, deposited on Si (100) with thick (a) and thin (b) thickness (No 6 and No 9, see Table 1). The size of the observed surface is 5 x 5 micron²

the surface of CdTe films. We observe row of objects on the surface for both thick and thin films grown on Si, as well as for thin films grown on glass. For such films grown on glass there is no such periodicity. Note, that the output square-like AFM images of the films deposited on Si were in 2 times larger in size than the films deposited on the glass, with sizes of 5 and 2.5 microns,

respectively. Frequency along the abscissa axis is more clearly visible (Fig. 4).

Table 1 – CdTe films thickness, deposited on Si (100) and glass

No sample	Substrate	d, microns
6	Si (100)	2.30
9		0.54
7	glass	1.62
9		0.54

From Fig. 4 we estimate the orientation of the series of objects on the surface of the film. It is (1 1) for the films deposited on the substrate Si, and (1 2) on the glass substrate (the marks of orientation of the objects written for case of planar objects). Also, we can estimate the distance between the rows by the number of maxima (Fig. 5): it is 35 nm for thick film and 31 nm for thin films on the case of silicon substrate, and 22 nm for thin film on glass substrate.

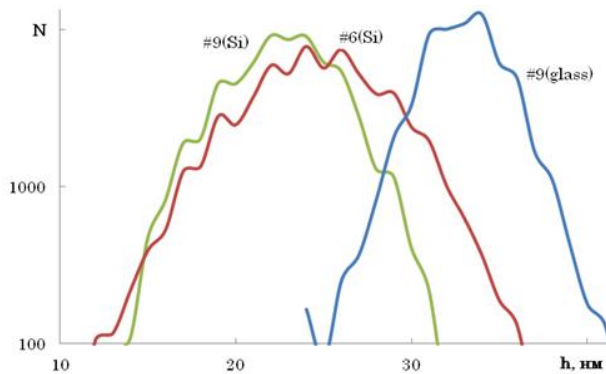


Fig. 3 – Distribution by height of the relief of CdTe film

The presence of periodic rows is manifested in images in the inverse space obtained by discrete Fourier transforms of 64 x 64 pixel images (Fig. 6) for films deposited on silicon. Coordinates of the maxima in rows for a thick film are (17; 39) and (47; 25), and for thin films are (27; 31) and (37; 32).

The lengths of the broadcasts of the inverse lattice for the thick film are 0.53 and 0.38 μm^{-1} , and broadcasting angle is 58°, and for the thin film – lengths are 0.52 and 0.51 μm^{-1} and the angle is 90° (Fig. 6). That is, the objects on the surface of thin film are arranged in square grid, and on the surface of thick film are in monoclinic lattice. We observe the reconstruction of the lattice through monoclinic to hexagonal as the thickness of the film increases. The length of one of the edges has decreased by 30%, and the angle change to 60°. In the usually space the lattice parameters are 49 and 35 nm, and the angle between the edges is 122° for the thick film, for the thin film – the lattice parameters is 30 and 31 nm, and the angle is 90°.

The lattice periods, that obtained by using of Fourier transformation are in good agreement with the such periods obtained by the auto-correlation functions.

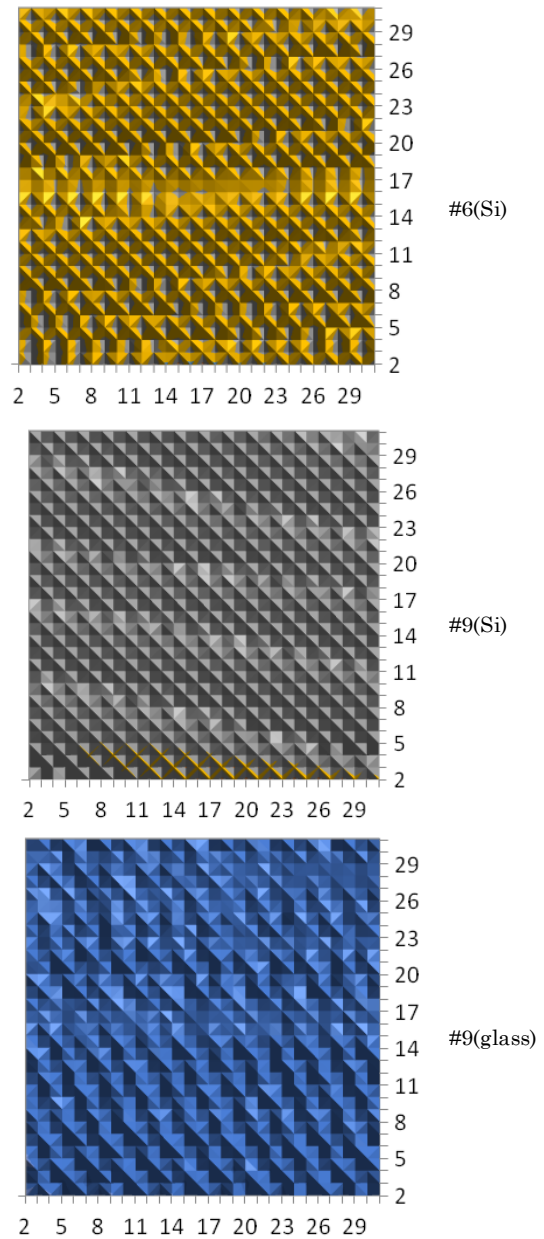


Fig. 4 – 2-D autocorrelation images

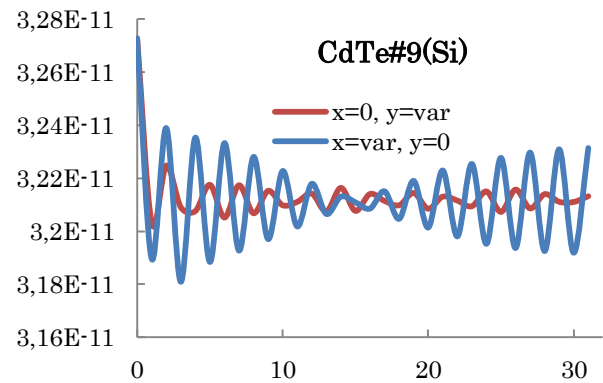


Fig. 5 – The values of a two-dimensional auto-correlation function along coordinate axes

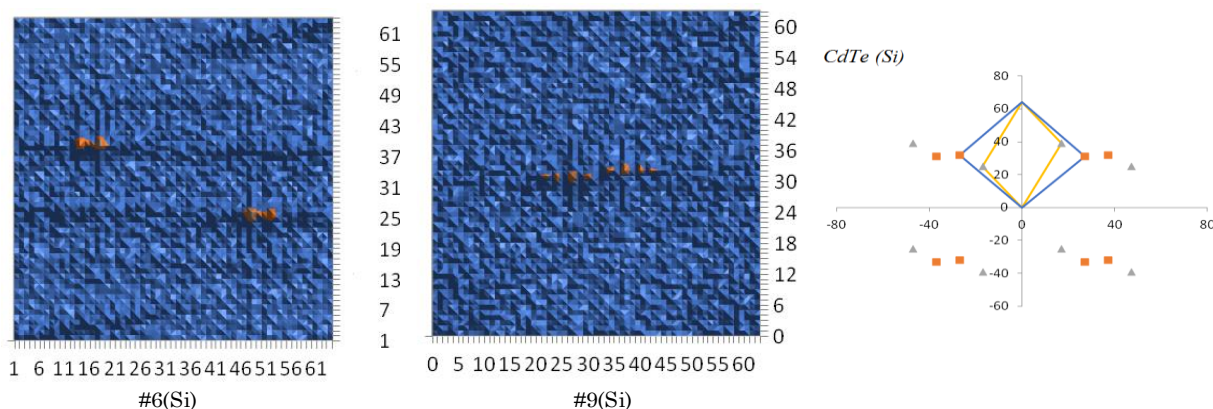


Fig. 6 – The Fourier images for films deposited on silicon. There are used the image 64×64 points for conversion. The Fourier maxima images and corresponding cells for thin (\square – squares) and thick films (Δ – triangles)

4. CONCLUSIONS

1. It has been established that the distribution of the heights of the CdTe films surface is normal, the mean square deviation is less than 10 nm.
2. It was found that the most probable heights of surfaces of films of the same thickness grown on glass are larger than one those grown on silicon.
3. It is shown that objects on the surface of thin films grown on silicon substrate are arranged periodically in a square lattice. The lattice is modified to hex

agonal with the increase of the films thickness.

4. It was established that objects on the surface of thin films grown on glass are arranged periodically, but with the increase in film thickness, the periodicity disappears.

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Морфологія поверхності тонких плінок CdTe отриманих методом відкритого випаровування в вакуумі

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Тонкі плівки CdTe різної товщини отримано методом відкритого випаровування в вакуумі на підкладках із скла і кремнію (100). Досліджено поверхню плінок за допомогою АСМ аналізу. Приміняючи двовимірне дискретне перетворення Фур'є та авто-кореляційну функцію вперше вивчено закономірності структури поверхні тонких плінок кадмій телуриду сформованих в процесі паро фазної конденсації. Виявлено періодичну сітку об'єктів. Період сітки пов'язаний з неузгодженням решіток підкладки і конденсації.

Ключові слова: Кадмій телурид, Тонкі плівки, Метод відкритого випаровування, Авто-кореляційна функція, Фур'є перетворення.

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