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Study of the effect of dynamic and temperature inhomogeneities on epitaxial processes in a horizontal CVD reactor

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Abstract. In order to investigate the effect of temperature and velocity inhomogeneities at the reactor inlet on the susceptor growth rate distribution, a numerical simulation of the flow in a horizontal CVD reactor was carried out. It was obtained that the velocity inhomogeneity can reach 60%, and this can considerably affect the growth rate distribution on susceptor. To simulate the temperature inhomogeneities, the temperature distribution at the reactor inlet was set separately for the bottom and the main inlet. The temperature inhomogeneity at the bottom inlet affects the growth rate distribution more drastically than at the main inlet. This influence is quite strong and should be taken into account for accurate simulation of the flow and growth processes in similar horizontal CVD reactors.

Keywords: ANSYS Fluent, CFD, numerical simulation, MOVPE, CVD

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Влияние динамических и температурных неоднородностей на эпитаксиальные процессы в горизонтальном CVD-реакторе

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Аннотация. Для исследования влияния температурных и скоростных неоднородностей на входе в реактор на распределение скорости роста на подложкодержателе было проведено численное моделирование потока в горизонтальном CVD-реакторе. Было получено, что неоднородность скорости может достигать 60%, и это может значительно повлиять на распределение скорости роста на подложкодержателе. Для моделирования температурных неоднородностей распределение температуры на входе в реактор задавалось отдельно для нижнего и основного входа. Температурная неоднородность на нижнем входе влияет на распределение скорости роста более сильно, чем на основном входе. Это влияние довольно сильное и должно учитываться для точного моделирования течения и процессов роста в подобных горизонтальных CVD-реакторах.

Ключевые слова: ANSYS Fluent, CFD, компьютерное моделирование, МОСГФЭ, химическая эпитаксия

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Introduction

Nitride monocrystals have unique physical properties. Such properties as high saturated electron velocity and the ability to form solid solutions make these semiconductor structures indispensable for high-frequency electronic devices. There are several ways to fabricate such structures, and one of the most popular is chemical vapour deposition (CVD) [1]. This method is based on growing a crystal on a susceptor out of gas-phase components as a result of surface chemical reactions. There are several types of such reactors; in this paper we consider a horizontal one. In contrast to vertical ones, horizontal reactors allow multi-parameter optimization over a wide range of parameters. Its relative cheapness is also an advantage. Therefore, the use of horizontal reactors is very prospective.

There are many publications on the physicochemical aspects of the growth of nitride structures in horizontal reactors. In particular, many papers analyze the dependence of epitaxial parameters on pressure [2], susceptor temperature [3], or reagent flow rate [4]. A much smaller number of studies concern hydrodynamic factors. For example, in [5] the influence of precursor supply configuration through different inlets on the epitaxial processes is investigated.

Due to the design features (including the complex reactant supply system) in a horizontal reactor, significant inhomogeneities in velocity and temperature at the reactor inlet can occur. Such effects as, for example, local overheating of the injector caused by irradiation from the susceptor can lead to a flow restructuring and a change in the pattern of the crystal parameters distribution over the susceptor. It is important to consider such effects when designing new reactors and determining its optimal operating conditions. This study was carried out in order to investigate the effect of possible inhomogeneities in a horizontal reactor on epitaxial processes.

Materials and Methods

In this paper the peculiarities of growth processes in the model of the experimental setup “Dragon 125” (125 is the diameter of a susceptor in millimeters), which is currently active in the Science and Technique Center of microelectronics (STC) [6], are analyzed by means of numerical simulation. Numerical simulation replicates in-situ experiments done at the STC. Figure 1 shows the computational domain (only half of the geometry was considered with the symmetry boundary condition). It includes the gas domain (Fig. 1, *a*, *b*) located inside a quartz reactor, which itself is placed inside a nitrogen tank (Fig. 1, *c*). Through the main inlet, aluminum trimethyl and hydrogen are fed. Ammonia is supplied through the bottom inlet. A long slit channel is placed in front of the main inlet, which is set aside in the figure for clarity. The susceptor is heated to a temperature of 1100 °C. External heat transfer boundary condition is set on the rest of the bottom wall. The walls of the nitrogen tank are water-cooled and the temperature on them is assumed to be 150 °C. A crystal is assumed to grow on all the inner walls. In the simulation, this is accounted for by a chemical surface reaction model [7]. The susceptor rotates slowly; its rotation has low effect on the growth processes and is taken into account in the postprocessing of the calculation results by averaging the crystal growth rate in the azimuthal direction.

In front of the bottom inlet the bottom injector is located. It is a mixing chamber from which the gas flows into the slotted channel. In this paper two cases are considered: with and without bottom injector (in the second case a uniform velocity profile on the bottom inlet was set). The flow inside the channels and the chamber is laminar; typical Reynolds number does not exceed 1.

In order to reproduce possible temperature inhomogeneities, temperatures at lines T_1^m, T_2^m, T_1^b, T_2^b and T_3 were varied in the simulation (Fig. 2). A quadratic distribution is set between T_1^m and T_2^m, as well as between T_1^b and T_2^b. A linear distribution is set between T_1^m and T_3.

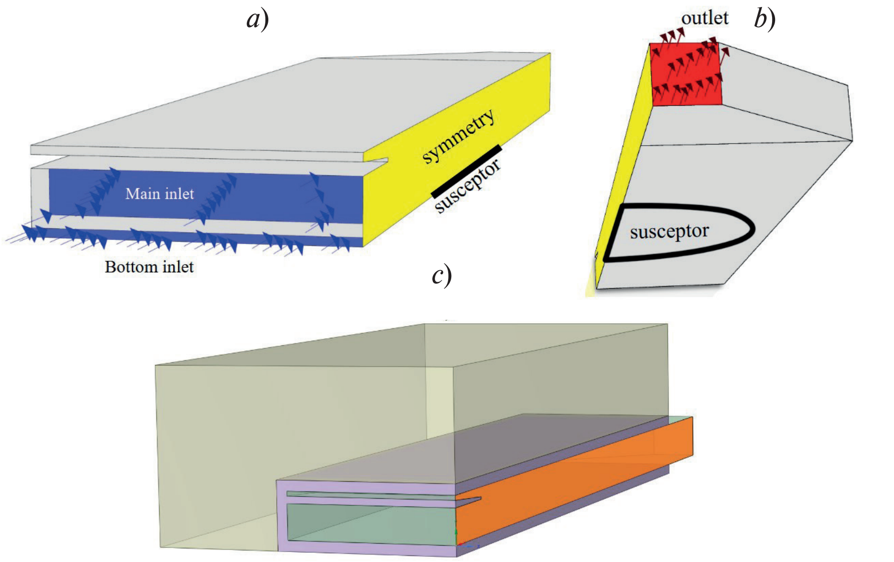

Fig. 1. Computational domain. Gas block (*a*, *b*) and the whole geometry (*c*)

Numerical simulation was performed using ANSYS Fluent. Second Order Upwind numerical scheme was used for spatial approximation. Green-Gauss Cell Based method was used for gradient discretization. SIMPLEC pressure-velocity coupling scheme was used to solve the equations of low-speed flow of a multi-component mixture.

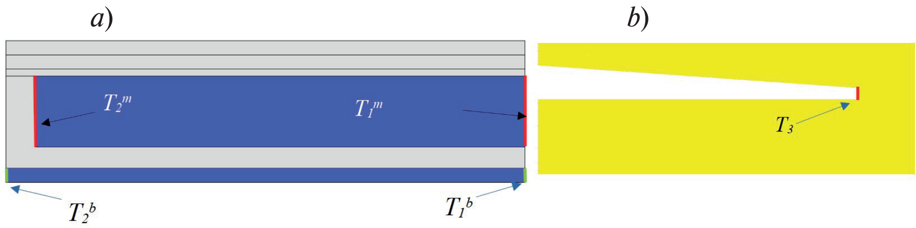

Fig. 2. Schematic diagram of setting temperature boundary conditions. Front view on inlets (*a*) and view on symmetry plane (*b*)

Results and Discussion

In the experiment at high flow rates, the velocity inhomogeneity at the bottom inlet with a local maximum on the symmetry plane ($z = 0$) can occur. The characteristic velocity distribution in the outlet section for this case is shown in Fig. 3. The maximum velocity can exceed the average value by 60%, so the assumption of the uniform velocity profile here is not correct.

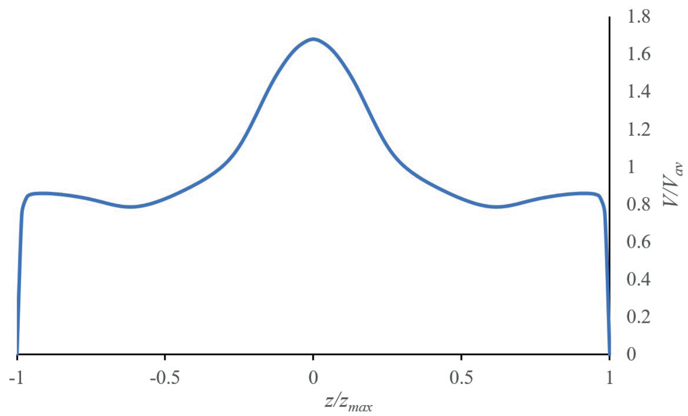

Fig. 3. Velocity distribution at the outlet of the bottom injector

By setting given velocity profile at the bottom inlet, the flow structure in the reactor changes considerably. Fig. 4 shows the field of the vertical velocity component at a distance of 1 calibre from the reactor inlet (1 calibre is bottom inlet height). It can be seen that in the case of a non-uniform profile, there is additional convective flow directed from the main inlet to the susceptor.

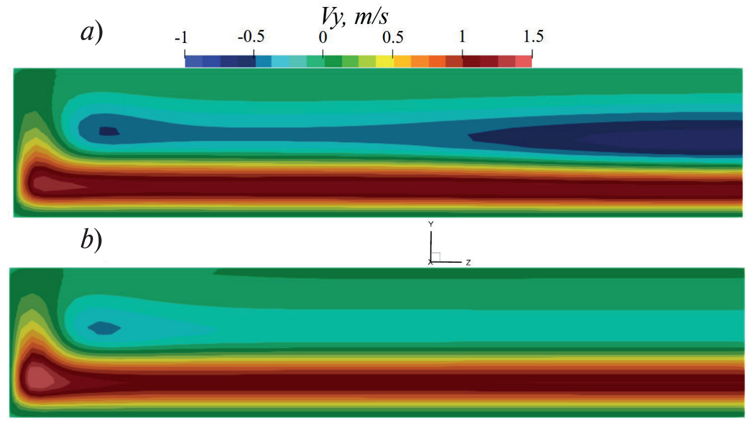

Fig. 4. Vertical velocity component at 1 calibre distance from the reactor inlet with non-uniform (*a*) and uniform (*b*) velocity profile at the bottom inlet

In case of non-uniform velocity profile, the growth rate distribution across the susceptor also changes significantly, as can be seen in Fig. 5, where the dependence of the angle-averaged growth rate on the distance from the center of the susceptor is shown. The growth rate at the center of the susceptor increases drastically and decreases at the periphery. Thus, results shown below are obtained with a non-uniform velocity profile at the bottom inlet.

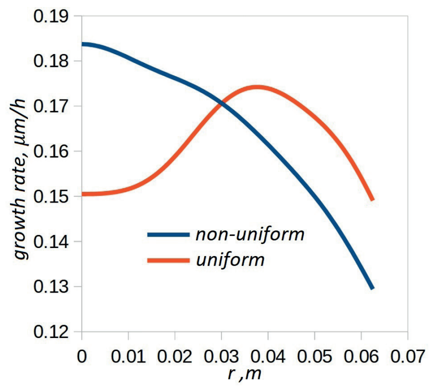

Fig. 5. Averaged growth rate profile obtained with uniform and non-uniform velocity profile at the bottom inlet

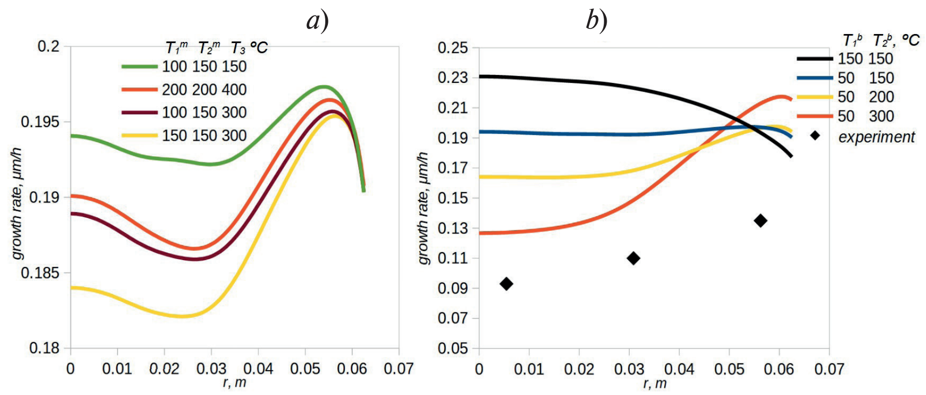

Fig. 6. Growth rate plots for temperature inhomogeneities at the main (a) and bottom (b) inlets

The effect of temperature inhomogeneity at the main inlet is shown in Fig. 6, *a*, where the plots of the averaged growth rate profile are shown. The growth rate decreases with increasing T_1^m, it also decreases with increasing T_3. It can be seen that these parameters have a stronger influence on the growth rate in the center than in the periphery. Increasing T_2^m only slightly increases the growth rate.

The growth rate profiles for varying temperatures T_1^b and T_2^b are shown in Fig. 6, *b*. It can be seen that the growth rate at the periphery increases with increasing temperature at the wall. The growth rate also increases when the temperature at the middle of the inlet decreases. Note that there is a qualitative agreement with the experimental trend (yellow and red curves).

Conclusion

Numerical simulations were carried out to establish the effect of inhomogeneities in reactor inlet velocity and temperature on the epitaxial processes. The results obtained are important for detailed modelling of the reactor. It is shown that due to the structure of the injector, significant velocity inhomogeneities are formed at the reactor inlet. These inhomogeneities have a significant impact not only on the growth rate level but also on the growth rate distribution over the susceptor. Temperature inhomogeneities at the inlet also affect the growth rate distribution over the susceptor. At the bottom inlet, a temperature lowering at the center (T1b) reduces the growth rate at the center and increases it at the periphery. In contrast, a temperature reduction at the wall (T2b) increases the growth rate at the center and decreases it at the periphery. Temperature inhomogeneities at the main inlet affect the distribution of the growth rate in the opposite way. It should be noted that this effect is weaker than the effect of inhomogeneities at the bottom inlet.

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