JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS Vol. 8, No. 1, February 2006, p. 144 - 147

Substrate thermal profiles in spray-CVD reactor

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The spray CVD technique is an interesting method for depositing coatings such as Transparent Conducting Oxides. The substrate temperature is the major factor, which determines the thickness uniformity of the deposited films. This paper summarizes recent simulation results of heat transfer in a reactor of Spray-CVD using an infrared (IR) lamp furnace. In order to establish the optimal deposition conditions, the substrate thermal profile is analyzed for different IR lamp temperatures.

(Received October 14, 2005; accepted January 26, 2006)

Keywords: Spray CVD, Numerical simulation, Substrate temperature uniformity

1. Introduction

Spray pyrolysis is a chemical vapor deposition (CVD) technique that has been successfully applied in the deposition of a variety of materials [1-3]. The main advantage of the spray pyrolysis process is to be an atmospheric pressure process, which allows depositing films on large area.

The deposition mechanism and the films properties depend on a significant number of parameters such as: the precursor solutions, the flow rates of the aerosol, the carrier gas, the temperature and the nature of the substrate. Finding the optimal conditions is a laborious work and many trials are necessary, consequently numerical simulations of such deposition system are of great utility.

In the paper [4] an overview of the application of numerical simulation in CVD process and equipment was given. In the paper [5] we presented the simulation results of a RTCVD (Rapid Thermal Chemical Vapor Deposition) reactor.

In other paper [6] we presented the fluid dynamics results (without heating), which appeared as a necessary preliminary work. The flow patterns for different substrate angle and different flow rates are depicted and the velocity profiles are drawn. From this previous work, it results that a small angle as 5^0 of the substrate with regard to the horizontal and a flow rate of about 1-2L/min lead to higher uniformity of velocity patterns near the substrate.

To investigate this problem in its high complexity, heat transfer and chemistry have to be taken into account. In this paper, numerical simulations are performed to examine the heating of the substrate using an IR lamp furnace.

2. Experimental procedure

The deposition apparatus consists of two parts, linked by a transport tube: the aerosol generator and the pyrolysis chamber. Aerosol of the solution generated in the ultrasonic atomizer is conveyed by the carrier gas through the transport tube to the substrate. The substrates are microscope glass slides of 75 x 25 mm in area and of 1 mm in thickness, heated using an IR lamps furnace. Substrates are placed in a quartz tube and a reflector is use on the inferior half of this tube, in order to improve the substrate heating. Three tungsten-halogen lamps are used as radiation source. A slide of silicon is used as susceptor. The distance between the furnace and the quartz tube is of about 10 cm.

3. Computational model

Simulations are performed using the finite volume commercial CFD package CFD-ACE [7]. The geometry of the system, built in two dimensions (2D), is shown in Fig. 1. The entire domain has been divided into elementary cells and the resulting mesh can be seen. The grids are structured and most of the cells have a rectangular shape, which makes the calculations easier. The total number of cells is 14556.

Governing equations required for the simulations are the conservation of mass (continuity equation), of momentum (Navier –Stokes equation) and of energy.

Black body radiation is calculated by the Stefan-Boltzmann law using Monte Carlo Method (MCM), where the radiative heat transfer equation is puzzled out by tracing the ways of a representative number of rays.

The flow is considered two-dimensional, incompressible (Mach number less than 10^{-5}) and in single-phase (air).

3.1 Flow solving routine

The equations are solved for the steady state case and the gravitational effect is taken into account. The second order differencing scheme (blending 0.1) has been used to discretise all terms and a convergence criterion of 1×10^{-4} was considered as satisfactory. A complete simulation takes between 16 min and 76 min of CPU time on AMD 64 processor with 1Gb RAM to reach the solution.

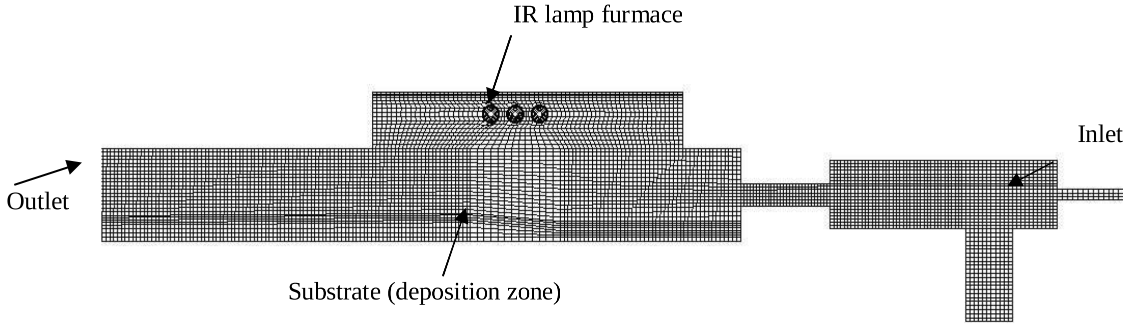

Fig. 1. Structured mesh.

Simulations have been performed by imposing the same temperatures to all the lamps, which means the lamp filaments are defined as walls at constant temperature. Pressure boundary conditions are fixed at 10^5 Pa for both inlet and outlet. The air flow rate was kept at 1.98×10^{-5} kg/s which, at 300 K, corresponds to 1L/min.

In order to establish the efficacy of the susceptor system, three sandwich arrangements are analyzed.

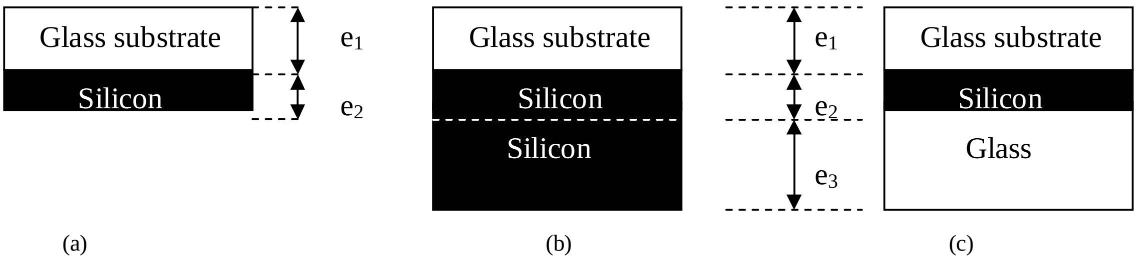

Fig. 2. Different susceptors: e_1= 1mm, e_2 = 0.5mm, e_3= 3.5 mm.

4. Results and discussion

The uniformity of films deposited by this method depends, on one hand, of the flow velocity patterns uniformity near the substrate and on other hand, on the substrate temperature uniformity.

The flow patterns for different substrate inclinations were analyzed in a previous study [6]. The velocity profiles pointed out that the most homogeneous flow fields are obtained for a horizontal arrangement with a 5^o inclined substrate with regard to the horizontal. For this reason, in the following, we analyzed the heat transfer only in an arrangement where the substrate is inclined at 5^o.

To maximize the thermal performance we have investigated the heat transfer by radiation, conduction and convection when IR lamp filaments are at different temperatures ranging between 1700 K and 2300 K, for the three susceptor arrangements (a), (b), (c).

The influence of the lamp filament temperature onto substrate temperature is investigated. As an example, Fig. 3 depicts the temperature profiles when the arrangement (b) is used and lamp filaments are at 2200 K.

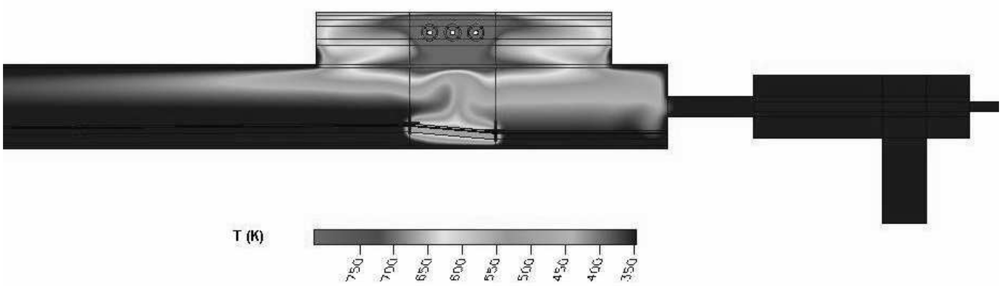

Fig. 3. Temperature patterns for an arrangement using a susceptor of (b) type and when lamp filaments are at 2200 K.

The profiles of substrate temperature determined by numerical simulations for different lamp filament temperature (1700 K, 1900 K, 2100 K and 2300 K) are presented in Fig. 4, for each of the three types of susceptors (a), (b) and (c). When lamp filament temperature is fixed at values ranging between 1700 K and 2300 K the substrate temperature, using (a) and (b) susceptors, reaches 500 K to 740 K, while by using (c) susceptor the substrate temperature is only of 440 K to 500 K.

Fig. 5 gives the relation between the lamp filament temperature and the temperature of the centre substrate for the three types of susceptors. We notice that the most efficient susceptor is (a) because the temperature is the highest for the same power supplied to the lamps. Quite similar results are also obtained using (b) susceptor but furthermore, in this case, the temperature onto the substrate is more homogenous.

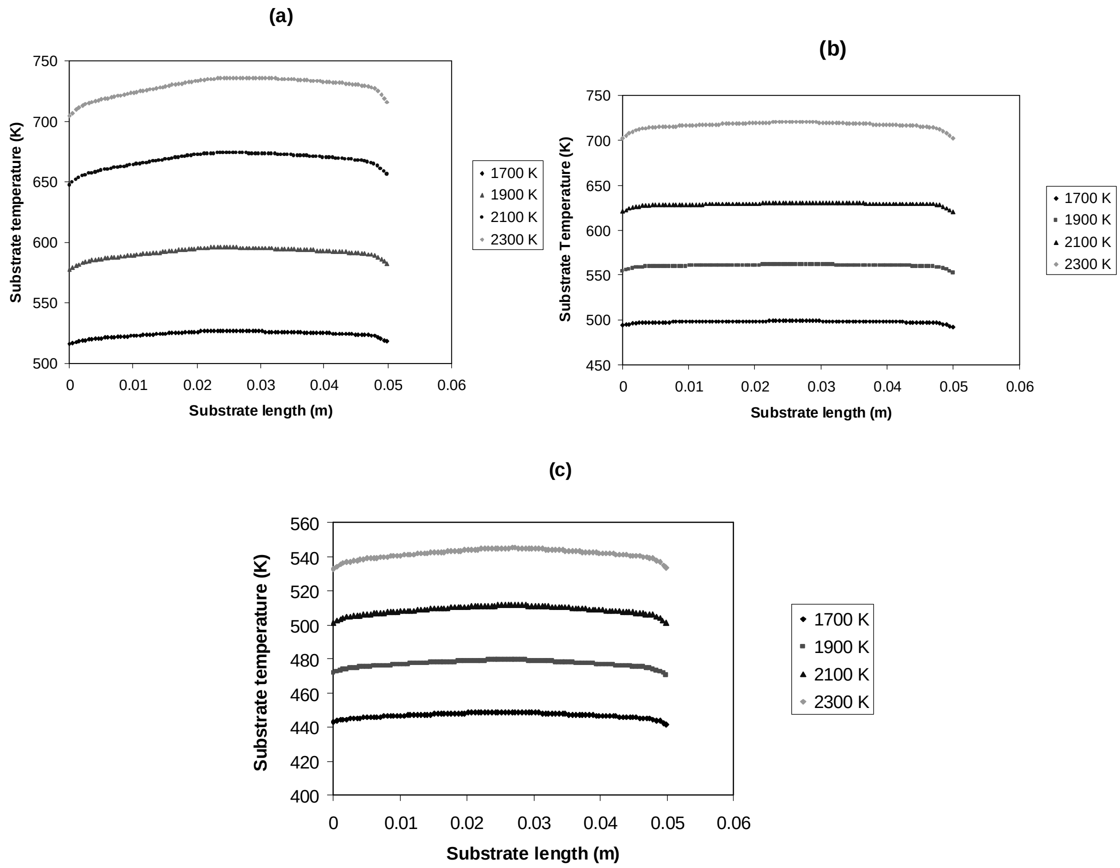

Fig. 4. Temperature along the substrate for the three susceptors (a), (b) and (c), when lamp filaments are at temperature of: 1700K, 1900K, 2100K and 2300K.

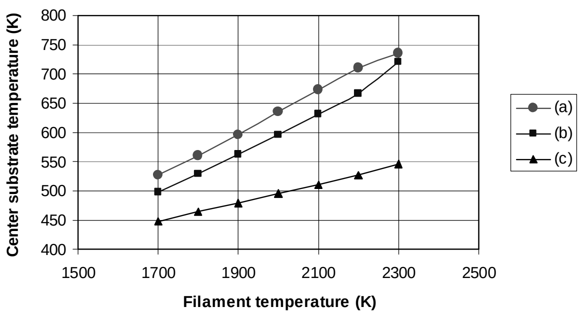

Fig. 5. The temperature in the center of the substrate, in function of the lamp filament temperature, for the three arrangements: (a), (b) and (c).

In Fig. 6a we compare the temperature profiles for the different susceptors when the lamp filament temperature is 2200K. We remark that the most homogenous temperature of the substrate is obtained when the susceptor (b) is used. The profile obtained in this case is detailed in Fig. 6.b.

Finally we analyzed the modifications on velocity patterns in the presence of IR heat source. The profiles are obviously influenced by the heating source [6] but the uniformity of these profiles near the substrate is still satisfactory.

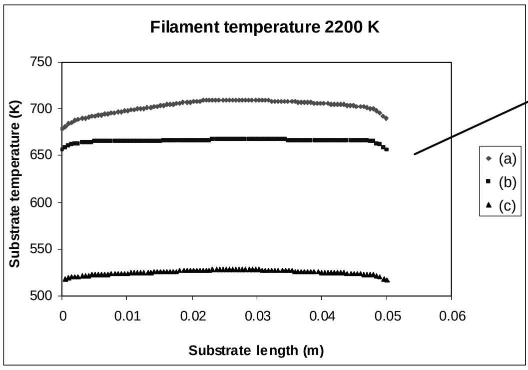

Fig. 6a. Temperature profiles for the different susceptors (a), (b), (c).

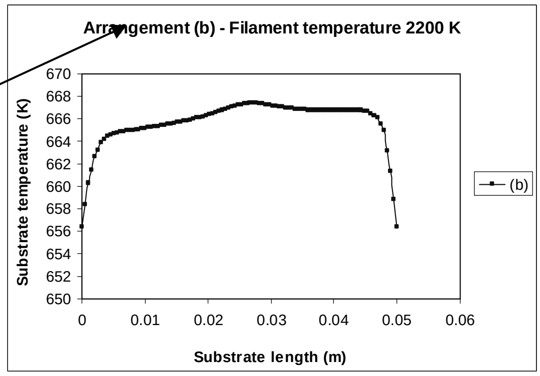

Fig. 6b. Temperature profile along the substrate for the susceptor (b).

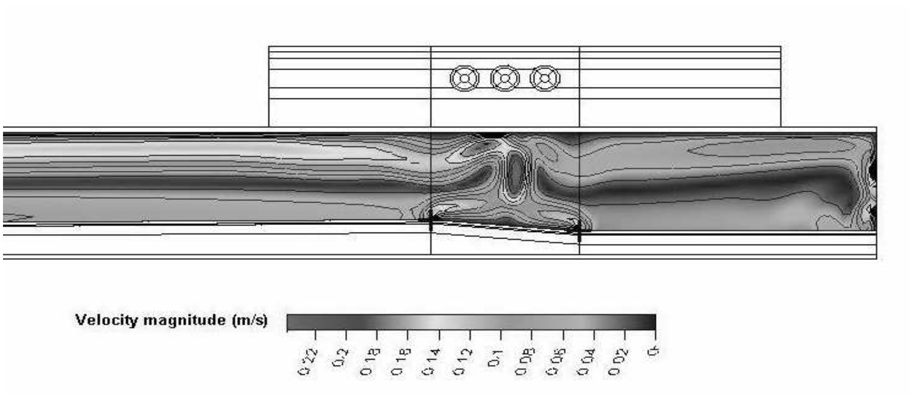

Fig. 7. Velocity patterns in the presence of heating sources (lamp filaments at 2200 K) for an arrangement using a (b) type susceptor. The air flow rate at the inlet is 1.98×10^{-5}kg/s.

5. Conclusions

In this paper we analyzed the heating of glass substrates into a Spray-CVD system, using an IR furnace. Different susceptors are compared in order to establish the best arrangement for obtaining the most uniform temperature profile onto the substrate.

The different substrate temperature profiles are presented in function of the temperature applied to the lamp filaments. Also the temperature in the center of the substrate is given in function of lamp filament temperature. It is shown that a temperature of about 725 K onto the substrate may be obtained when the lamp filaments are at 2300 K

The simulations results showed that a silicon susceptor having a thickness of 0.5 mm is sufficient to heat the substrate between 500 K and 740 K when power supplied to the lamps corresponds to a filament temperature ranging between 1700 K and 2300 K. However more uniform profiles are obtained when the silicon susceptor thickness is about 4 mm.

References

[1] K. L. Chopra, S. Major, D. K. Pandya, Thin Solid Films **102**, 1 (1983).
[2] H. L. Hartnagel, A. L. Dawar, A. K. Jain , C. Jagadish, "Semiconducting Transparent Thin Films", Institute of Publishing, Bristol and Philadelphia, 1995
[3] Manifacier, Thin Solid Films **90**, 297 (1982).
[4] A. Bouteville, J. Optoelectron. Adv. Mater. **7**(2), 599 (2005).
[5] M. Girtan, P. O. Logerais, L. Avril, F. Gonzatti, A. Bouteville, J. Optoelectron. Adv. Mater. **7(**2), 665 (2005).
[6] Mihaela Girtan, P. O. Logerais, Anne Bouteville, Study on the possibilities of modelling the physical processes involved in spray CVD, Proceeding, EUROCVD -15, September 4 - 9, 2005, Bochum – Germany.
[7] CFD Research Corporation, CFD'ACE (U) User Manual, Version (2003).

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