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SHAPE OPTIMIZATION OF A SHOWERHEAD SYSTEM FOR THE CONTROL OF GROWTH UNIFORMITY IN A MOCVD REACTOR USING CFD-BASED EVOLUTIONARY ALGORITHMS

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Aiming at a high degree of spatial uniformity of the growth rate across the substrate, MOCVD reactors are commonly equipped with showerhead systems above the heated substrates. In these cases, the interplay of chemical reactions and transport phenomena can be controlled through the degree of precursor mixing, as determined by the design of the gas delivery system [1]. Consequently, a shape-optimization problem arises, with regard to the uniformity of the film grown over the substrate.

Most conventional MOCVD systems are designed for a narrow range of operating conditions and, therefore, have limited flexibility for improving the process, particularly regarding the quality of the films. Moreover, the evaluation of the effects of different designs on the process outcome is a task difficult to be addressed by experimental effort. Numerical methods have shown many advantages over trial-and-error experimental methods, as the reactor geometry is easier to be modified and evaluated. To improve the efficiency of computational fluid dynamics (CFD) modeling in the shape design of novel MOCVD systems, an evolutionary algorithm (EA) is incorporated in a CFD software.

The particular MOCVD system under study is described in detail in [2]. The vertical reactor is equipped with a showerhead system above the silicon substrate. The diameters of the susceptor and the shower plate are 58mm and 60mm, respectively. The plate consists of 1450 holes of diameter of 0.76mm. Its thickness is 1mm.

Numerical modeling was used based on the CFD model reported previously [3]. The set of the coupled partial differential equations, along with the boundary conditions, are implemented in PHOENICS software [4]. The optimization analysis was carried out using the optimization platform EASY [5] that implements a multilevel structure based on evolutionary algorithms [6]. The optimization problem is concerned with the design of the shower plate for minimum non-uniformity (NU) of the growth rate across the substrate. The design variables are

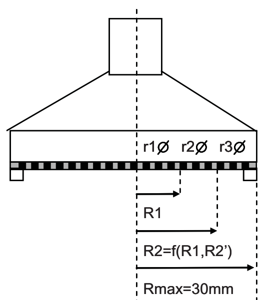

Fig. 1. 5-variable parameterization of the shower plate.

Table 1. Shape-optimization problem: range and optimal values of the design variables.

Design variable	Minimum value	Maximum value	Optimal value
R1 (mm)	1	28	6.806
R2'	0	1	0.115
r1 (mm)	0.250	0.635	0.631
r2 (mm)	0.250	0.635	0.362
r3 (mm)	0.250	0.635	0.262

depicted in Fig.1, while the range of their values is summarized in Table 1. The optimal values of the design variables that correspond to the minimum value of the objective function (NU = 4.27%) are also shown in Table 1. There seems to be a preference of the algorithm to use holes with the maximum permissible value of diameter in the inner zone, and in contrast, holes with the minimum possible value of diameter in the outer ring.

Fig. 2 presents the distribution of the growth rate for the actual and the optimal design of the shower plate. The non-uniformity of the growth-rate distribution decreases from NU=7.52% in the actual design to NU=4.27% in the optimal design. Further improvement in growth-rate uniformity is desirable if the actual restrictions set by the end users of the films are to be restricted. This calls for trying alternative shape-optimization scenario, involving more and carefully selected geometric parameters.

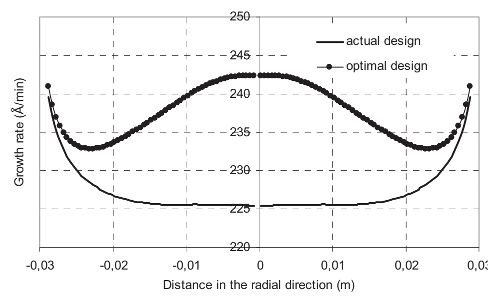

Fig. 2. Growth-rate distribution in the radial direction of the 58mm-substrate for actual and optimal design of the shower plate.

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