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NUMERICAL STUDY OF THE GROWTH CONDITIONS IN A MOCVD REACTOR: APPLICATION TO THE EPITAXIAL GROWTH OF CdTe

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A 2-D model to simulate the gas flow in a horizontal MOCVD reactor has been developed. This model takes into account the conservation equations coupled with heat transfer and mass transport of the chemical species. For the mathematical solution a commercial solver, that can be run in a conventional personal computer, has been used. The influence of different parameters such as total flow, partial pressures of precursors, reactor pressure and substrate temperature on the gas flow and growth rate has been studied. Diisopropyltelluride (DIPTe) and dimethylcadmium (DMCd) have been used as precursors and H_2 as carrier gas. The capabilities of the used model for the numerical study in a conventional research or production laboratory will be shown. The main goal of this paper is both to offer a valuable tool for the numerical simulation of the MOCVD system and to suggest some practical reflections for the MOCVD experimental grower in order to facilitate the optimization process in a reduced time.

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1. Introduction

CdTe is a well-established material essentially used for the fabrication of solar cells [1] and gamma ray and X-ray detectors [2]. Mixed with HgTe, it is a component of the alloy $Hg_{1-x}Cd_xTe$ (MCT) [3, 4] used in IR detection and it is also used, when mixed with a small fraction of ZnTe, as substrate for the epitaxial growth of MCT [5]. Several methods have been developed for the crystal growth of CdTe and the Metalorganic Chemical Vapour Deposition (MOCVD) has been largely applied for the deposition of CdTe layers [6].

Nowadays MOCVD has become an important industrial technique for manufacturing thin solid films to be used in optoelectronic devices [7]. The success of this technique primarily stems from its flexibility and the high compositional control that it offers.

Nevertheless, several problems remain among them the large number of parameters which must be precisely controlled to reach the necessary uniformity and reproducibility. The MOCVD process is critically dependent on the fluid dynamics of the reacting and carrier gases. Quantitative and qualitative understanding of basic fluid dynamics associated with a determined reactor is a key point to achieve improvements in efficiency, crystal production and growth uniformity.

Numerical studies appear to be a valuable tool in crystal growth [8]. In recent times there has been an increasing effort on the simulation of the crystal growth processes. This effort joined to the availability of commercial codes to solve the involved mathematical equations facilitates the simulations and numerical studies.

In this context, the development of accurate theoretical models applied to the MOCVD growth is particularly attractive in order to study, for a given reactor, the influence of various operating parameters and to reduce the number of experiences and, consequently, the cost for the optimisation of the process.

Several numerical and analytical approach can been found in literature. Van de Venn et al. [9]

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studied the growth rate of GaAs as a function of both lateral and axial position in a horizontal reactor under controlled diffusion conditions. A general conclusion from this work was that the study of the growth rate distribution, as a function of the position on the susceptor, gives very valuable information on the properties of the flow and the epitaxial growth mechanism. A numerical model of a three-dimensional horizontal reactor was presented by Ern et al. [10] in order to study the growth of gallium arsenide. Fluid flow and temperatures inside the reactor were obtained using the vorticity-velocity form of the three dimensional steady-state equations coupled with an energy balance equation inside the reactor and on its walls. The influence of the susceptor temperature and inlet composition on the growth rate was analysed.

With regard to the CdTe epitaxial growth, only some few models have been developed to analyse the growth rate. Liu et al. [11] use a boundary-layer model incorporating a catalytic reaction to simulate the kinetics of CdTe deposition in a horizontal cold wall reactor. On the other hand, Irvine et al. [12] explain, with a kinetic model based on experimental results obtained by reflectometry measurements, the low and high temperature regimes. The low temperature regime is limited by the surface catalysis of tellurium organometallics bound to group II surface atoms and the high temperature regime is limited by the tellurium desorption. More recently, Kuhn et al. [13] made a two-dimensional numerical simulation of the reactor hydrodynamics in a horizontal MOCVD system. This simulation was applied to the CdTe epitaxial growth. Deposition uniformity was analysed by numerical simulations and growth rates were evaluated as a function of susceptor position. Some drawbacks were pointed out related to the particularities of the MOCVD reactor and some simplifications were proposed.

In spite of the increasing interest above mentioned, it is frequent to find that the theoretical and the experimental works do not follow parallel ways. Complexity and difficulties to an easy and low cost implementation of numerical models can be, in some cases, a significant limitation.

Following our previous study about HgTe growth [14], our main purpose in the present study is to show how a numerical simulation, which can be run in a personal computer, can help to know the features of a particular MOCVD growth system and, consequently, to optimise the growth conditions. That is, a 2-D modelization to simulate the flow and thermal environment in a horizontal organometallic MOCVD reactor has been developed. This model takes into account the momentum conservation equation coupled with heat transfer and mass transport of the chemical species. For the mathematical solution of the problem we have used a commercial solver (FLUENT). The influence on the gas flow and growth rate of different parameters such as reactor pressure, partial pressures of precursors, total flow and substrate temperature is analysed and discussed. As precursors we have used diisopropyltelluride (DIPTe) and dimethylcadmium (DMCd), the most classical precursors for the MOCVD CdTe growth in the substrate temperature range from 350 to 400 ºC [15]. This substrate temperature has proved to be optimum for the growth of MCT by the Interdiffused Multilayer Process (IMP) [3], where the HgTe/CdTe layers can completely interdiffuse but still permitting the growth of junctions [15]. As carrier, H_2 has been employed.

It will be demonstrated that numerical simulation can be used to improve the film thickness uniformity and to optimise the choice of precursor partial pressures.

The main goal of this paper is both to offer a valuable tool for the numerical simulation of the MOCVD system and to suggest some practical reflections for the MOCVD experimental grower in order to facilitate the optimization process in a reduced time.

2. System description and numerical simulation

The study has been made on a horizontal MOCVD system (Quantax 226 refurbished by EMF Ltd). The reactor consists of a tapered silica reaction cell which longitudinal section is shown in Fig. 1. The system is well adapted to the growth of mercury compounds and it has two gas inlets, one for the metalorganic precursors and the other one for the Hg-gas entry, also the system has an outlet for throwing out the residues. The Hg-inlet is purged by a continuous H_2 flow when no Hg compounds are going to be grown. Inside the reactor, two 2” wafers can be placed on a graphite susceptor with a surface of 63×151 mm^2, which is heated by a radiofrequency system, allowing to reach the necessary temperature for the pyrolysis of metalorganic precursors.

As suggested by Kuhn et al. [16], a preliminary analysis of the regime and characteristics of the gas flow is of interest in order to evaluate the possibility to incorporate some simplifications in the numerical simulation. In fact, a first hydrodynamic characterisation of flow in the reactor can be made by means of the Reynolds (Re) and Rayleigh (Ra) dimensionless numbers [17].

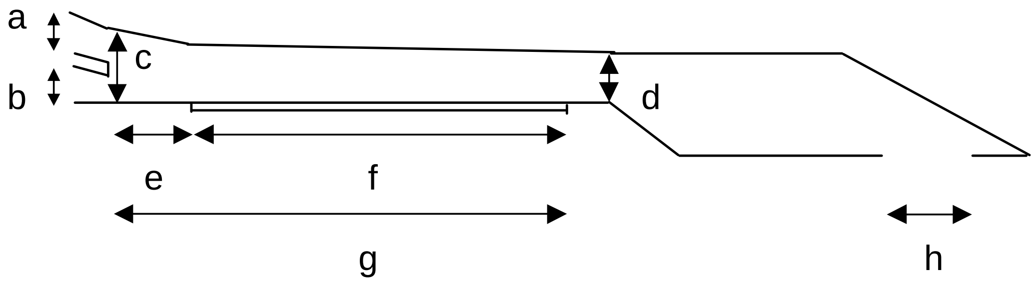


Fig. 1. Scheme of the two-inlet reactor cell. a = upper inlet (15 mm), b = lower inlet (9 mm), c = 19 mm, d =15 mm, e = 38 mm, f = substrate zone (120 mm), g = susceptor (150 mm) and h = outlet (25 mm). Width of the reactor cell is 66 mm.

The Reynolds number

$$\mathrm{Re} = \frac{\rho v h}{\mu} \tag{1}$$

where ρ is the fluid density, v the fluid velocity, h the reactor height and μ the fluid viscosity, as compared with the critic Reynolds number (≈ 2100), informs about the transition between laminar flow to turbulent one [17]. The calculations for the range of temperatures and flows which can be used in the epitaxial growth of CdTe have been achieved. To calculate the Reynolds number the physical properties of the fluid have been taken into account at a mean temperature of 295 ºC only for H_2 because the concentration of precursors is very small. Values of the Reynolds number ranging from 5 to 30 have been obtained. These values depend on the flow velocity, therefore on the total flux, and on the position inside the reactor. Nevertheless in all cases are far from the critic Reynolds number.

On the other hand, in our reactor the susceptor is hotter than the upper wall. The tendency to free convection can be estimated from the Rayleigh number (Ra)

$$\mathrm{Ra} = \frac{\alpha g c_p \rho^2 h^3 \Delta T}{\mu \kappa} \tag{2}$$

where α is the coefficient of thermal expansion, g is the gravity acceleration, c_p is the specific heat of the fluid, ΔT is the temperature difference between the susceptor and upper wall and κ is the thermal conductivity of the fluid.

The Rayleigh number (Ra) was also evaluated for values of the H_2 properties taken at the mean temperature of the reactor. The upper wall temperature was considered 140 K lower than the susceptor one according to our experimental measurements. Values of the Rayleigh number ranging from 1 to 10 were obtained, depending on the reactor pressure (100-760 Torr) and on the position inside the reactor. These values are lower than $\mathrm{Ra}_{\mathrm{crit}} \approx 1707$ for the transition from no convection to free convection in horizontal reactors [18]. Then, the free convection of the gas flow will not be taken into account further.

With respect to the processes in the reactor, it can be said that there are two main consecutive processes: the arrival of precursor molecules at the substrate and the surface reaction between them. The first process is controlled by the flow field inside the reactor which is determined for the governing equations that, in case of laminar flow, forced convection and steady state, are:

- Continuity equation:

$$\nabla\cdot\rho\vec{v} = 0 \tag{3}$$

- Momentum conservation equation:

$$\nabla\cdot\rho\vec{v}\vec{v} + \nabla p + \nabla\cdot\bar{\bar{\tau}} = \rho\vec{g} \tag{4}$$

- Energy conservation equation:

$$\nabla\cdot\rho\vec{v}\hat{H} + \nabla\cdot\vec{q} + p\nabla\cdot\vec{v} + \nabla\cdot\hat{H}\vec{J}_{i,j} + \bar{\bar{\tau}} : \nabla\vec{v} = -S_h \tag{5}$$

Where p is the static pressure, $\bar{\bar{\tau}}$ is the conventional stress tensor, m_i is the mass fraction of specie i, $\hat{H}$ is the enthalpy per unit mass, q is energy flux relative to mass average velocity and S_h is a source term that includes sources of enthalpy due to chemical reactions [17].

Additionally we need to consider the diffusion flux of species i in carrier j ($\vec{J}_{i,j}$):

$$\vec{J}_{i,j} = -\rho D_{i,m}\nabla m_i - D_i^T \frac{1}{T}\nabla T \tag{6}$$

where T is the temperature of fluid, $D_{i,m}$ is the diffusion coefficient for species i in the mixture and D_i^T is the thermal coefficient for species i. The expression of the diffusion coefficient is:

$$D_{ij} = 0.00186 \frac{\left[T^3\left(\frac{1}{M_i} + \frac{1}{M_j}\right)\right]^{\frac{1}{2}}}{p_{op}\sigma_{ij}^2\Omega_D} \tag{7}$$

where M_i is the molecular weight of species i, p_{op} is the reactor pressure, σ_{ij} is the mean value of the Lennard-Jones diameters of species i and j [19]. Ω_D is a correction factor provided for the rigid sphere approximation given by

$$\Omega_D = F\left(\frac{T}{\left(\frac{\varepsilon}{k}\right)_{ij}}\right)$$

where F is a tabulated function [17] and

$$\left(\frac{\varepsilon}{k}\right)_{ij} = \left[\left(\frac{\varepsilon}{k}\right)_i\left(\frac{\varepsilon}{k}\right)_j\right]^{\frac{1}{2}}$$

ε is an energy parameter and k is the Boltzmann constant. The rate $\left(\frac{\varepsilon}{k}\right)$ can be calculated for each species from

$$\left(\frac{\varepsilon}{k}\right) = 1.21T_b$$

where T_b is the boiling temperature. In our case, the second term of eq. (6) is negligible, due to the thermal conditions and the low value of D_i^T (D_{DIPTe}^T, D_{DMCd}^T << $D_{DIPTE,H2}$, $D_{DMCd,H2}$), so we have not considered the mass diffusion due to thermal gradients (Soret effect).

The solution of coupled governing equations permits to obtain the local concentration of different species and to evaluate the second process (surface reactions) which is described by the velocity of reaction k (A+B $\Rightarrow$ C+D) between species i (R_{ik}).

$$R_{ik} = \nu_{ik}M_iA_k \prod_{j reactants} C_j \exp(-E_k/RT) \tag{8}$$

where ν_{ik} is the stoichometric coefficient of species i in reaction k, C_j is the molar concentration of specie j, A_k is a pre-exponential factor and indicates the frequency of reaction between the precursor molecules, E_k is the activation energy that takes into account the minimum amount of energy necessary for producing the reaction. A_k and E_k are known as the Arrhenius parameters, and R is the ideal gas constant. To simplify the chain of reactions present [20] in the CdTe growth, we have used a global surface reaction [13]:

$$DIPTe_{(g)} + DMCd_{(g)} \Rightarrow CdTe_{(s)} + Res_{(g)} \qquad (9)$$

where $Res_{(g)}$ represents the by-products.

The presence of two consecutive processes makes the growth rate to be basically limited by the slowest one. If the growth rate is limited by the arrival of the constituents to the substrate, the growth takes place in a mass transport regime, while if it is limited by the second process (surface reaction) the growth takes place in a kinetics regime. One criterion to know the dominant growth regime is to analyse the experimental dependence of the growth rate with temperature [21]. If this dependence follows a function of $T^{3/2}$, as the diffusion coefficient (see eq. 7), the dominant regime is the mass transport. On the contrary if the temperature dependence follows a exponential form, as in eq. (8), [$\propto \exp(-E_k/RT)$], the kinetics regime will be the dominant one.

As boundary conditions we need to consider that for the epitaxial MOCVD process values of the parameters such as total flux, pressure of precursors at the inlet, substrate temperature, reactor pressure can be adjusted in order to optimise the growth conditions. These adjustable parameters have been used as variable boundary conditions. The metalorganic precursors and the H_2 carrier gas are introduced in the reactor through the higher gas inlet (see Fig. 1), while the lower one is purged by a continuous H_2 flow of 0.25 slm. The other boundary conditions have been fixed as follows: the gas inlet temperature was 300 K, and the emissivity coefficient of the silica at the upper wall was taken constant (0.9) [22] because the contribution related to the weak CdTe deposition on the quartz wall was not taken into account.

For the numerical calculations of the fluid flow, temperature and concentration fields, the computational fluid dynamics (CFD) code FLUENT [23] was used. In this code the discretisation of the conservation equations is based on a finite difference/control volume technique. This technique guarantees the conservation of all quantities in every volume element of a discretised domain. The set of conservation equations (conservation of mass, momentum and energy) is solved by a semi-iterative scheme, with iterations continuing until all equations are satisfied at all volumes. The criterion for the solution of the numerical problems is the residual error for each conservation equation in each volume, which must decrease to a required value.

In this study, for reducing the computational time, we have made use of a 2D approach because the aspect ratio (width to height ratio) is approximately 4 and the sidewalls have not significant influence on the flow field in almost all the susceptor width [10]. This fact, joined to the hypothesis of absence of transverse rolls predicted by the Rayleigh number, justifies good lateral growth rate homogeneity.

We have used a computational domain of 2624 (82×32) cells adapted to the geometry of the reactor (Fig. 1). In order to avoid divergence problems and mathematical difficulties related to the local variations of flow values, the density of cells in the grid has been taken not uniform but higher near the susceptor where the gradients of species concentration are strong. Consequently the size of these cells is smaller than the rest. We have tested the results with a double cell density and we have verified that similar results are obtained which justify the validity of the chosen grid. With this domain cell no divergence problems, as reported in ref. [13,16], were detected. The calculations have been made in a personal computer and the memory requirements were 32 MB of RAM.

3. Results of numerical simulation

As already mentioned, numerical simulation permits a detailed knowledge of several magnitudes in a particular reactor on determined flux, substrate temperature and partial pressure conditions.

In this study we will focalise on the low and middle substrate temperature range which includes the optimum range for the MCT growth by IMP process [15].

In most cases the study has been conducted in the whole region where the substrates should be positioned. Nevertheless in some cases we have focused our calculations on the point in which the centre of the first substrate should be positioned, that is at 9.4 cm from the beginning of the reactor.

3.1. CdTe growth rate dependence on the substrate temperature in the range 260 to 380 °C

For the range of substrate temperature of 300 to 350 °C a dominant process cannot be established and both regimes (transport mass limited and kinetic limited) should be considered. The Arrhenius parameters have been evaluated from the experimental data of ref. [12]. These are an activation energy of $E_k \approx 20.5$ kcal/mol and a estimated pre-exponential factor of $A_k \approx 10^{10}$ S.I. (see equation 8) for a VI/II ratio of 2.

In Fig. 2 we show the CdTe growth rate at a point on the susceptor situated at a length along the reactor of 9.4 cm as a function of the inverse substrate temperature. Similar results can be found for the other points of the susceptor. In this figure we can see that, for the whole temperature range, the growth rate decreases when the temperature decreases too. In the low temperature range (260-300 °C) there is a strong dependence of the growth rate with the temperature, indicating that a kinetics regime dominates. In the temperature range of 300 to 350 the two processes (transport mass limited and kinetic limited) coexist. For middle temperatures (350-380 °C), the temperature dependence is smooth; we can consider the growth rate basically limited by mass transport. We have not analysed the high temperature range because our interest is on the middle temperatures where the IMP process is optimum. In the high temperatures region other processes as the desorption of molecules from the epitaxial surface [12, 24] and the depletion of reactants due to the upper wall temperature, which increase the upper wall deposition [9] should be considered.

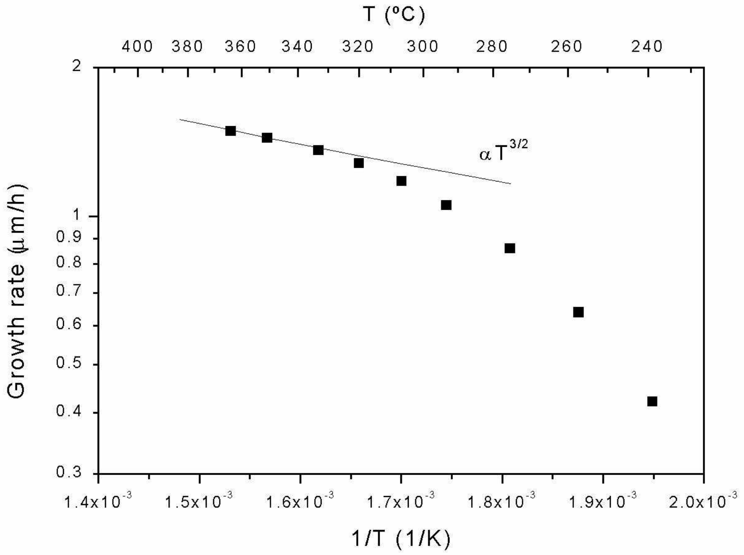


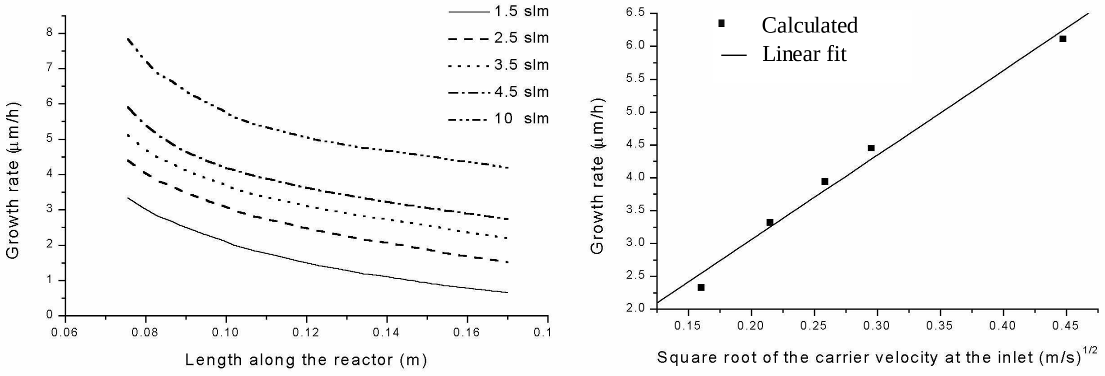
Fig. 2. CdTe growth rate in a point situated at 9.4 cm from the beginning of the reactor versus inverse temperature. $n_{DIPTe} = 20.4$ μmol/min, VI/II ratio = 2, total flux = 3.5 slm (3.25 through the upper inlet and 0.25 through the lower inlet) and $p_{op} = 1$ atm.

Anyway, as it has been calculated (see Fig. 2), in the substrate temperature range 350-380 °C, it can be considered that the mass transport regime is dominant and the next studies have been made under mass transport limited conditions. The numerical calculations have been thus conducted under the assumption of a fast surface reaction.

Due to the different values of the VI/II ratio (between 0.5 and 2) in the experimental work, for example [13, 24, 25], we have done the most of the next numerical calculations for a VI/II ratio of 1. Nevertheless the basis of conclusions are the same.

3.2. CdTe growth rate dependence on the total flux

In a MOCVD growth experiment, the parameters that appear to be more directly related to the growth rate are the total flux and the partial pressure of precursors. Thus, generally, the partial pressure of precursors can be fixed at a certain value and the total flux would be changed until the desired growth rate is obtained. Trying to reproduce this process, we have studied the CdTe growth rate in the susceptor using the total flux as a parameter. We have maintained constant the partial pressures of both precursors at a value of 1.3×10^{-4} atm. and we have varied the total flux from 1.5 to 10 slm. The CdTe growth rate is pictured in Fig. 3-a as a function of the length along the reactor, for different total fluxes. As a general characteristic, it can be seen that the CdTe growth rate increases when the total flux increases. Another important information which can be obtained by the numerical simulation is the uniformity of the growth rate along the susceptor. From Fig. 3-a, it can be seen that this uniformity remains almost invariable for different total fluxes when the partial pressure of precursors is constant. We can conclude that apparently the total flux does not affect the growth rate uniformity when the partial pressures are maintained constant. It is noteworthy that when the total flux is increased, keeping constant the partial pressures of precursors, the individual flux of precursors need to be also increased. Furthermore we have calculated the CdTe growth rate, at the point on the susceptor situated at 9.4 cm from the beginning of susceptor, as a function of the square root of the inlet carrier velocity (see Fig. 3-b). We find that this rate follows a fairly behaviour with the square root of the fluid velocity at the inlet, as the boundary layer theory [26] predicts in the mass transport regime, here considered. This result is also in agreement with the experimental data shown in [27] for the GaAs growth at the same mass transport limited regime.



a b

Fig. 3. a) CdTe growth rates as a function of the length along the reactor for different values of total flux. $p_{DIPTe} = 1.3 \times 10^{-4}$ atm., VI/II ratio = 1 , $p_{op} = 1$ atm and $T_{sus} = 365$°C. b) CdTe growth rate in a point situated at 9.4 cm from the beginning of the reactor versus square rate of gas velocity at the upper inlet. Same boundary conditions of Fig. 2.

On the other hand an alternative way to work could be to keep constant the amount of precursors, and not the partial pressures. Under these conditions an increment of the total flux implies obviously a reduction of the partial pressures. The numerical simulation of the growth rate has been studied using, as before, the total flux at the higher inlet as a parameter. The amount of precursors (DIPTe and DMCd) have been kept constant, respectively at a value of $n_{DMCd} = 20.9$ μmol/min for DMCd and $n_{DIPTe} = 20.4$ μmol/min for DIPTe (same partial pressures, VI/II = 1). The total flux has been ranged from 1.5 to 10 slm. In Fig. 4 the CdTe growth rate is plotted as a function of the length along the reactor, for different total fluxes. When the total flux increases, the CdTe growth rate significantly decreases. Under these conditions the total flux affects the growth rate uniformity along the susceptor making a significant difference with the formerly constant partial pressure conditions.

As a first conclusion, according to our numerical results, good uniformity along the susceptor can be reached without a important decrease in the CdTe growth rate at total flux rates of 3.5 – 4.5 slm.

and values of partial pressures in the order of 1 - 1.5 × 10^{-4} atm. This result is also in good agreement with experimental results obtained in a similar reactor (see ref. 13).

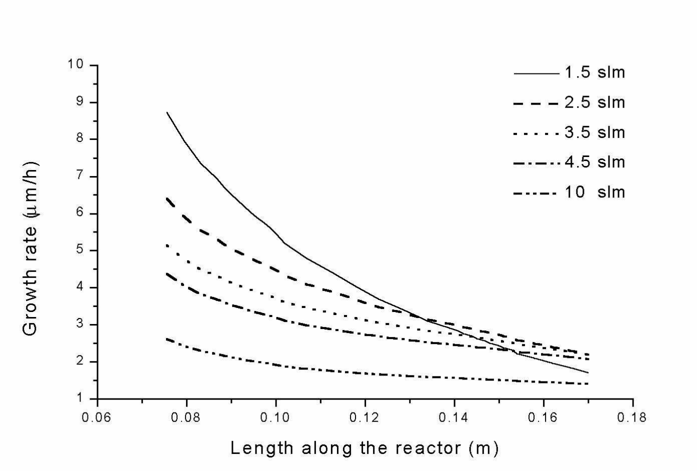


Fig. 4. CdTe growth rates as a function of the length along the reactor for different values of total flux. n_{DIPTe} = 20.4 μmol/min, VI/II ratio = 1 , p_{op} = 1 atm and T_{sus} = 365 °C.

3.3. CdTe growth rate dependence on the DIPTe and DMCd ratio

Without regarding the surface morphology which cannot be numerically analysed in the theoretical study presented here, we will next analyse the influence on the growth rate of the precursors ratio, i.e. the relative amount of precursors. We have set constant the amount of DMCd at a value of 20.9 μmol which is a standard experimental value [25] and we have varied the DIPTe amount. Typical results for the growth rate as a function of the length along the reactor using the ratio of precursors as a parameter are plotted in Fig. 5. The growth rate uniformity is nearly unchanged for different precursor ratios, except for values near the saturation effect which appears for VI/II ≥ 1.5.

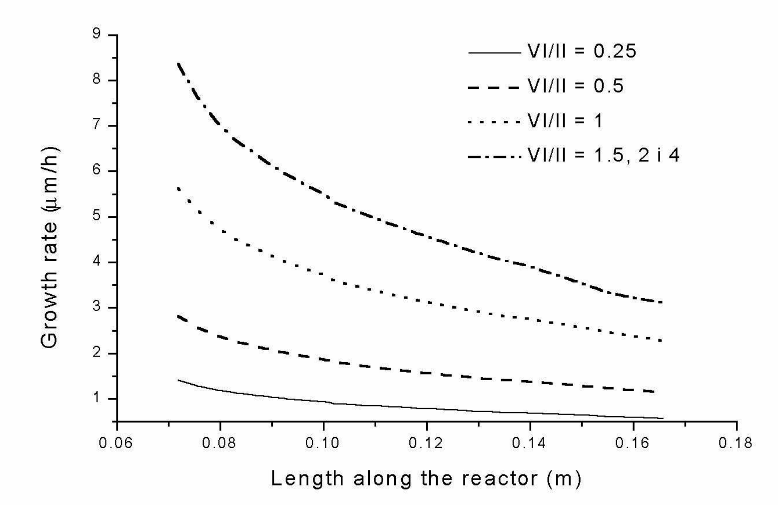
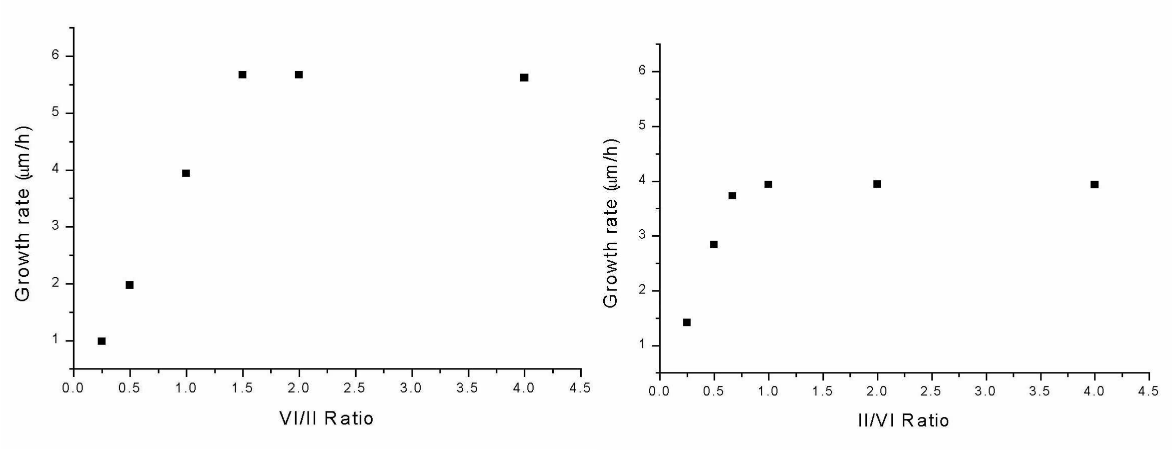


Fig. 5. CdTe growth rate as a function of the length along the reactor for different values of VI/II ratio. n_{DMCd} = 20.9 μmol/min, total flux = 3.5 slm (3.25 through the upper inlet and 0.25 through the lower inlet), p_{op} = 1 atm and T_{sus} = 365 °C .

In order to analyse in more detail the influence of the relative amount of precursors over the growth rate, we have calculated it at the point situated at 9.4 cm from the beginning. In Fig. 6-a and

6-b, the saturation effect mentioned above is clearly seen. The growth rate saturates for a certain ratio of the precursors, but it can be observed that the saturation is smoother when the DMCd partial pressure is fixed and the variation of the VI/II precursors ratio is due to DIPTe partial pressure changes (see Fig. 6-a) than when the DIPTe partial pressure is the fixed one. These results have been experimentally found [25, 28]. Otherwise, the asymptotically growth rate reached in fig. 6-a is greater than those reached in Fig. 6-b. Numerical simulation shows that DIPTe is the minority compound which determines the growth rate, depending on its mass transport to the susceptor point, DIPTe being the first precursor to be exhausted. The behaviour shown in figs. 6-a and 6-b can be explained if we calculate from eq. (8) the value of the diffusion mass coefficients. At the substrate temperature of 365 ºC, the diffusion coefficients are $D_{DIPTe,H2} \approx 1\ cm^2/s$ and $D_{DMCd,H2} \approx 2\ cm^2/s$. Due to the fact that $D_{DIPTe,H2} < D_{DMCd,H2}$, the arrival of DIPTe molecules at the substrate will be slower than the DMCd one. The first precursor will limit reaction (11) and, therefore, the CdTe growth rate. We have supposed that DIPTe and DMCd molecules are pyrolised in the hotter zone of the reactor cell, just over the susceptor, ignoring intermediate species. We have not considered the difference between the pyrolysis temperature of DIPTe and DMCd molecules. When we apply this discussion to experimental data, we would need to consider a correction factor, for example when DIPTe and DMCd are both at 370 ºC, the 40% of DMCd and 30% of DIPTe molecules are unreacted [20]. Nevertheless the basis of the discussion continues to be the same. In reference [29] the precursor of tellurium was DETe, Fig. 6-a and 6-b qualitatively agree also with experimental data of that paper [29] because the diffusion coefficient of the Te precursor is also lower than those of the Cd precursor.



a b

Fig. 6. a) CdTe growth in a point situated at 9.4 cm from the beginning of the reactor versus VI/II ratio. $n_{DMCd} = 20.9$ μmol/min, total flux = 3.5 slm (3.25 through the upper inlet and 0.25 through the lower inlet), $p_{op} = 1$ atm and $T_{sus} = 365$ ºC. b) CdTe growth in a point situated at 9.4 cm from the beginning of the reactor versus II/VI ratio. $n_{DIPTe} = 20.4$ μmol/min, total flux = 3.5 slm slm (3.25 through the upper inlet and 0.25 through the lower inlet), $p_{op} = 1$ atm and $T_{sus} = 365$ ºC.

3.4. CdTe growth rate dependence on the reactor pressure

With the aim of testing the simulation model and also of determining the influence of reactor pressure on the particular characteristics of our reactor, a study of the growth rate in the susceptor has been undertaken, using the reactor pressure as parameter. The total flux and the molar fractions of the precursors (χ_{DIPTe} and χ_{DMCd}) have been kept constant, and the reactor pressure has been varied from 100 to 760 Torr. The CdTe growth as a function of the length along the reactor is, practically, the same for different reactor pressures.

As it is well known from the boundary layer theory [26] and predicted by eq.6 ($\rho \propto p_{op}$ and $D_{i,m} \propto 1/\ p_{op}$), when the system is working in the mass limited diffusion regime and the molar fraction of precursors is constant, the CdTe growth rate is constant for different reactor pressures. However, when the partial pressures of precursors are fixed at a constant value the molar fraction increases when the total reactor pressure decreases. So that, when the partial pressures of DIPTe and DMCd are constants the CdTe growth rate increases when the total reactor pressure decreases (see Fig. 7). Thus aspect needs to be considered in order to use the reactor pressure as an effective experimental parameter.

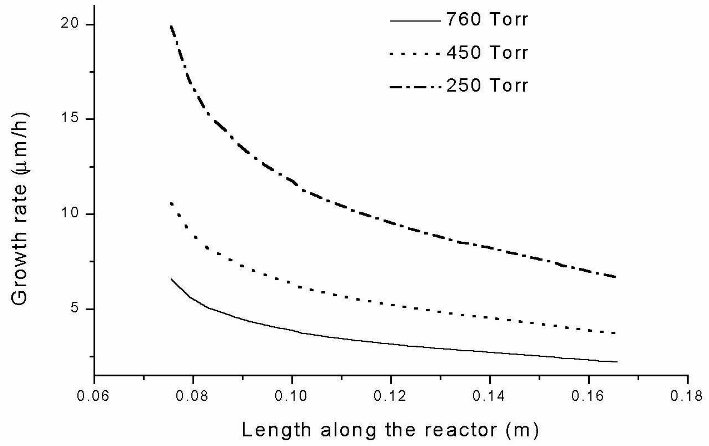


Fig. 7. CdTe growth rates as a function of the length along the reactor for different values of reactor pressure. $p_{DIPTe} = 1.3 \times 10^{-4}$ atm, VI/II ratio = 1 , total flux = 3.5 slm and $T_{sus} = 365$ °C.

4. Summary and conclusions

This numerical simulation permits a preliminary determination of the experimental conditions. From this study, the value of different adjustable parameters can be chosen in order to optimise the growth rate and uniformity under the best economical and technical conditions.

In summary, a numerical simulation of the CdTe MOCVD growth in a horizontal quartz reactor with DIPTe and DMCd as precursors and H_2 as the carrier gas, has been achieved, using a commercial code for the mathematical solution of governing equations. This two-dimensional numerical simulation has allowed the determination of the CdTe growth rate dependence on several experimental parameters.

The study has been made in mass transport and kinetics regimes at low and middle temperatures. In the mass transport regime this study has permitted to determine quantitatively some of the general trends of the process:

- For a constant amount of precursors at the inlet, the CdTe growth rate decreases as the total flux increases, and the uniformity of the growth rate along the susceptor increases.
- For a constant partial pressure of precursors at the inlet, the CdTe growth rate increases linearly with the square root of the gas velocity at the inlet.
- The DIPTe is the limiting reactant.
- For a constant amount of total flux and molar fraction of precursors (χ_{DIPTe} and χ_{DMCd}) at the inlet, the CdTe growth rate is invariable with the reactor pressure.

As a practical conclusion, we can say that if a uniform growth rate along the susceptor is wanted (a common aim in MOCVD growth experiments), there are three complementary ways which are:

- To change the amount of precursor raising the growth rate at an appropriate value.
- To change the total reactor pressure, with the partial pressure of precursors constant, raising the growth rate at an appropriate value.
- To increase the total flux.

These alternatives are compatible between them and a good combination can give excellent results.

In other words, the numerical simulation here presented reproduces qualitatively the trend of experimental data [4,12,13,25,27,28,29] with respect to the CdTe growth rate variation due to different experimental parameters: total flux, precursors amount and ratio, total reactor pressure and substrate temperature. This fact shows that the numerical simulation is a helpful tool in the analysis of the behaviour of a MOCVD reactor, that can improve the understanding of the growth process and the growth rate and the thickness uniformity dependence along de susceptor on different adjustable parameters. This fact can be very useful in order to reduce the number of experiments and, consequently, the economic cost. The generalisation of this study and analysis for other compounds is straight.

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