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MCT epitaxial films: discrete solution of a non linear diffusion problem numerical stability study

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$Hg_{1-x}Cd_xTe$ (MCT) is the most important semiconductor for infrared detection. MCT films have been obtained by ISOVPE technique. Thin film growth is described by a nonlinear convective diffusive model. The evolution of the nonlinear diffusion problem with boundary values was numerically solved by means of discrete mathematics. Two finite differences methods (explicit and implicit iterative algorithms) were used. The obtained results were compared. The experimental results are compared with the predictions of the model, the discrepancies between them are discussed.

1. Introduction

HgCdTe(MCT) is an excellent material for the manufacture of infrared detectors. It has a high optical absorption coefficient, a high electron mobility, a low thermal carrier generation rate and a tunable bandgap[1]. Also this material is very suitable for emission devices operating in the 2-5 μm range for which there has been an increasing interest in recent years. In every case the material must be singlecystalline. Several bulk and epitaxial growth techniques have been developed to get MCT singlecrystals. Among the epitaxial techniques (MBE, MOCVD, LPE, ISOVPE) the last one is the most appropiate for small enterprises owing to its low cost and versatility [2] . Besides, this technique enables the obtention of MCT epitaxial films with good radial compositional uniformity, surface morphology and electrical properties. In this work is applied a model that attempts the prediction of compositional profiles of MCT films grown by ISOVPE. The experimental results are compared with the predictions of the model, the discrepancies between them are discussed.

2. Calculation Procedure

Djuric Model

The following steps are considered [3]:

1) source sublimation and dissociation:

$$HgTe(s)\ \circledR\ Hg(g)\ +\ ½\ Te_2\ (g)$$

It´s supposed that this step does not determines the film growth rate.

2) *Hg* and Te_2 transport from the source to the substrate

Since the Hg partial pressure is at least three orders of magnitude higher than the Te_2 partial pressure, the rate of this step is controlled by Te_2 transport:

$$v(u,T) = 2\ D_{Te}\ [\ P_{Te}(HgTe) - P_{Te}(MCT)] \,/\, k\ Td\ N$$

D_{Te}: diffusion coefficient of Te_2 in $Hg(g)),P_{Te}(HgTe)$:Te_2 partial pressure over *HgTe* at a temperature T, P_{Te} (MCT): Te_2 partial pressure over MCT at a temperature T, *k*: Boltzmann constant, *d*: source-substrate distance,N: atomic density in *HgTe.*

If the Te_2 partial pressures are expressed in terms of the dissociation equilibrium constants of *HgTe* and $Hg_{1-u}Cd_uTe$ and the *Hg* partial pressure then:

$$v = 2\ D_{Te}\ [\ (K_{HgTe})^2 - (K_{Hg(1-u)Cd(u)Te})^2\ ] \,/\, kTd\ N\ (P_{Hg})^2$$

K_{HgTe} : *HgTe* dissociation equilibrium constant
$K_{Hg(1-u)Cd(u)Te}$: $Hg_{1-u}Cd_uTe$ dissociation equilibrium constant

For the employed experimental conditions ($T = 883\ K$, $d = 5.10^{-2}\ m$, no Hg overpressure) the convective term results:

3) reaction at the epitaxial surface:

$(1-u)\ Hg(g) + (1-u)\ Te_2(g) + u\ CdTe(s) \rightarrow Hg_{1-u}Cd_uTe$

It´s supposed that this step does not determines the film growth rate.
4) Hg and Cd interdiffusion in the epitaxial film with the coefficient $D(u) = 1{,}84\ 10^{-13}\ exp.\ (\ -6{,}705\ u)\ \ m^2\ s^{-1}$ [4].

The net rate of the process is determined by the steps 2) and 4). Therefore, if the epitaxial surface is selected as the origin (x = 0), an unidimensional diffusion-convection problem results, wich is described by a partial differential equation with no linear coefficients. In fact, the so-called “ convective term “ corresponds to the Te_2 diffusion in a Hg vapor phase.

Numerical Resolution of the Nonlinear Diffusion-Convection Problem

For the study of the expossed process, it has been resolved the nonlinear diffusive-convective partial differential equation:

$$\frac{\partial}{\partial x}\left[D(u)\frac{\partial u}{\partial x}\right] - v(u)\frac{\partial u}{\partial x} = \frac{\partial u}{\partial t} \qquad (1)$$

with the initial condition: $u(x,0) = 1$,

and the boundary conditions: $D(u)\dfrac{\partial u}{\partial x} = v(u)\ u(0,t)$ at $x = 0$, and $u(\infty,t) = 1$, that is to say, Robin boundary condition (or third class condition, in which appears the unknown value and its gradient) and Dirichlet boundary condition (or first class, which provides the value of the unknown in a boundary), in a semiinfinite medium.

The equation has been trasformed to the form:

$$D(u)\frac{\partial^2 u}{\partial x^2} + \left[D_u(u)\frac{\partial u}{\partial x} - v(u)\right]\frac{\partial u}{\partial x} = \frac{\partial u}{\partial t} \qquad (2)$$

and it has been discretized simultaneously with the boundary conditions. The problem has been resolved by the finite differences method. It has been employed centered differences (that is to say, an interval of *2h* lenght has been considered, where h is the grid step with the node to be resolved in the central point), for the convective term.

Explicit Method

The explicit method has been employed in a first resolution. Its use corresponds to calculate the unknown value in each grid node, only employing nodes of the $v = 5{,}98\ 10^{-9}\ [\ 1 - (1-u^2)\ exp.\ (1{,}3\ u^2\ )\ ]\ m\ .\ s^{-1}$ previous temporal step. Since the domain is semiinfinite, an adequate amount of nodes has been used in order to situate far away the boundary condition $u(\ \ , t) = 1$, so that the solution does not change at the *n*-1 node, if we call n the last node of the grid. It has been studied the properties of the transition matrices (these matrices enable to generate the composition profile at a given temporal level, knowing the previous solution), particularly its diagonal dominance and spectrum, also it has been shown the consistency of the calculation scheme and the differential problem. It has been investigated the numerical stability of the scheme and with the appropriate assumptions on the existence and boundedness of the derivates of the solution, the operators result bounded.

Implicit Method

In a second resolution it has been elaborated an algorithm that iterates at each time level, that uses implicit discretization. In this case, for each iteration, the coefficients are actualized, maintaining the profile corresponding to the previous time. At each time step, the iteration procedure finishes when the sup-norm of the difference between two solutions is lower than an?? (prefixed

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As in the first method, the characteristics of the transition matrices (in this case inverse operators) have been investigated, verifing the necessary properties of diagonal dominance and spectral conditions for numerical stability.

The discretization of the convective term in diffusion-convection problems generates numerical dispersion or viscosity. This quantity adds to the physical diffusion, introducing perhaps an unreal diffusion coefficient. A control of this quantity has been made, and it has been verified that its value is of limited signification with respect to the physical diffusion.
In figure 1 the graphs of the curves that represent the approximate solutions obtained with the two methods are exhibited, and it can be seen the similitude between them.

3. Comparison between the experimental results and the model predictions. Model modification

MCT epitaxial films (obtained by ISOVPE technique at 883 K without Hg overpressure) were clived at {110} planes and the composition profiles were determined with a wavelength dispersive microprobe.
Additional experimental details and film´s properties can be found elsewhere [5].

The experimental composition profiles differ markedly from the theoretical ones. Djuric et al have argued that the MCT epitaxial films grown in closed ampoule generally have lower thicknesses because a surface substrate oxidation [3]. However, other authors have observed a

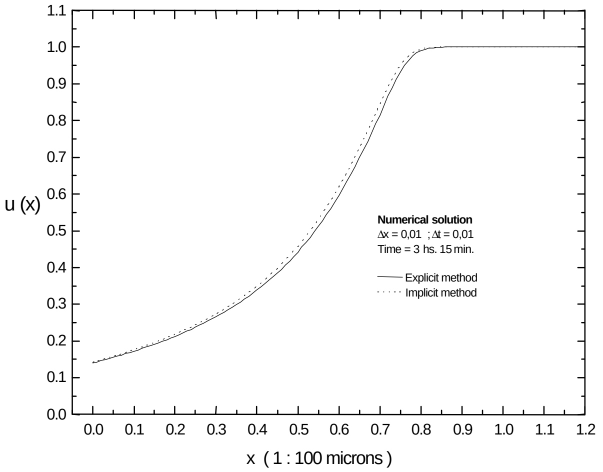

Fig. 1. Approximate solutions of the problem obtained with implict and explicit methods.

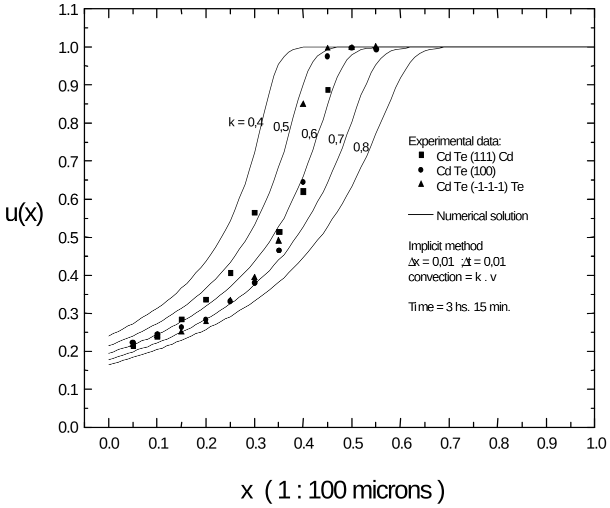

Fig. 2. Curves corresponding to the modified model and experimental data.

similar discrepancy in MCT epitaxial films grown with hydrogen flow [6]. This experimental fact would enable the neglect of that hypothesis.

These authors have supossed that the surface reaction of the step 3) takes place with a so slow rate that influences the net process rate. With this consideration in mind the " convective " term results: V = k .v , k is a function of d, D_{Te} and the rate reaction constant of the step 3) and $0 < k < 1$. As long as k is not a function neither of u nor of x, a similar equation to (1) results. Adopting this criterion the problem has been resolved again. In figure 2 are exhibitted the corresponding curves. It can be see that the modified model with k ≈ 0.6 fits the experimental data.

4. Conclusions

The boundary and initial conditions problem corresponding to Djuric model has been numerically solved, by discrete mathematics with the diffusive-convective form given by the equation (2). It has been verified the theorems that enable to assert the numerical stability of the scheme and the conditions that allow to say that the results are admissible approximations to the solution of the problem. The plots of the obtained results with the explicit and implicit schemes are exhibitted. In every time the diffusive term controls the equation, and so treated, the equation behaves as the parabolic heat equation. In the comparison between the experimental data and the model predictions, it can be seen a marked difference in accordance with other authors [6]. However, by supossing a finite rate in the surface reaction a good fit is found.

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