High Productivity Numerical Computations for Gas Dynamics Modelling Based on DFT and Approximation

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Abstract— **In article questions of high productivity numerical computations for gas dynamics modelling based on discrete Fourier transform and approximation are considered. The offered method is based on use of piecewise and analytical approximation of the equations of dynamics of gas and application of discrete transformations of Fourier. It allows to increase the accuracy of calculations and to increase the speed of convergence of the solution of the equations in space of three dimensions and in time. The iterative scheme of calculations is offered. Speed of convergence and an error of approximation is estimated. The possibility of approximation is considered by various approximating kernels. The computing algorithm was developed for fast calculation of a stream of gas and heat conductivity in the reactor of a vapor-phase epitaxy for crystal growth on computing systems of small productivity.**

Keywords*—Gas dynamics*; epitaxy; approximation; thermal field

I. INTRODUCTION

Active scientific research on heat transfer from a rotating disk has been underway for several decades. The main results of these studies can be found in a number of papers and monographs [1-4]. This increased interest in the problem is due to the fact that the rotation of the flow initiated by the rotation of the mechanical system can be found in a variety of engineering applications and industrial installations. Systems containing rotating discs are used in gas-turbine and electrochemical plants, chemical reactors, in brake systems of transport, etc.

For today, interest in this issue is not decreasing, as evidenced by the materials of many relevant scientific and technical conferences and articles. In a limited number of cases, the flow above the rotating surface can be viewed as a modified flow above a fixed surface, provided that the observer is on a rotating surface, that is, moves along with it. However, in most cases, the action of centrifugal forces or the nature of the spatial boundary layer causes the formation of significant additional flows, which can not be neglected.

In this case, the description of the resultant flow can be very complex and, according to [5], "practically any rotating system releases new and unexpected flow characteristics in the case of a complete stability analysis or in experimental studies due to the widest variation of the hydrodynamic variables". Due to the fact that in convective heat transfer in the rotating systems the strongest and most complicated way is connected with the flow, these two phenomena in the complex are also the subject of scientific and practical interest.

II. FORMULATION OF THE PROBLEM

Based on the description of the reactor unit for the installation of gas-phase epitaxy, cited in [2], in order to optimize the epitaxy process taking place in it, it is also necessary to investigate the processes of heat transfer and the motion of an external forced flow for the case of a rotating disc whose rotation plane, in general, is at an angle to the main flow.

III. PHYSICAL STATEMENT OF THE PROBLEM

Gas phase epitaxy is the process of growing epitaxial layers of semiconductors by deposition from the vapor-gas phase, which is most often used in the technology of growing wide-band and narrow-band semiconductor heterostructures of compounds of elements of the II-V group, and silicon, as well as semiconductor heterostructures of organometallic compounds of group III nitrides.

The process takes place in special reactors of a vertical or horizontal type. The reaction proceeds on the surface of the substrates (semiconductor wafers), heated to 400 - 1200 ° C, depending on the deposition method, process speed and pressure in the reactor. The required temperature of the substrates is provided by means of infrared sources, by a resistive method or by induction heating. Lowering the temperature below the limit for these particular precipitation conditions leads to the formation of a polycrystalline layer. On the other hand, it makes it possible to reduce the width of the diffusion transition region between the epitaxial layer and the substrate, the presence of which degrades the characteristics of the resulting devices.

In the gas phase epitaxy (VEP-VAPOR-Phase Epitaxy, VPE), a multicomponent gas mixture is used that includes the precursor molecules needed for epitaxial growth and a carrier

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gas (Figure 1). The carrier gas is usually hydrogen with an operating pressure in the range of 102-105 Pa, depending on the type of reactor and the characteristics of the growing process regime.

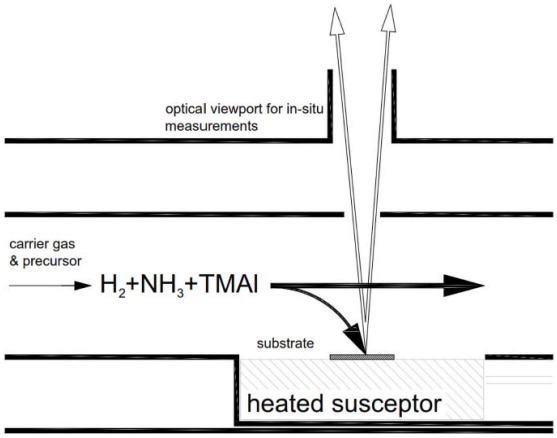

Fig. 1. Schematic representation of the gas phase epitaxial growth process for the case of GaAs and AlAs / GaAs MOVPE

For the growth of III-V semiconductor structures of a group of elements for which standard organometallic (mainly alkyl) compounds of Group III elements and hydrides of Group V elements are used, the process of chemical vapor deposition of metalorganic compounds is used (Metalorganic Vapor Phase Epitaxy, MOVPE). For these precursors, pressures in the range of 103-105 Pa (10-2-1 Bar) are typical. It is worth noting that, due to the many undesirable properties of alkyls and hydrides, today new organic compounds ("alternative precursors") are being searched for the technology of MOVPE.

To the greatest extent it is the carrier gas that determines the total pressure of the gas mixture and many of its physical properties.

The main type of structures used in research laboratories and on production lines is a horizontal reactor, shown in Figure 2.

IV. Gas Phase: Mass Transfer

To ensure the specified growth parameters for VPE, it is necessary to provide the appropriate parameters for the chemical reactions of the gas phase, that is, to control the presence of the necessary elements on the growth surface and the parameters determining the transfer of these elements to the growth surface. The latter is especially important in the case of growth determined by transfer, when the transfer has a strong effect on the uniformity of growth. The transport processes depend primarily on the velocity and temperature profiles in the reactor.

The mass transfer, i.e., the flow $\mathbf{j}_i$ of reagent *i* to the interface between the gas and solid media, is determined by the convective flow, diffusion in the concentration gradient, and thermal diffusion determined by the temperature gradient. The mass transfer can be described as follows:

$$\mathbf{j}_i = \frac{p_i \mathbf{v}}{kT} - \frac{D_i}{kT}\left[\nabla p_i + \frac{\alpha_i}{T} p_i \nabla T\right]$$

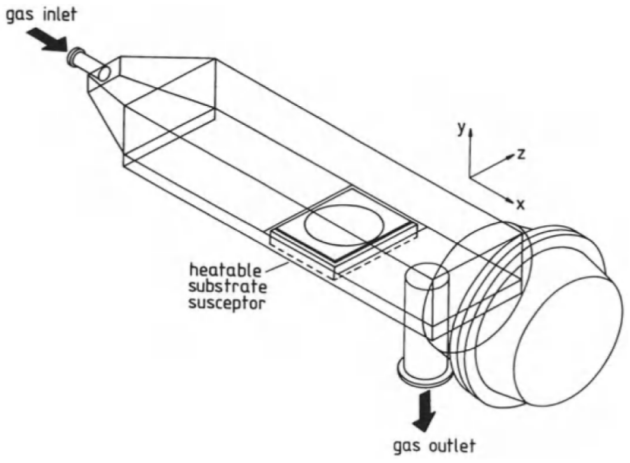

Fig. 2. The horizontal reactor for gas-phase epitaxial growth

where pi – is the partial pressure of reagent *i*, *Di* is the diffusion coefficient of reagent *i* in the carrier gas, and α_i is the coefficient of thermal diffusion.

In a record of the form (1), multicomponent diffusion and gas-phase reactions are neglected. Under these conditions, the main parameters determining the flow are the velocity v, temperature T, and partial pressures. While the partial pressures of the elements providing the epitaxy process will be determined by the ongoing chemical reactions of the gas phase, the gas flow rate and its temperature are essentially properties only of the carrier gas. This is due to the large difference in the partial pressures, which makes it possible in good approximation to neglect the influence of the precursor and the products of its reaction on the gas-dynamic and thermodynamic properties of the gas mixture. Thus, for the calculations of v and T, as well as for their determination by experimental means, it is sufficient to consider only the carrier gas. This simplifies experimental studies, without requiring the need to take precursors into account, and theoretical calculations - by reducing the number of equations necessary for their implementation.

V. Main Tasks of Modeling and Analysis

Summing up, it is possible to formulate the main tasks of modeling and analysis, the solution of which will help to improve the quality of growing layers and the speed of epitaxy:

1. Development of differential equations and boundary conditions describing the transfer of heat and mass in a chamber of a horizontal reactor with a rotating heated disk (a susceptor) (as the most general, ie, a three-dimensional problem).

2. Development of equations and boundary conditions describing the transfer of heat and mass in the region of the

thermal boundary layer above the substrate (susceptor) in the chamber of a horizontal reactor with a rotating susceptor.

3. Development of equations describing the spatial distribution of molecules (flow) of impurities (precursors) in the carrier gas flow, taking into account heat and mass transfer in the chamber of a horizontal reactor with a rotating heated disk.

4. Creation of software complexes for the calculation of heat and mass transfer fields in the chamber of a horizontal reactor with a rotating susceptor, which allow calculating the thermal field on the substrate surface and transfer in the thermal boundary layer above it with sufficient accuracy, as well as the spatial distribution of the precursor molecules and the thermal field in the region of this distribution.

5. Creation of software complexes for calculating the intensity and spatial distribution of radiation sources for heating the susceptor, allowing to increase the uniformity of thickness, stoichiometry and carrier concentration on the entire surface of the substrate, along with an increase in the rate of epitaxy in the specified ranges of operating conditions of the reactor. The calculation must take into account the disturbing effect of the oncoming gas flow on the uniformity of the thermal field on the surface of the substrate and the thermal boundary layer above it.

6. Development of algorithms to optimize transport processes, including transport for the precursor flux, and intensity and spatial distribution of radiation sources in order to increase the uniformity of thickness, stoichiometry and carrier concentration on the entire surface of the substrate, along with an increase in the epitaxy rate in given ranges of operating conditions reactor.

VI. Statement of the Model

Adequate modeling and analysis of processes in the reactor will solve problems of structural and parametric synthesis, as well as synthesis of optimal control aimed at achieving the main goal: increasing the thickness uniformity, stoichiometry and carrier concentration on the entire surface of the substrate, along with an increase in the epitaxy rate.

In order to calculate the profiles of temperatures and velocities in the reactor chamber, it is necessary to solve a set of equations describing the laws of conservation of momentum, mass, and energy for given boundary and initial conditions. As a rule, numerical solutions of this system of equations are realized with the help of finite element methods. In this case, because of the complex geometry and nature of the processes, as a rule, it is not possible to solve a complete three-dimensional model. Therefore, in modeling, the reactor chamber is considered to be symmetric in the middle plane along the flow direction.

Two-dimensional solutions in this plane give fairly accurate approximations, and calculations, although they require extremely high computational powers, can be performed for real boundary conditions.

However, for horizontal reactors with a rotating susceptor, it is impossible to make such assumptions, and the problem becomes three-dimensional.

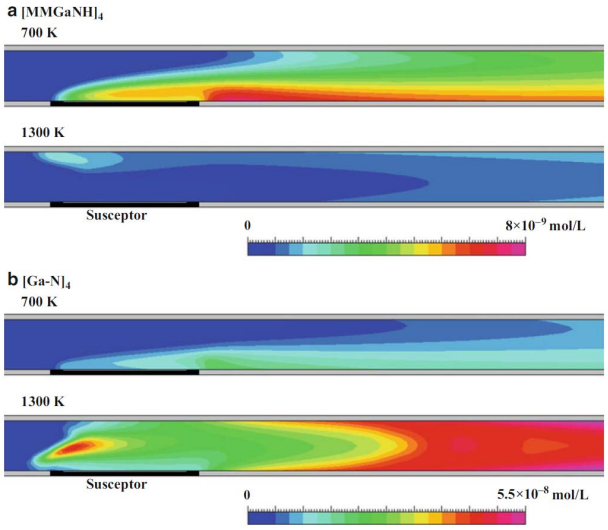

Fig. 3. Spatial distribution of [(CH3) GaNH] 4 and [GaN] 4 molecules at the entrance to the growth region where a large temperature gradient is observed

VII. Conclusions

An essential problem in the preparation of Group III nitrides is the absence of nitride substrates that are most suitable for the parameters of the crystal lattice and the coefficient of thermal expansion for the growth of GaN structures, because large bulk GaN single crystals can not be grown by conventional methods. Because of the high melting point of GaN (~ 2500 ° C) and the high equilibrium nitrogen pressure above the melt, a sufficiently low decomposition temperature of GaN (~ 1000 ° C), it is impossible to grow a large single GaN single crystal by standard methods and then cut it into substrates. Therefore, the main method for growing heterostructures based on III-N compounds is epitaxy from organometallic compounds. As an alternative to GaN substrates for the growth of nitride structures, sapphire and 6H-SiC crystals are widely used. However, neither sapphire nor SiC prevents the epitaxial growth of GaN without the use of special techniques for the nucleation of III-N crystals on them. These methods are empirical in nature, and there are few published studies on the relationship between growth conditions and the formation of nitride layers.

To some extent, this is due to the lack of attention to the processes occurring in the reactor with the growth of the VP- the relationship between the rate of decomposition and the synthesis of nitrides, their dependence on the already-grown growth conditions of the MOVPE method.

An understanding of the nature of the epitaxial process leads to an understanding of the processes of formation of epitaxial layers on foreign substrates and there is a conscious management of growth conditions to achieve the necessary characteristics of the growing layers. Therefore, the aim of this paper is to simulate the main processes that determine the quality and rate of growth of structures in the reactor.

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