

NUCLEATION AND GROWTH MECHANISMS OF CdTe THIN FILMS ON SILICON SUBSTRATES WITH SILICON CARBIDE BUFFER LAYERS

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Abstract. The kinetics of the initial growth stages of cadmium telluride (CdTe) films on silicon substrates covered with silicon carbide (SiC) buffer layers grown by the method of topochemical substitution of atoms is investigated theoretically. The model based on the classical nucleation theory is proposed to depict the CdTe film growth by the method of thermal evaporation and condensation in vacuum. The model accounts for the mechanical stresses caused by the lattice mismatch and difference of thermal expansion coefficients of CdTe film and substrate. The influence of substrate and evaporator temperature on the nucleation mechanism and kinetics of the initial growth stages of CdTe film is estimated. The different growth regimes of CdTe films on the SiC/Si substrates are discussed, and the optimal growth conditions are found. It is shown that the elastic stresses in the CdTe/SiC/Si structure are approximately three times lower than the elastic stresses in the CdTe film grown coherently on the Si substrate without the SiC buffer layer. This leads to the large difference in the nucleation rates of the CdTe films on the SiC/Si substrate and Si substrate. The diagram of the nucleation rates of CdTe islands on the SiC/Si depending on the substrate and evaporator temperature is presented.

Keywords: thin film; CdTe; SiC; Si; silicon substrate; silicon carbide buffer layer; growth; nucleation; thermal evaporation.

1. Introduction

At present time considerable efforts of researchers are aimed at study of A^{II}B^{VI} group semiconductors and development of methods for growth of thin films of these materials [1-3]. Such semiconductors are of great practical interest and can be used for creation of various optoelectronic devices, solar batteries, photodetectors and ionizing radiation sensors [4, 5]. Cadmium telluride (CdTe) outstands among the semiconductors of this group, since it is widely applied in the solar batteries production [6]. CdTe is used as an absorbing layer because it is a direct-band semiconductor with a bandgap of 1.49 eV and has a high absorption coefficient in visible range. To create efficient solar batteries, thin CdTe films of high quality grown on conductive or semiconductive substrates are needed. This will greatly simplify the production of optoelectronic devices, since there is no need to add additional contacts. Materials such as indium tin oxide (ITO) [7], indium antimonide (InSb) [8], gallium arsenide (GaAs) [9], silicon (Si) [10], and many others [11] are often used as substrates. Silicon has a number of advantages, since silicon substrates are widely available and most well developed from a technological point

of view. However, various problems arise during the growth of CdTe directly on silicon. The film grows polycrystalline [12] often. In case of chemical deposition of thin CdTe films, the silicon reacts with precursors and forms Si_2Te_3 , which significantly degrades the properties of the resulting structures. In this regard, it was proposed in [13] to use Si substrates with a buffer layer of silicon carbide (SiC) formed by the method of topochemical substitution of atoms [14] for deposition of CdTe. Silicon carbide does not interact with elements of group VI practically. In addition, SiC layer grown by the method of atoms substitution on Si substrate has a number of advantages over silicon carbide carved from SiC single crystals. According to [14], the feature of SiC epitaxial layer growth by the method of atoms substitution is that an ensemble of pores is being formed between the layer and the substrate during the synthesis. As a result, the contact area of the silicon substrate and the structure grown on SiC is being significantly reduced. Silicon substrates covered by SiC buffer layer that "hangs" above the pores in Si become elastically "compliant". They adapt well to growth conditions and nature of the films deposited on their surface. As a result, elastic stresses arising due to mismatch of the lattice parameters and difference in the thermal expansion coefficients of the substrate and the film materials are being significantly reduced. More details on the SiC/Si films obtained by the method of topochemical substitution of atoms, theoretical basis of this growth technology and the study of SiC/Si samples are presented in the review [14] and original paper [15].

There are various methods [16] for deposition of cadmium telluride films, such as magnetron sputtering [17], thermal evaporation and condensation in vacuum [18], chemical vapor deposition [19], etc. Thermal evaporation in vacuum has a number of advantages, since it ensures high deposition rate and does not require high material costs. However, to the best of our knowledge, despite a significant amount of experimental works on the growth of CdTe [20, 21], there is no quantitative theory describing the processes of CdTe formation, which would allow estimating of various parameters of the resulting films depending on growth conditions: pressures, temperatures. The present paper is a continuation of a series of papers on the growth of CdTe on SiC/Si substrates [13] by thermal evaporation and condensation in vacuum, and is devoted to the theoretical aspects of the growth of thin CdTe films. In the first part of the paper a model of the film growth is developed on the basis of the classical nucleation theory and estimates for the parameters necessary for calculations are made: the diffusion lengths of Cd and Te adatoms, their lifetimes, equilibrium concentrations and diffusion coefficients. In the second part, the calculation results within the framework of the model are compared with the experimental data [13] and growth regimes of CdTe under conditions other than in Ref. [13] are analyzed.

2. Model of the initial stages of CdTe thin film formation on Si/SiC substrate upon evaporation and condensation

Usually two-zoned reactor is being used for growth of CdTe films by the method of thermal evaporation and condensation in vacuum, in one of the zones of which the powdered cadmium telluride is being evaporated, and in the other one condensation of CdTe onto the substrate occurs. The principal scheme of the reactor, shown in Fig. 1, was proposed by I.P. Kalinkin and his group [22]. We note that this type of the reactor can be used both for the growth of films by the method of thermal evaporation in vacuum and for the growth in a quasi-closed volume. In the latter case, it is being lowered onto the substrate holder and it completely covers the substrate.

In the evaporation zone sufficiently high temperature T_g is maintained, so that the powdered CdTe evaporates by dissociating into Cd and Te_2 chalcogen molecules as a result of the reaction:



We note that in the general case it is necessary to take into account the fact of the possible formation of individual tellurium atoms in vapor that can get onto the substrate. However, during thermal evaporation, this process is not very probable and in this study we will not take it into account. The mechanisms of evaporation of $A^{II}B^{VI}$ compounds, to the group of which CdTe belongs, are mostly completely described in the monograph [22].

After evaporation of CdTe and formation of Cd and Te_2 in vapor phase, the process of mass transfer through the gas phase towards the condensation zone (in which the substrate is located) begins. As a consequence, fluxes of Cd and Te_2 onto the substrate appear. Since the substrate is maintained at temperature T_s , which is lower than T_g , the flux of material coming to the surface from the vapor exceeds the flux of material evaporating from the substrate. As a result, significant supersaturation appears on the substrate, which is sufficient to initiate the nucleation of CdTe islands. The nucleation is the main reason for the growth of CdTe film. The influence of the growth conditions, in particular, temperature of the evaporator and the substrate on possible growth regimes and conditions under which their change occurs will be estimated below.

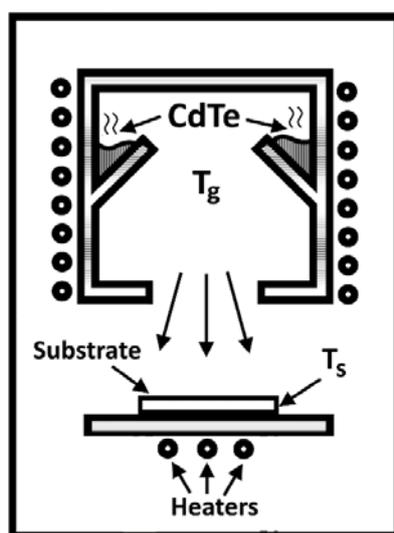


Fig. 1. Scheme of two-zoned reactor for the growth of CdTe by the method of thermal evaporation and condensation in vacuum [22].

We note that within the framework of the present model, it is believed that SiC film affects the nucleation of CdTe islands through three main parameters: the adsorption energy of Cd and Te (we suppose that Te_2 molecules are being completely dissociated into atoms on the surface of the substrate); diffusion and, as a consequence, the mobility of Cd and Te adatoms; the field of mechanical stress σ , which arises due to the difference in lattice parameters of SiC and CdTe and which will be taken into account during calculation of the dependence of nucleation rate of CdTe islands on supersaturation. For simplicity in this paper we assume that diffusion lengths, lifetimes, and diffusion coefficients of adatoms during the growth of the first cadmium telluride layers directly on SiC surface coincide with these parameters on the surface of CdTe, although this is certainly not the case in real growth process. However, since the studies of evaporation processes of Cd and Te adatoms from the SiC surface are not available yet to the best of our knowledge, we are using this approximation, and in the future we will try to estimate these parameters from quantum-chemical calculations. We should also note, that increase in the thickness of the growing film, leads to rapid decrease in the influence of the existing differences in parameters, and since the films of thickness of the order of hundreds nanometers or more are of main practical interest, we believe that this assumption is quite reasonable.

3. The growth mechanism and nucleation rate of CdTe islands on the SiC/Si substrate

The nucleation rate of CdTe islands is determined by the equation [23]

$$I = N_0 W^+(n_c) Z \exp(-\Delta F(n_c)/kT), \quad (2)$$

where N_0 is the number of adsorption sites on the substrate, $N_0 \sim 1/l_0^2$; l_0 is the lattice constant of SiC, n is the number of Cd atoms in the island (equals to the number of CdTe pairs); n_c is the critical size of island; $W^+(n_c)$ is the diffusion coefficient in the size space for the island of the size n_c ; $W^+(n_c)$ depends on the island growth mechanism and is of order of the number of CdTe pairs that attach to the critical island per second; $\Delta F(i)$ is the free energy of the island formation without the entropy correction; k is the Boltzmann constant; T is the growth temperature; $Z = \sqrt{-\Delta F''(n_c)/2\pi kT}$ denotes the Zeldovich factor. The free energy of the island formation $\Delta F(i)$ equals [23]

$$\Delta F(i) = \alpha n^{1/2} - (\Delta\mu - w)n, \quad (3)$$

where $\alpha = 2\pi^{1/2} \gamma(h\Omega)^{1/2}$ for the disk-shaped islands of the radius r and height H ; γ is the effective surface energy of the island sides, Ω is the volume of the CdTe pair in solid state; $\Delta\mu$ is the difference of chemical potential per CdTe pair between the two-dimensional gas of adatoms and bulk solid; $\Delta\mu = kT \ln(C_{Cd}C_{Te}/K^{eq})$, C_i are the atomic concentrations of Cd and Te atoms on the surface of substrate; $K^{eq} = C_{Cd}^{eq}C_{Te}^{eq}$ is the equilibrium constant of the chemical reaction $Cd + Te \rightarrow CdTe$, C_i^{eq} is the equilibrium concentration of the i -th element; w is the elastic energy per CdTe pair produced by the lattice mismatch of the substrate and CdTe film. The difference $\Delta\mu - w$ is the driving force of nucleation. The supersaturation of the two-dimensional gas of adatoms ξ relates to the difference of chemical potentials $\Delta\mu$ by the formula $\Delta\mu = kT \ln(\xi + 1)$ and, consequently, $\xi = C_{Cd}C_{Te}/K^{eq} - 1$. It is noteworthy that in our model we assume that the Te_2 molecule absorbed on the substrate dissociates into two Te atoms. Therefore, the kinetics processes on the substrate (the island formation and growth) are governed by the diffusion of Te adatoms (not Te_2 molecules) and their interaction with the Cd adatoms. We suppose that tellurium in molecular form desorbs easily from the substrate and is not involved in the nucleation process of CdTe islands. In the general case, the several possible growth mechanisms can be considered. Herein, we focus only on the mechanism mentioned above but, in the further studies, we will investigate other possible mechanisms. For instance, the Te_2 molecule can interact with the Cd adatom and, as a result, the "free" Te adatom is produced on the surface. Also, one should consider the possibility of the reaction between the Te_2 molecule in the vapor phase and two Cd adatoms on the surface [23]. Thus, we suppose that the following reaction on the substrate results in the formation of CdTe islands



where $Cd(ad)$ и $Te(ad)$ are the cadmium and tellurium adatoms, $CdTe(s)$ is the cadmium telluride in solid state. It is well known that the critical size of island and nucleation barrier can be expressed by the formulas $n_c = \alpha^2/4(\Delta\mu - w)^2$ and $\Delta F(n_c) = \alpha^2/4(\Delta\mu - w)^2$, correspondently. Following to Zeldovich [24], the diffusion coefficient in the size space $W^+(n)$ can be defined by the formula

$$W^+(n) = - \frac{kT dn/dt}{\partial \Delta F / \partial n}, \quad (5)$$

where dn/dt is the island growth rate; it depends on the mechanism of material transport. In the general case, the different growth mechanisms of islands can be considered depending on the substrate temperature [25]. In this paper, we consider the most realistic mechanism that can occur at the growth conditions similar to those used in the work [13]. We assume that the island

has the shape of the thin disk of the radius r and height H . The height H equals to one monolayer and is a constant at the nucleation stage of the islands. Therefore, the radius of island, i.e. its lateral size, only changes during the growth. This assumption is reasonable because the number of atoms in the islands is usually about ~ 10 -100 at the nucleation stage and the islands have the size of ~ 1 nm [23]. At the initial growth stage, the average distance between islands is much larger than their sizes. Therefore, we assume that the island growth is limited by the surface diffusion of Cd and Te adatoms at the growth conditions [13]. In this case, we can use the following formula for the growth rate of island [25]

$$\frac{dn}{dt} = \frac{2\pi\gamma\Omega N_0 D_{CdTe}}{kT r} \left(\frac{r}{r_c} - 1 \right), \quad (6)$$

where

$$D_{CdTe} = \left(\sum_{i=Cd,Te} \frac{v_i^2 \ln \lambda_i / r_c}{D_i C_i^{eq}} \right)^{-1} \quad (7)$$

is the generalized diffusion coefficient; D_i and λ_i are the diffusion coefficient and diffusion length of the i -th element on the surface, correspondently, such that $\lambda_i = \sqrt{D_i \tau_i}$, τ_i is the adatom lifetime; v_i is the stoichiometric coefficient of the i -th element that corresponds to the reaction (4), $v_{Cd} = 1$, $v_{Te} = 1$; $r_c = \gamma \Omega / \Delta \mu_c$ is the radius of the critical island. To calculate $W^+(i_c)$, we differentiate (3) with respect to n and substitute the derivative in (5) then simplify the result using the formula (6). Finally, we obtain the formula [26]

$$W^+(i_c) = 2\pi D_{CdTe} N_0, \quad (8)$$

where

$$D_{CdTe} = \frac{D_{Cd} D_{Te} C_{Cd}^{eq} C_{Te}^{eq}}{D_{Te} C_{Te}^{eq} \ln(\lambda_{Cd}/r_c) + D_{Cd} C_{Cd}^{eq} \ln(\lambda_{Te}/r_c)}. \quad (9)$$

Substituting (8) in (2) and calculating the Zeldovich factor, we rewrite the formula (2) for the nucleation rate of CdTe islands in the following form

$$I = \frac{N_0^2 D_{CdTe} (\Delta \mu - w)^{3/2}}{\gamma (h \Omega k T)^{1/2}} \exp \left(- \frac{\alpha^2}{4kT(\Delta \mu - w)} \right). \quad (10)$$

Let us estimate the values of the material constants of our model to use the formula (10). The adatom lifetime of Cd and Te can be found by means of the formula [25]

$$\tau_i = \tau_{0i} \exp \left(\frac{E_{a,i}}{kT} \right), \quad (11)$$

where $\tau_{0i} \sim 1/\nu_{p,i}$, $\nu_{p,i}$ is the frequency of normal vibrations of the i -th element on the substrate; $\nu_{p,i}$ equals approximately $\sim 10^{13} s^{-1}$ [27]; $E_{a,i}$ is the activation energy of adsorption of the i -th element. The diffusion coefficient of the Cd and Te adatoms D_i is calculated using the equation

$$D_i = \frac{l_i^2 \nu_{t,i}}{z} \exp \left(- \frac{E_{d,i}}{kT} \right), \quad (12)$$

where $E_{d,i}$ is the activation energy of the surface diffusion; l_i is the diffusion jump distance of the i -th element; we put $l_i \sim l_0$ for simple estimates; the lattice constant of CdTe l_0 equals to 0.648 nm [28]; $\nu_{t,i}$ is the frequency of tangential vibrations of the i -th element on the substrate, $\nu_{t,i} \sim 10^{13} s^{-1}$ [28]; z is the number of neighboring sites which the adatom can hop to; z equals to 3 for the triangular lattice.

The activation energy of adsorption $E_{a,i}$ is estimated using the results of the work [29], $E_{a,Cd} \sim 0.5$ eV and $E_{a,Te} \sim 1.5$ eV. The activation energy of diffusion $E_{d,i}$ equals to $E_{d,Cd} \sim 0.17$ eV and $E_{d,Te} \sim 0.5$ eV [30]. After the activation energies were found, it easy to estimate the adatom lifetimes and diffusion coefficients according to the formulas (11) and (12). The calculated dependences of τ_{Cd} and τ_{Te} and, also, D_{Cd} and D_{Te} on the substrate temperature are presented in Fig. 2a. In order to estimate the temperature dependence of the evaporation and condensation fluxes of Cd and Te at the vapor-surface interface and, correspondently, the

equilibrium concentrations of adatoms, we use the data on the saturated vapor pressure of Cd and Te_2 over the congruently sublimating crystal of CdTe [22, 31]. According to the work [31], the logarithm of the saturated vapor pressure of Te_2 molecules equals to $\log P_{\text{Te}_2} = -10^4/T + 6.346$, where the temperature T is measured in degrees of Kelvin and the pressure P_{Te_2} is measured in atmospheres. The saturated vapor pressure of Cd is calculated by means of the equation $P_{\text{Cd}} = 2P_{\text{Te}_2}$ [31]. The flux densities of Cd and Te atoms coming to the substrate from the vapor phase are equal to $J_{\text{Cd}} = P_{\text{Cd}}/(2\pi m_{\text{Cd}}kT)^{1/2}$ and $J_{\text{Te}} = 2P_{\text{Te}_2}/(2\pi m_{\text{Te}_2}kT)^{1/2}$, correspondently, where m_{Cd} and m_{Te_2} are the mass of Cd and Te_2 , correspondently.

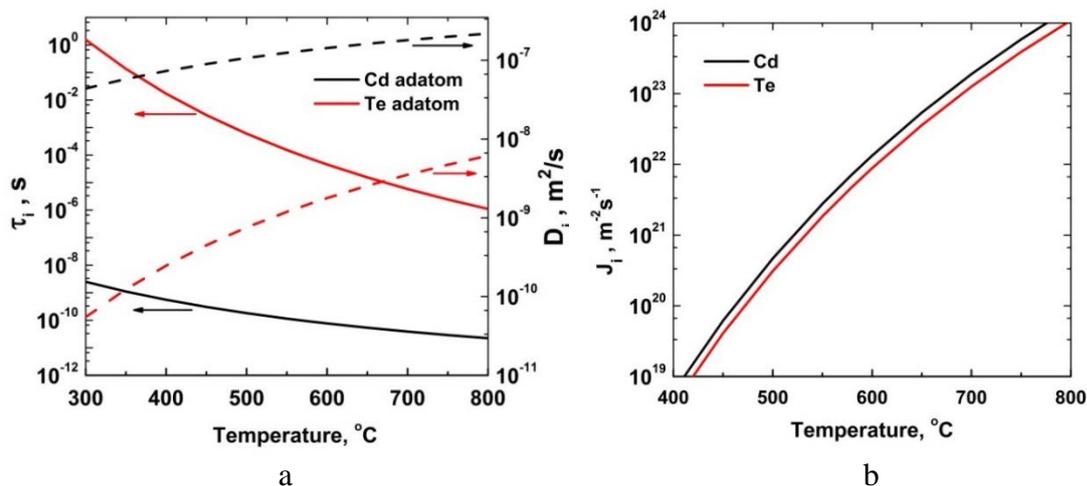


Fig. 2. The dependences of the adatom lifetimes, diffusion coefficients and flux densities of Cd and Te atoms on the substrate temperature; (a) the dependences of the adatom lifetimes (τ_{Cd} , τ_{Te}) and diffusion coefficients (D_{Cd} , D_{Te}); (b) the dependences of the flux densities of Cd and Te atoms.

The results of the calculation of J_{Cd} and J_{Te} are shown in Fig. 2b. After the flux densities are calculated, it is easy to estimate the adatom concentrations using the formula $C_i = n_i/N_0 = J_i\tau_i/N_0$, where n_i is the surface density of the i -th adatom. To determine the value of the effective surface energy of island γ , the results of the work [32] on the surface energy calculation of CdTe are used. Thus, we equal γ to $0.65 \text{ J} \cdot \text{m}^{-2}$ in the further computations.

The mechanical stress σ produced during the growth of the CdTe film on the SiC/Si substrate is estimated by means of the analysis of the Raman spectrum of the CdTe/SiC/Si structure [13]. The Raman measurements performed at room temperature [13] show that the Raman shift ω of the E(TO) phonon peak has the value of about 141 cm^{-1} . According to the work [33], the Raman shift ω_0 of this peak of the CdTe crystal in the unstressed state has the value of about 140 cm^{-1} . The value of the mechanical stress σ in the CdTe/SiC/Si structure is estimated by means of the formula derived in the work [34], $(\omega - \omega_0)/\omega_0 = k\sigma$, where $k \approx -(0.36 \pm 0.1) \text{ cm}^{-1}/100 \text{ MPa}$. Thus, the CdTe film grown on the SiC/Si substrate has the residual compressive stress of about 200-400 MPa. Note that at the growth temperature the value of the mechanical stresses can be higher or lower than the calculated value depending on the presence of misfit dislocations, lattice mismatch and difference of thermal expansion coefficients of CdTe film and substrate during the growth process [35]. However, in this paper, we assume that the mechanical stress in the volume of CdTe film equals approximately $\sim 300 \text{ MPa}$. During the heteroepitaxy growth, the island-substrate interface is often semicoherent. Therefore, the effective mechanical stress is lower than that in the volume of CdTe film. Our estimates show that its value is about 120-150 MPa. It is also important to note that in the case of CdTe growth on the Si substrate the residual stress is several times higher,

about 0.6-1.0 GPa [36]. Moreover, the use of the nanopatterned substrates does not lead to the relaxation of CdTe film on the Si substrate [36].

As a result, the model allows the estimation of the values of the parameters of the CdTe film growth on the SiC/Si substrate at the growth conditions [13]. At the substrate temperature $T_S = 500$ °C, the Cd adatom lifetime equals $\tau_{Cd} \sim 2 \cdot 10^{-10}$ s. The Te adatom lifetime is much larger, $\tau_{Te} \sim 6 \cdot 10^{-4}$ s (Fig. 2a). The estimates of the equilibrium concentrations of adatoms, C_{Cd}^{eq} and C_{Te}^{eq} , show that their ratio equals $C_{Cd}^{eq}/C_{Te}^{eq} \sim 10^{-7}$. Such a large difference in the adatom lifetime and equilibrium concentrations is caused by the difference in the binding energies of Cd and Te adatoms with the substrate. The binding energy of Cd adatom is approximately three times less than that of Te adatoms. As the material source, the CdTe powder heated up to the temperature of $T_g = 580$ °C was used in the work [13]. The calculated values of the flux densities of Cd and Te atoms coming to the substrate at $T_g = 580$ °C equal, correspondently, $J_{Cd} \sim 7 \cdot 10^{21} \text{ m}^{-2}\text{s}^{-1}$ and $J_{Te} \sim 5 \cdot 10^{21} \text{ m}^{-2}\text{s}^{-1}$. Note, the values of J_{Cd} and J_{Te} are very close to the value of the flux density of CdTe molecules at the same temperature T_g obtained experimentally in the work [22]. The concentration of Cd and Te adatoms at such fluxes equal $C_{Cd} \sim 10^{-7}$ and $C_{Te} \sim 1$. The values of C_{Cd} and C_{Te} correspond to a very large value of the supersaturation ξ . In the real growth process, such a large excess of adatoms will be consumed rapidly by the growing islands. This will lead to the decrease of the supersaturation down to the regular value of $\xi \sim 0.1$. It can be shown that $D_{Te}C_{Te}^{eq} \ln(\lambda_{Cd}/r_c) \gg D_{Cd}C_{Cd}^{eq} \ln(\lambda_{Te}/r_c)$ (equation (9)) in the considered temperature range. Consequently, the growth of the CdTe film is limited by the diffusion of Cd adatoms on the substrate and the equation (9) can be represented in the following form $D_{CdTe} \approx D_{Cd}C_{Cd}^{eq} / \ln(\lambda_{Cd}/r_c)$. The elastic stresses due to the lattice mismatch between the SiC/Si substrate and CdTe film cause the decrease of the driving force of nucleation compared to the case of unstrained structure. The value of this decrease equals $\sim 15\%$ that corresponds to $w \sim 0.048$ eV per atom. As a result, the nucleation rate decreases by three orders of magnitude. However, in the case of nucleation on the Si substrate the driving force is several times lower because the value of the mechanical stresses is several times larger. Our calculations show that the nucleation rate of CdTe islands on the Si substrate is several orders of magnitude lower than the nucleation rate on the SiC/Si substrate. Therefore, the formation of the CdTe film is much easier on the SiC/Si substrate than on the Si substrate.

4. Diagram of the nucleation intensity of CdTe nuclei on the SiC/Si surface. Conditions of optimal epitaxial growth of the CdTe films on SiC/Si

Using the formula (10), it is possible to estimate the nucleation rate $I(T_g, T_s)$ for different temperatures of the evaporator T_g and the substrate T_s . Fig. 3 demonstrates a diagram of the relative intensity of the CdTe islands nucleation on SiC/Si substrate in T_g and T_s axes. The color corresponds to the value $I(T_g, T_s)/I(580 \text{ °C}, 500 \text{ °C})$, i.e. to the ratio of the intensity of the islands nucleation calculated from the formula (10) for the temperatures T_g and T_s to the intensity of the islands nucleation under the growth conditions of the paper [13]. Note that the use of such a relative value is convenient in view of the fact that the growth mechanism of the CdTe film under the conditions of the paper [13] has already been determined experimentally and the film growth rate is known to be about 0.3–0.5 $\mu\text{m/s}$. Comparing the values $I(T_g, T_s)$ and $I(580 \text{ °C}, 500 \text{ °C})$, it is possible to estimate the regimes and rate of CdTe film growth under other conditions as well. Thus, in Fig. 3 one can distinguish 5 characteristic regions with different rates of CdTe nucleation. It is expected that in the region I (see Fig. 3), the mechanism of CdTe film growth will be similar to that observed in the experiment [13]. In the region II corresponding to much lower values of the supersaturation and more equilibrium conditions of

the film growth, one can get epitaxial layers of high quality. However, it should be taken into account that the growth rate in this case will be much lower. In this regard, if the vacuum is not sufficiently high in the system, the concentration of other substances which present in the gas phase in the reactor will be higher in the resulting CdTe film.

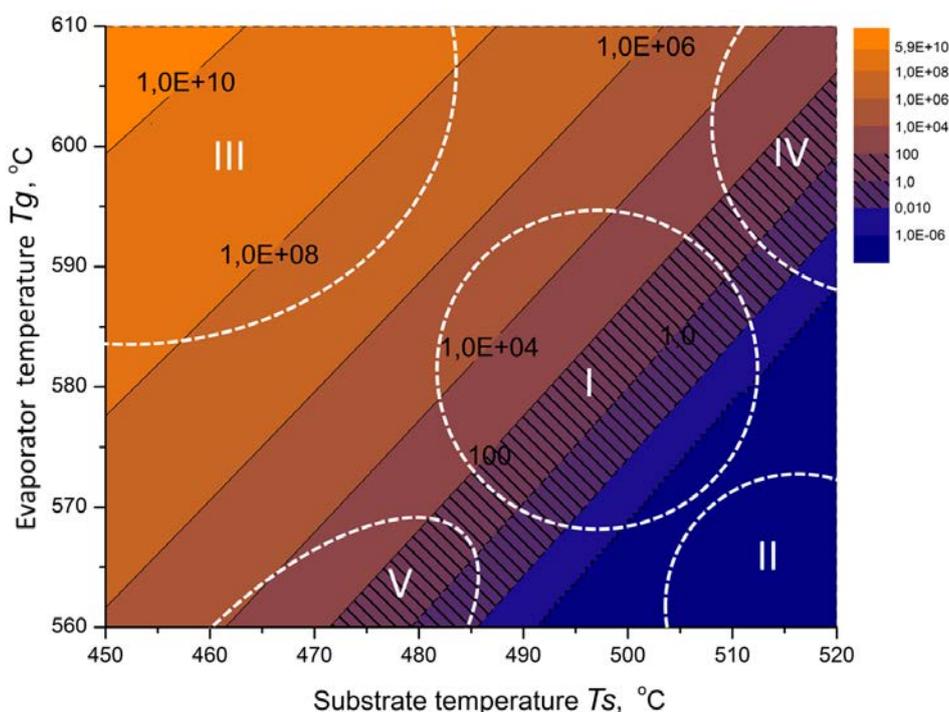


Fig. 3. Dependence of the relative intensity of nucleation $I(T_g, T_s)$ of CdTe islands on evaporator temperature and substrate temperature. The normalization was carried out on the nucleation intensity under the experimental conditions of paper [13].

Moreover, taking into account the small supersaturation and the extremely low nucleation rate, a change of the film growth regime for the two-dimensional growth due to the diffusion of adatoms to the growth steps or to the exit points of screw dislocations is possible. In the region III large supersaturations are observed and the nucleation intensity significantly exceeds the values corresponding to [13]. The growth in such non-equilibrium conditions can lead to the appearance of polycrystals. In addition, significant supersaturation can lead to the development of morphological instability and increase of surface roughness [37, 38]. The region IV corresponds to nucleation rates comparable to [13], but the growth occurs at high substrate temperatures. As a result, the diffusion length of adatoms of cadmium and tellurium becomes smaller, which can also contribute to the development of roughness at scales comparable to the diffusion lengths of adatoms [37]. An advantage of the region IV is higher partial pressures of Cd and Te_2 in the reactor and, as a consequence, lower concentrations of impurities in the film. In the region V, vice versa, the partial pressures of cadmium and tellurium are small, and a large concentration of impurities can be observed. However, the diffusion lengths of the adatoms in this region are much larger, which can lead to smoothing of the roughness with a short spatial wavelength [37].

5. Conclusions

The process of cadmium telluride film growth on SiC/Si substrates by the method of thermal evaporation and condensation in vacuum is considered. The model for the formation and growth of CdTe film is developed on the basis of the classical nucleation theory, which takes into account the influence of mechanical stresses that arise in CdTe due to difference in the

parameters of crystalline lattices of the film and the substrate. It is shown that the presence of elastic stresses reduces effective difference of chemical potentials for Cd and Te by $\sim 15\%$, which corresponds to ~ 0.048 eV per atom. Such a decrease in the difference of chemical potentials has a significant effect on the nucleation rate, and as a consequence, on the growth mechanism of thin films. Estimates of the mechanical stresses arising in CdTe films grown on SiC/Si and Si substrates showed that in the case of coherent coupling between the film and the substrate in CdTe/SiC/Si heterostructure elastic stresses are of the order of ~ 0.2 - 0.3 GPa, whereas in CdTe/Si heterostructure the elastic stresses will be ~ 0.6 - 1 GPa, which are approximately three to four times higher. Such a difference in the elastic stresses significantly affects the activation barriers for CdTe nucleation on Si substrate with a buffer layer of SiC and on pure Si substrate without a buffer layer. The main constants determining the nucleation rate, namely the lifetimes of Cd and Te adatoms are calculated, as well as the generalized adatom diffusion coefficient, which determines the growth rate of CdTe islands. On the basis of these data, a theoretical diagram of the nucleation rate of CdTe nuclei on SiC/Si surface in the temperature range of the evaporator 560 - 610 °C and of the substrate 450 - 520 °C was calculated. The various growth regimes of the film are discussed. It is shown that change in the temperature of the substrate/evaporator by 10 °C can lead to a sharp (up to several orders) change in the rate of nucleation, which significantly affects the mechanism and growth rate of thin film, impurity concentration, degree of crystallinity and, ultimately, quality of the grown CdTe films.

Acknowledgements

This work was supported by the Russian Science Foundation (№ 14-12-01102). The experimental results were partially obtained using the unique scientific facility "Physics, chemistry and mechanics of crystals and thin films" (IPME RAS, St. Petersburg).

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