SIMULATION OF EPITAXIAL SILICON DEPOSITION AND DOPANT INCORPORATION IN A INDUSTRIAL BARREL REACTOR

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ABSTRACT

Customarily, the deposition of thick epitaxial silicon layers over substrates up to 5", 6" and 8" diameter, nowadays used for *discretes* and *IGBTs* devices, is performed in the so-called "cold wall barrel reactors Because the high temperature to which epitaxial deposition are performed, and because the external bell wall has to be maintained at a significantly lower temperature, such reactors are characterised by the presence of very high temperature gradients that are quite responsible of their peculiar fluid dynamics behaviour that results in a mixed flow regime (i.e., natural + forced convection). Moreover, in the usually adopted process conditions, also the dissociation chemistry of precursors plays a significant role.

Because of the peculiar barrel geometry, a satisfactory answer to the industrial priorities can be obtained only through fully 3D models (that accounts for all the geometry details) embedding a realistic chemical kinetics (ref. (2) and (3)). These requirements are somewhat in contrast with the industrial necessity of "fast solutions". Thus the full 3D model should be adopted only to verify solutions previously identified through simplified models addressing only partial aspects of the problem. Accordingly, the procedure here developed to analyse the problem was the following:

- To derive a lumped kinetic expression able to substantially represent the detailed chemistry in the temperature and pressure ranges of interest by means of a very fast running simplified 1D model (ref. (1) and (4)).
- To verify the lumped kinetics previously derived through a 2D model of the reactor. In that case the calculations are also repeated through the detailed mechanism to compare the accuracy of the calculations (ref. (2)).
- To embed the now verified lumped kinetics into the detailed 3D model to perform the reactor optimization and design, after the final comparison of the model prediction on experimental test runs.
- To perform a sensitivity analysis to identify the construction features affecting in larger extent the reactor performances.

The advantage of the above procedure is in the independent estimation of the lumped kinetic parameters whose values resulted not influenced by any particular fluid dynamic regime insisting inside the reactor.

The system here analyzed, the epitaxial silicon deposition from $SiHCl_3$-H_2-PH_3 mixtures, has a great industrial importance and thus the industrial data of two reactors having *the geometric standard LPE configuration* (Table 1) were adopted to verify the modeling procedure. The data refer to two different operative conditions and they were obtained in two different industrial sites. Because the provenience of the data, all the comparison were reported in a normalized way. Some other papers have been previously published on barrel reactors (c.f.: ref (2) and (3)) but, for our knowledge, this is the first one were simulated growth rate and resistivity data are compared with experimental data on both directions (i.e., longitudinal and transversal) of the deposition plane (Figures 1-3).

REFERENCES

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Table 1. Main features of the LPE 2061 barrel reactor and of process parameters

	case 1	**case 2**
Geometry	Standard x inch	Standard x inch
Q_{H2MAIN} [A.U.]	1	0.91
Bell-jar wall temperature [°C]	400	400
Susceptor Temperature [°C]	1110	1150
$SiHCl_3$ mass fraction	0.51	0.56
PH_3 inject [A.U.]	1	0.7
Angular velocity [rpm]	5	5

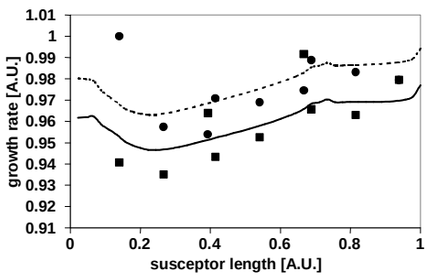

Fig. 1. Experimental (▪ case 1; • case 2) vs. calculated Growth Rate (— case 1; - - - case 2) along the susceptor, *"top-bottom"* line

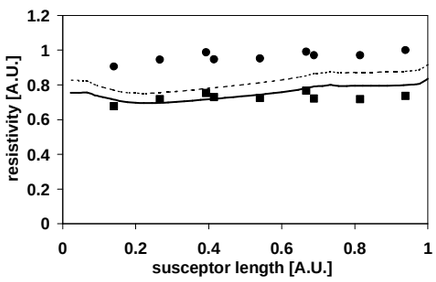

Fig 2. Experimental (▪ case 1; • case 2) vs. calculated resistivity (— case 1; - - - case 2) along the susceptor *"top-bottom"* line.

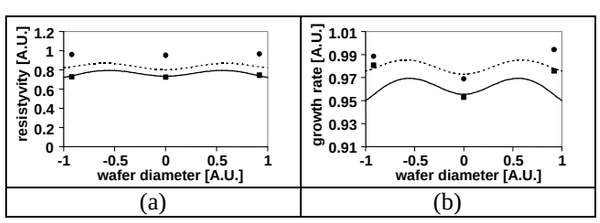

Fig. 3. Experimental (▪ case 1; • case 2) vs. calculated (— case 1; - - - case 2): (a) growth rate along the middle wafer,*"left-right"* line; (b) resistivity along the middle wafer,*"left-right"* line.