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Influence of the Au interlayer on the contact resistance and morphology of CdTe films deposited on molybdenum substrate $\stackrel{\text{trans}}{\approx}$

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Abstract

Development of a proper electrical contact between CdTe and the metallic substrate is one of the hurdles in the fabrication of flexible solar cells on metal foils. From the point of view of matching thermal expansion coefficient; Molybdenum (Mo) is favored as the substrate material. However, the large difference in work, function of CdTe and Mo necessitates a no-rectifying interlayer. In this work we are presenting some preliminary results of our efforts on developing a pseudo-ohmic layer between CdTe and Mo substrate. A thin interlayer of Au seems to reduce the contact resistance. The dependence of the film morphology on the substrate material as well as the substrate temperature is discussed.

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1. Introduction

The high absorption coefficient and nearly ideal band gap of 1.45 eV makes CdTe a potential candidate for photovoltaic applications. Close spaced sublimation (CSS) is one of the most successful methods in developing CdTe thin films due to the large grain size, high material utilization, fast process, and economical experimental facilities. The

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difficulty in getting a good ohmic contact between CdTe and Molybdenum (Mo is preferred owing to the matching thermal expansion coefficient) is one of the major problems in developing CdTe solar cells on metallic substrates. In an effort to develop a reasonably good contact layer between Mo and CdTe, we have deposited a thin layer of Au on the Mo substrate. The CdTe was deposited on top of this layer by CSS. In this work we are reporting the influence of the Au interlayer and substrate temperature on the contact resistance, morphology and surface roughness of the CdTe film.

2. Experimental

Approximately 20 nm thick Au interlayer was deposited on a clean Mo substrate by sputtering. The CSS system for the CdTe deposition was operating at a pressure of 10 mb with 5 mb partial pressure for both He and O₂. The source temperature of the CSS system was maintained constant at 570 °C, and the substrate temperature (T_{su}) was varied from 480 to 540 °C. The selection of the substrate temperature was on the basis of our earlier studies [1]. After the deposition, a routine CdCl₂ treatment at 400 °C was carried out to promote the recrystalization and to enhance the electrical properties of the CdTe film. The structure of the film was analyzed with a Rigaku X-ray diffractometer with Cu K_α radiation at 1.54056 Å. The morphology and the roughness of the surface were studied with AFM.

3. Results

We have analyzed the XRD spectra of the as prepared and $CdCl_2$ treated CdTe films on Mo and Mo/Au substrates deposited at different substrate temperatures. From the spectra, the texture coefficient was calculated utilizing the equation [2,3];

$$P_{i} = \frac{N(I_{i}/I_{i0})}{\sum_{i=1}^{N} (I_{i}/I_{i0})},$$
(1)

where P_i is the texture coefficient corresponding to the plane *i*, I_i is the XRD intensity of the reflections from plane *i*, I_{i0} is the corresponding intensity of the powder sample (JCPDS) and *N* is the number of planes considered for the analysis. The texture coefficient is a measure of the orientation of the crystallites in comparison with the powder sample. A value more than one indicates a preferential orientation in that direction. For this analysis seven structural planes of cubic Zinc blende CdTe has been considered. The degree of preferential orientation in the case of each film has been evaluated from the standard deviation σ of all the values calculated from the P_i of each film [4].

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N} (P_i - P_{i0})^2}{N}}.$$
(2)

The value of σ was utilized to compare the degree of preferential orientation among the films. The value zero for σ indicates that the film is oriented randomly. The results of the comparison are given in Table 1. From table it can be seen that the degree of preferential orientation has a dependence on the substrate (Mo or Mo/Au) as well as the substrate temperature. The CdCl₂ annealing treatment at 400 °C has no significant effect on the orientation of the films which is evident from the values of the texture coefficient and σ .

Table 1

The values of the texture coefficient and the standard deviation σ estimated for CdTe films deposited on Mo and Mo/Au, and treated with CdCl₂

Substrate	T _{su} (°C)	Texture coefficient							σ
		(111)	(220)	(311)	(400)	(331)	(422)	(511)	
Мо	480	1.28	0.18	0.73	1.34	0.37	0.90	2.16	0.62
Мо	480-CdCl ₂	1.48	0.15	0.81	1.41	0.41	0.61	2.10	0.64
Mo/Au	480	0.67	0.97	1.18	1.25	1.13	0.63	1.13	0.23
Mo/Au	480-CdCl ₂	0.67	0.85	1.00	0.98	0.86	1.02	1.58	0.26
Mo	500	1.58	0.06	0.58	1.42	0.30	0.77	2.27	0.73
Мо	500-CdCl ₂	1.75	0.06	0.52	1.36	0.30	0.86	2.12	0.71
Mo/Au	500	0.66	0.79	0.95	1.12	0.93	1.02	1.49	0.25
Mo/Au	500-CdCl ₂	0.70	0.97	1.08	1.16	1.05	1.18	0.83	0.16
Mo	520	1.23	0.14	0.75	1.52	0.46	0.96	1.92	0.57
Мо	520-CdCl ₂	1.25	0.07	0.76	1.37	0.24	1.18	2.11	0.65
Mo/Au	520	0.80	0.88	0.98	0.96	0.85	1.03	1.47	0.21
Mo/Au	520-CdCl ₂	0.77	0.86	1.01	1.04	0.92	1.05	1.31	0.16
Mo	540	1.65	0.31	0.80	1.01	0.55	0.90	1.76	0.49
Мо	540-CdCl ₂	1.73	0.26	0.87	0.98	0.52	0.99	1.64	0.50
Mo/Au	540	0.69	0.86	1.04	0.83	1.01	1.15	1.38	0.21
Mo/Au	540-CdCl ₂	0.60	0.87	0.98	1.16	0.98	1.20	1.18	0.20



Fig. 1. The changes in the lattice parameter **a** with temperature of the substrate.

This is due to the fact that the films were developed at relatively high temperature. The X-ray diffraction patterns also show the presence of MoO_2 [5]. The co-existence of Mo with some oxide phases has been reported earlier [6].

The lattice parameter has been calculated by utilizing the method developed by Nelson and Taylor [7,8] and the results are shown in Fig. 1. It can be observed that the films developed on Mo and Mo/Au at all temperatures has a lattice parameter in the range of the powder sample (powder = 6.481) which indicates that there is no significant stress

along the plane parallel to the substrate. The $CdCl_2$ vapor treatment at 400 °C also does not make significant change in the lattice parameter.

The results of the morphological studies of CdTe films deposited on Mo and Mo/Au at substrate temperatures of 480 and 540 °C are demonstrated in Figs. 2 and 3. As expected the grain size increases with the increase in substrate temperature. From figures it can be seen that the films deposited on Mo and Mo/Au substrates show different microstructures. The grain size of the films deposited on Mo/Au are much larger than those deposited on Mo. This is important since the grain size determines the grain boundaries and hence the electrical transport. The roughness of the films deposited on Mo/Au has larger grain size compared to that deposited on Mo, this is reflected in the higher surface roughness of the films (Fig. 4). The microstructures of the films deposited at a temperature of 500 °C and annealed in CdCl₂ vapor showed a significant reduction of grain boundaries which may improves the electrical properties of the material (Fig. 5).



Fig. 2. The AFM pictures of CdTe films grown on Mo at temperatures in the range 480-540 °C.



Fig. 3. The AFM pictures of CdTe films grown on Mo/Au with temperatures in the range 480-540 °C.

The resistivity of the film as a function of the substrate temperature has been determined utilizing the two point technique in a sandwich configuration metal/semiconductor/metal and utilizing the equation

$$\rho = \frac{\partial V}{\partial I} \frac{A}{d},\tag{3}$$

where A is the area of the electrode and d is the thickness of the film. The graphs in Fig. 6 show the variation in the resistivity of the film with the substrate temperature. It can be noticed that as the substrate temperature increases the resistivity decreases and reaches a minimum value at $T_{\rm su} = 520$ °C. This tendency may be due to increase in the grain size with the increase in substrate temperature and hence reducing the grain boundaries leading to better conductivity of the film.

The contact resistance between CdTe and the substrates (Mo and Mo/Au) has been determined from the model of vertical transmission (VTM) corrected by Ghosh et al. [9].



Fig. 4. A comparison of the surface roughness of the films deposited on Mo and Mo/Au.



Fig. 5. AFM pictures of CdTe films on (a) Mo substrate and (b) Mo/Au substrate grown at 500 $^{\circ}$ C and annealed in CdCl₂ vapor at 400 $^{\circ}$ C.

The contact resistance has been calculated by plotting the total resistance ($R_T = 1/A[2R_C + \rho d] + R_0$) as a function of inverse of area of contact. The slope of the straight line gives the contact resistance

$$m = 2R_{\rm C} + \rho d,\tag{4}$$

where *m* is the slope, ρ the resistivity, *d* is the thickness of the film. Fig. 7(a) shows the total resistance of CdTe deposited on Mo and Mo/Au as a function of contact area. For these measurements circular gold contacts of different diameters were deposited on the CdTe surface. Fig. 7(b) shows the variation of the contact resistance of CdTe as a function of temperature and the type of the substrate. From Fig. 7(b) it can be seen that the films deposited on Mo shows a significant decrease in the contact resistance as the substrate temperature increases. This may be due to the larger grain growth or the formation oxides (MoO₂) on the substrate surface. The films developed on Mo/Au shows a lower R_C



Fig. 6. Resistivity of CdTe films deposited on Mo and Mo/Au at different substrate temperatures.



Fig. 7. (a) Variation of $R_{\rm T}$ as a function area of contact and (b) variation of $R_{\rm C}$ as a function of substrate temperature.

compared to the films developed on Mo, this is because Au has higher work function than Mo. However, above 520 °C the R_C increases and this can be due to the degradation of the pseudo ohmic interlayer.

4. Conclusions

The effect of interlayer and substrate temperature on the growth of CdTe films on Mo substrate is studied. A thin interlayer of Au between CdTe and molybdenum substrate reduces the contact resistance. Substrate temperatures higher than $520 \,^{\circ}$ C shows an increase in contact resistance, which can be due to the degradation of the interlayer. The CdTe films developed on Au/Mo substrates has larger grains compared to films deposited on Mo substrate.

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