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# MULTISCALE MODELLING OF LOW-PRESSURE CVD OF SILICON BASED MATERIALS IN DEEP SUBMICRONIC TRENCHES: A CONTINUUM FEATURE SCALE MODEL

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ABSTRACT

The ability to predict feature profile evolution across wafers during filling from equipment scale operating conditions is one important goal of process engineers for power component fabrication. We develop an integrated approach for simulating the multiple length scales needed to address this problem for Low Pressure CVD processes of silicon based materials in deep submicronic trenches (aspect ratio can exceed 50). In this approach, continuum models at the reactor ($10^0$m) and feature ($10^{-7}$m) scales are tightly coupled in order to predict micro- and macro- loading effects in a transient environment. First, the main principles and assumptions of the reactor and trench scale models are presented. Then, some characteristic examples of numerical results at the trench scale are analysed and compared with the predictions of the deterministic Ballistic Transport-Reaction Model (BTRM) *EVOLVE*. This comparison shows that our continuum approach gives results as accurate as those of the BTRM one even for highly non conformable layers, for computations times up to 3 times lower.

## INTRODUCTION

More than ever, increasing the scale of integration and the performances of microelectronic components constitutes one major issue of process engineers for power device fabrication. For example, concerning the integration of capacitors, the purpose is to form deeper and deeper 3D structures within the silicon substrate. Thus, instead of enlarging the area on the substrate surface, the whole capacitor area and the planar capacitance can be increased within a small substrate area. Then reach higher capacitances today involves etching and filling 3D structures of more and more important aspect ratios (AR - ratio of width to depth of the trench). One major process to fill such deep structures is Low Pressure CVD to deposit intrinsic silicon, stoechiometric silicon nitride $Si_3N_4$, *in-situ* boron-doped silicon and *in-situ* phosphorus-doped silicon. The challenge is to form conformal films, i.e. without any void and with a perfect uniformity along the trench, in terms of film thickness, chemical composition and nanostructure. It is worth noting that industrial LPCVD reactors can simultaneously treat up to 200 etched wafers of 6 to 12 inches in diameter. A good uniformity in the deposition features must

also been reached everywhere on a wafer and along the wafers load, which is not a trivial task.

CVD involves complex and strongly coupled phenomena occurring at multiple length and time scales. Fast elementary processes such as migration of adsorbed molecules on the film surface or chemical reactions occur on typical time scales of $10^{-12}$-$10^{-15}$s and involve atomic motion of approximately $10^{-10}$m. Conversely, the formation of active regions on the submicron to nanometer scale on substrates held in a meter sized deposition chamber requires usually $10^{2}$-$10^{4}$s. Then a simulation model accurately describing all the phenomena involved should implement the equations governing interactions and molecular motions over wide length and time scales. The development of such a model remains a target out of range (1). In contrast, advances have been made in multiscale modelling strategies for thin film growth by CVD techniques and are now becoming convenient. In particular, the approaches developed by Merchant, Cale et al. (2-6) and Rodgers and Jensen (7) appear to be two of the most interesting in the field, but their resulting large calculation times can be replaced by faster approaches, depending on study objectives.

This article presents a new contribution to the multiscale modelling of an industrial LPCVD process for the filling of deep submicronic trenches by silicon-based films. This work aims to develop a self-consistent models package to represent physical and chemical phenomena occurring from the reactor (macroscopic) scale to the feature (microscopic) scale, generating reasonable computational times. The reactor and trench scale models we have developed using the Computation Fluid Dynamics (CFD) software package *FLUENT* (8) will be first described. Some characteristic results will be then commented and compared with those obtained using the Ballistic Transport-Reaction Model (BTRM) based on a determinist code developed by Cale et al. (2-6) for conditions involving high Knudsen numbers and implemented in the etch and deposition processes simulator called *EVOLVE*.

## DESCRIPTION OF INDIVIDUAL MODELS

The governing equations of mass, momentum, heat, and reactive species transport have been solved through the CFD *FLUENT* 6.1 package to predict gas flow, temperature and species concentrations versus position and time at the reactor and trench scales.

### Macroscopic model statements

The LPCVD reactor is an industrial tubular horizontal hot-wall furnace, 2.15 m in length and 0.11 m in tube radius. A load of 130 wafers 6’ in diameter and 500 µm in thickness has been considered. The main assumptions are (i) steady state conditions have been assumed; (ii) the presence of the quartz wafers boat, profile thermocouple sheathes and gas injector tubes has been neglected thanks to their small surface areas and the reactor is axially symmetric; (iii) the Reynolds number is very small, so the gas flow is laminar; (iv) compressibility effects have been considered; (v) gas is ideal; (vi) a detailed heat transfer model including radiation and heat of reactions has been used to predict wafers and gas temperatures knowing those of the reactor walls and doors. A 2D modelling domain of 25000 rectangular cells has been build.

For intrinsic silicon films, typical process parameters are a temperature of 620°C, a total pressure of 40 Pa, and 300cm$^3$/min STP of pure silane $SiH_4$. The classical chemical scheme and kinetic scheme for silicon deposition from $SiH_4$ used by Gris et al. (9) has been used. It involves 2 homogeneous reversible chemical reactions, [1] and [2], and 2

heterogeneous ones, [3] and [4], whose respective deposition rates are called in the following sections $R(SiH_4)$ and $R(SiH_2)$.

$$SiH_4 \leftrightarrow SiH_2 + H_2 \qquad [1]$$

$$SiH_4 + SiH_2 \leftrightarrow Si_2H_6 \qquad [2]$$

$$SiH_4 \rightarrow Si<s> + 2H_2 \qquad [3]$$

$$SiH_2 \rightarrow Si<s> + H_2 \qquad [4]$$

Microscopic model statements

The Knudsen number, i.e. the ratio between the mean free path of gaseous molecules and the characteristic length of the system, is roughly equal to 100, for our LPCVD conditions in a 1µm in width trench. This means that the gas flow regime is molecular and that the conventional hydrodynamic equations even with slip boundary conditions are no more valid. The integro-differential Boltzmann equation should be then approximated and solved either deterministically (BTRM) or probabilistically (Monte Carlo methods). Such approaches when tightly interconnected with reactor scale models today involve complex and time-costly numerical algorithms, slightly compatible with industrial engineering purposes. In the present work, our strategy has been to develop a continuum trench scale model through the *FLUENT* software package, then to interconnect it with the reactor scale model presented above so as to build an efficient, rapid and easy-to-use software package. In order to ascertain the validity of our continuum approach and ever to refine our results, we also use the BTRM *EVOLVE* code.

For our continuum trench scale model, infinitely long rectangular trenches have been considered, allowing 2D modelling. Within the trench, the frequency of collisions between gas phase species is small relative to the frequency of collisions between gas phase species and surfaces and it is reasonable to neglect particle-particle collisions. In such situations any potential homogeneous reactions can be neglected within the feature while they exist in the gas phase source volume immediately above the feature. Thus, as presented in Figure 1, the geometrical domain considered presents 2 parts. The first one corresponds to the region immediately above the trench (zone 1) in which classical continuum phenomena occur (i.e. molecular diffusion and homogeneous reactions). The second one is the trench itself (zone 2) in which homogeneous reactions are neglected. The kinetic laws are treated in a similar way as at the reactor scale. In addition, the Knudsen number being high within the trench (zone 2), special considerations must be taken into account to enable a continuum treatment of free molecular gas phase transport along the depth of the trench. In this way, species fluxes have been expressed in terms of Knudsen diffusion and gradients in the species concentrations. In the model formulation, a local value for the Knudsen diffusivity is calculated depending of the local trench width along the depth of the trench after each nodes motion of the feature sidewall profile. Moreover, note that our continuum model makes it possible to simulate the homogeneous chemical reactions above the trench (zone 1), thus allowing a tightly coupled multiscale simulation. However we do not have simulated them for the purpose work in order to only evaluate the ability of our continuum model to simulate gas phase transport within the trench (zone 2). Thus, the assumptions for the BTRM and our continuum diffusion-reaction model are the same and only their treatment of gas phase transport differs; the BTRM being the most fundamental since the flux of each species to the local surface is calculated taking into account the flux of each species leaving all others surfaces in the feature as opposed to the local averaging volumes inherent to continuum models.

As a first approach, so as to interconnect this model with the reactor one, the height of the first zone has been taken equal to 50 µm, which corresponds to the normal distance to the wafer surface of the mid points of the first mesh layer present near the wafer in the reactor scale model. Inlet mass fluxes and mass fractions are then fixed from data given by the macroscopic model. 2D modelling domains involving till 20000 dynamic triangular cells whose resolution can reach 100 nm have been used in this work. In the present work, we will see that inlet species mass fractions have been arbitrary fixed in order to test our continuum feature scale model over a large range of non-conformable deposits. Simulations are performed in transient conditions.

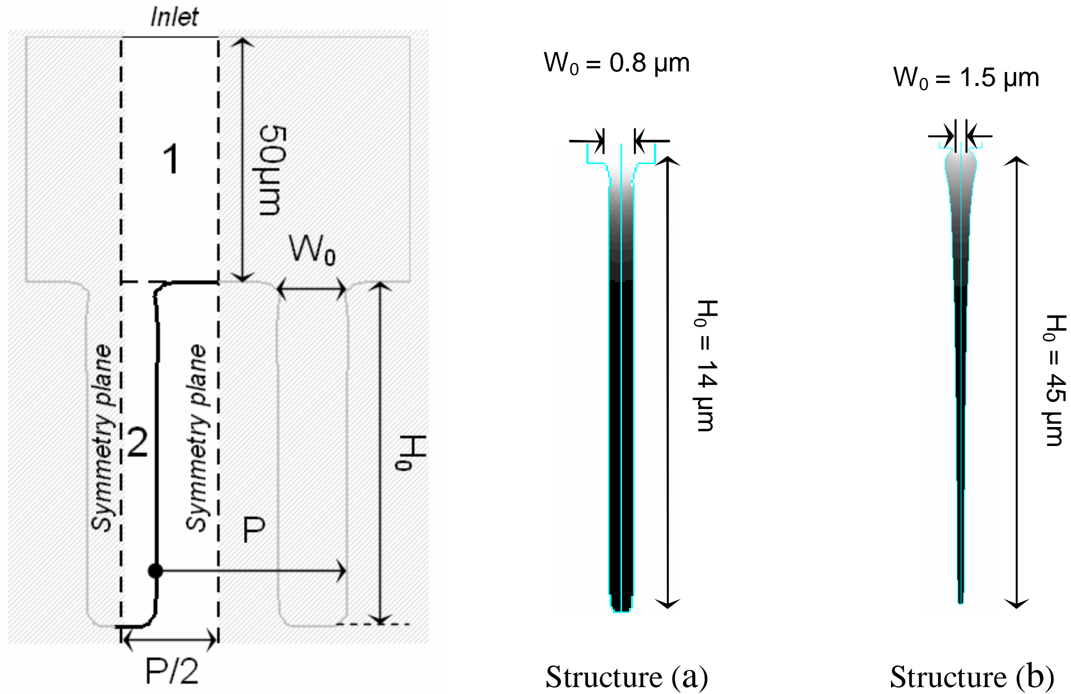


Figure 1: The 2D geometrical domain for the trench scale model [zone 1: gas phase source volume and wafer surface – zone 2: gas phase volume within the trench and trench surface] and the studied 2D trench initial profiles [(a), (b)]

Figure 1 shows the two initial profiles of 2D trench structures we have studied. The structures (a) and (b) present respectively an AR of 17.5 and 30 with an initial aperture of 0.8µm and 1.5µm in width. The structure (b) is deeper than the structure (a) (it has been subjected to a longer etching time), and presents a larger bowing ('local' enlargement) at its top and a sharper ending at its bottom. The study of bowings and sharp endings presents a strong interest because it is a remnant default of etching, occurring once one try simultaneously to reach deeper and deeper structures and shrink the whole surface structure area within a smaller and smaller substrate surface area. Usually, these phenomena are typical of very large AR structures of a hundred of microns in depth but, in order to reduce the time cost of the dynamic mesh procedures development we have simulated them for the 45µm depth structure (b). In this conditions, our model must be able to manage dynamic geometrical domains evolving very strongly with time due to deposition, especially when they present particularly marked etching defects (as those previously discussed but also numerous other ones, intentional or not). So it was important that the dynamic triangular mesh of our continuum feature scale model can be subjected to important deforming processes without deteriorate the mesh quality and without generating negative volume cells near the trench surface. However, *FLUENT*

does not allow to perform grid adaptation of moving and deforming meshes. So, it has been needed to develop a customized dynamic adaptation and moving mesh procedure, suitable for all structure profile. Consequently, today we can simulate 2D trench structures with an identical dynamic mesh procedure for all of them involving at each time step: (i) calculation step of the new trench surface nodes coordinates on the feature surface (ii) adaptation of the nodes positions on the new calculated structure profile (iii) moving step of the structure surface defined with a constant number of boundary nodes; (ii) deforming step of the lateral volume source boundaries; (iii) a local re-meshing and smoothing step of the volume mesh in order to maintain a good cell quality.

## RESULTS AND DISCUSSION

All results presented in this article have been obtained for a fixed temperature of 620°C and a pressure of 40Pa. For the sake of brevity, numerical predictions we have obtained at the reactor scale are not presented here. However, the first results obtained at this scale are in good agreement with the corresponding experimental layers thicknesses. As often used in the following discussion, a key parameter to quantify the conformality of a layer is Step Coverage (SC), corresponding here to the ratio of deposition thicknesses on the wafer plane surface and at a given position along the trench surface.

### Pure silicon and *in-situ* boron-doped silicon

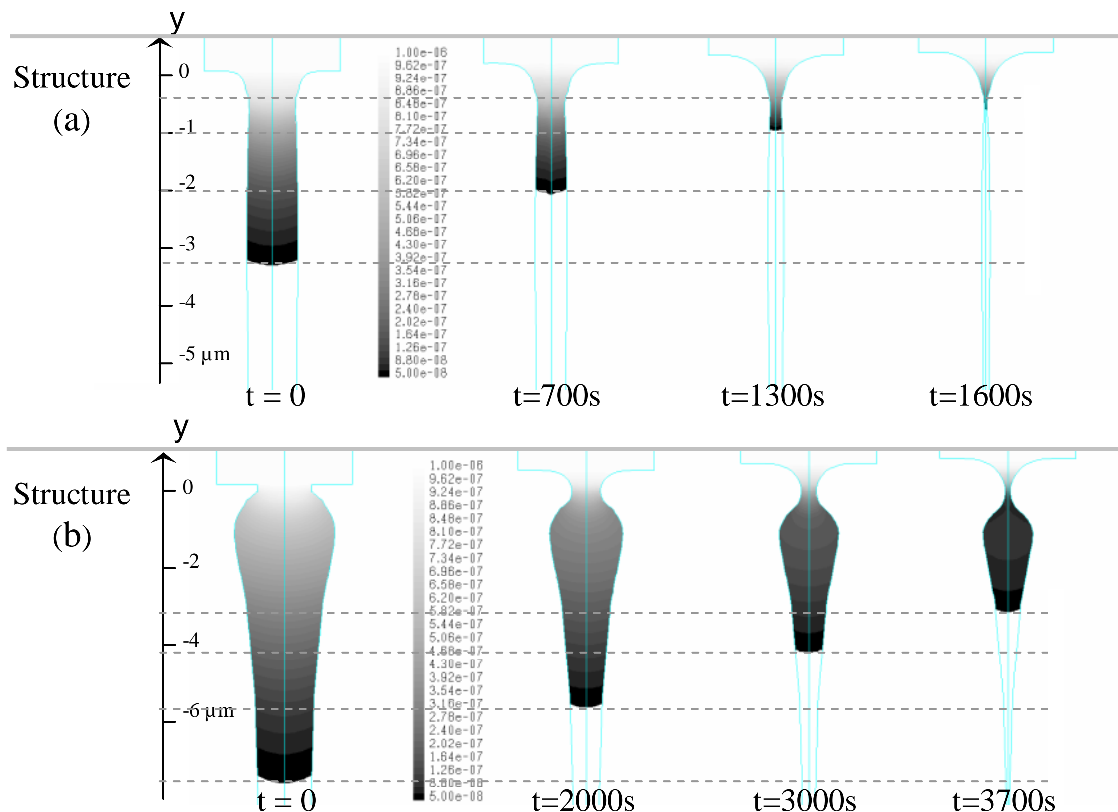


Figure 2: Trench profile and $SiH_2$ mass fraction evolutions versus the deposition time for trenches (a) and (b)

As a characteristic example of results obtained for pure silicon at the trench scale, Figure 2 presents top trench profile evolutions with time obtained for the two trenches of

Figure 1. $SiH_2$ mass fraction profiles inside the trench are also represented with a threshold value at $5.10^{-8}$ for a better visualization.

Intrinsic silicon deposition from $SiH_4$ and *in-situ* boron-doped silicon deposition from $SiH_4$ and $BCl_3$ involve predominantly lowly reactive species for conventional LPCVD operating conditions. Indeed calculations show a very low contribution of the extremely reactive radicalar species $SiH_2$ to the overall silicon deposit and consequently, the deposition rate ratio $R(SiH_2)/R(SiH_4)$ tends to zero. As a consequence, the kinetic behaviour in terms of deposit conformality of *in-situ* boron-doped silicon films and of pure silicon layers are very similar : they lead to very conformable deposits with quasi-perfect final step coverage (SC), whatever the initial trench geometry and AR. Note that $SiH_2$ is everywhere lowly concentrated (mass fractions comprised between $10^{-6}$ and $10^{-8}$) and that it reacts rapidly at the entrance of the pattern before being continuously and highly spatially depleted along the trench depth. Moreover, we observe an increase of this spatial depletion versus the deposition time. Indeed, during the deposition process, the surface to volume ratio increases and the probability for a very reactive unsaturated species to reach the trench surface at a given depth decreases.

<u>Other LPCVD films of lower conformability – Comparison with BTRM (*EVOLVE*)</u>

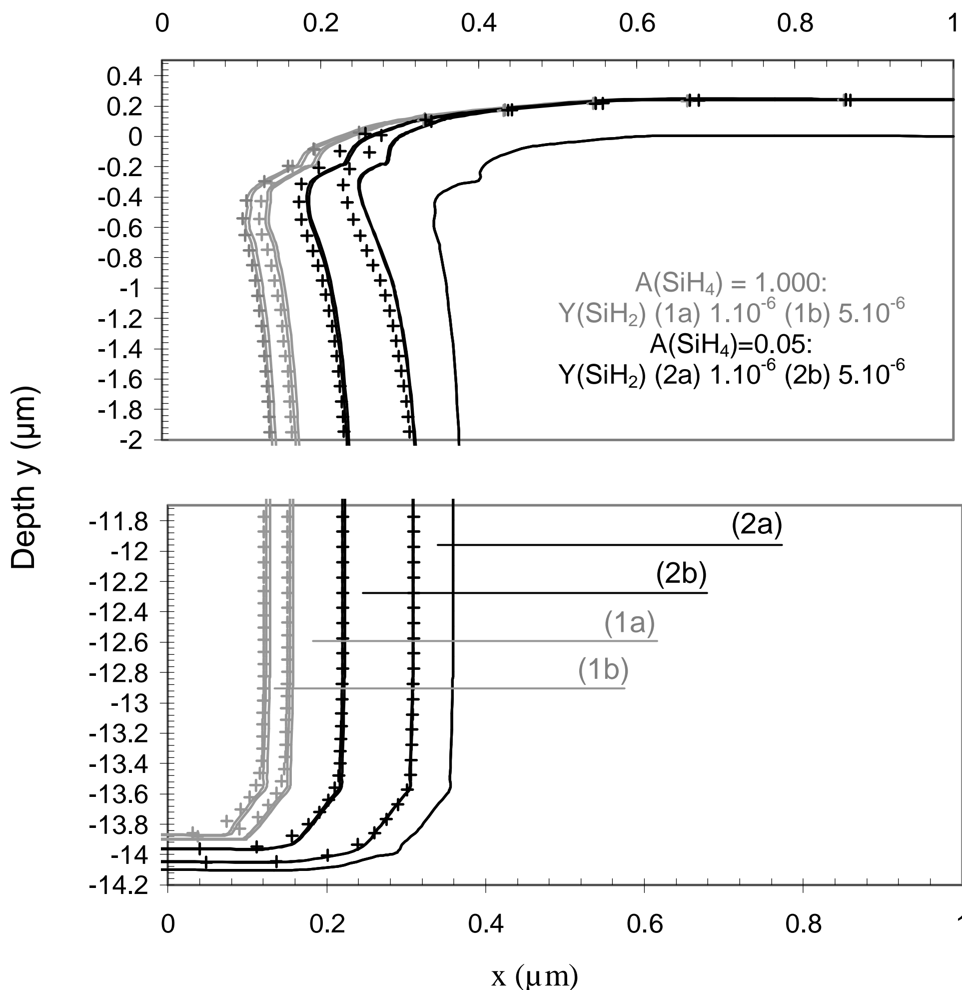


Figure 3: Thickness profiles at the top and bottom of the structure (a) for a 250 nm deposit thickness on the wafer plane surface predicted with (+) the continuum diffusion-reaction model and (——) the BTRM

In the case of in situ phosphorus-doped silicon deposition from mixtures of $SiH_4$ and phosphine $PH_3$, a previous study (9) has shown that a closure of the rectangular trenches systematically occurs before a complete filling, leading to a void inside the features. This result is a well-known consequence of the contribution of the very reactive radicalar species $SiH_2$. The $SiH_4$ contribution decreases when the $PH_3$ percentage in the gas-phase increases (10). Indeed, the presence of phosphorus (N-type doping) inside the film blocks the chemisorption of the poorly reactive $SiH_4$ molecule, due to the high electronegativity of phosphorus in comparison with silicon (10). This leads to a greater contribution of the lowly concentrated radicalar species $SiH_2$ to deposition, and to a sharp decrease of the overall deposition rate. Consequently, the $R(SiH_2)/R(SiH_4)$ ratio increases and can reach values greater than 0.5 (9,10), resulting in non-conformable layers with low SC. SC is clearly a function of the $R(SiH_2)/R(SiH_4)$ ratio. When this ratio tends to zero, SC tends to 100% and conversely, when this ratio tends to upper values, SC decreases dramatically. Moreover, when using important $PH_3$ inlet concentrations, it is possible to observe up to a 95% drop in the deposition rate from $SiH_4$. So, in order to consider this decrease in our models, we add a multiplicative factor $A(SiH_4)$ (<1) to the numerator of the well-known Langmuir-Hinshelwood law describing the deposition of pure silicon from $SiH_4$ as a function of partial pressures of $SiH_4$ and $H_2$ (11).

Then, to evaluate our model ability to predict trench profiles evolutions for non conformable layers, we have analysed the influence of the inlet $SiH_2$ mass fraction $Y(SiH_2)$ and of the multiplicative factor $A(SiH_4)$, on the trench model results. We have fixed arbitrary values of $Y(SiH_2)$ and $A(SiH_4)$. In order to cover a large range of non-conformality level we allow $Y(SiH_2)$ and $A(SiH_4)$ variations from $1.10^{-9}$ to $5.10^{-6}$ and from 0.05 to 1 respectively. The whole results has then been compared with the BTRM *EVOLVE* ones. In the following, the discussed results have been obtain for a 250 nm layer thickness simulated deposition on the plane surface wafer separating two trenches of initial structure (a).

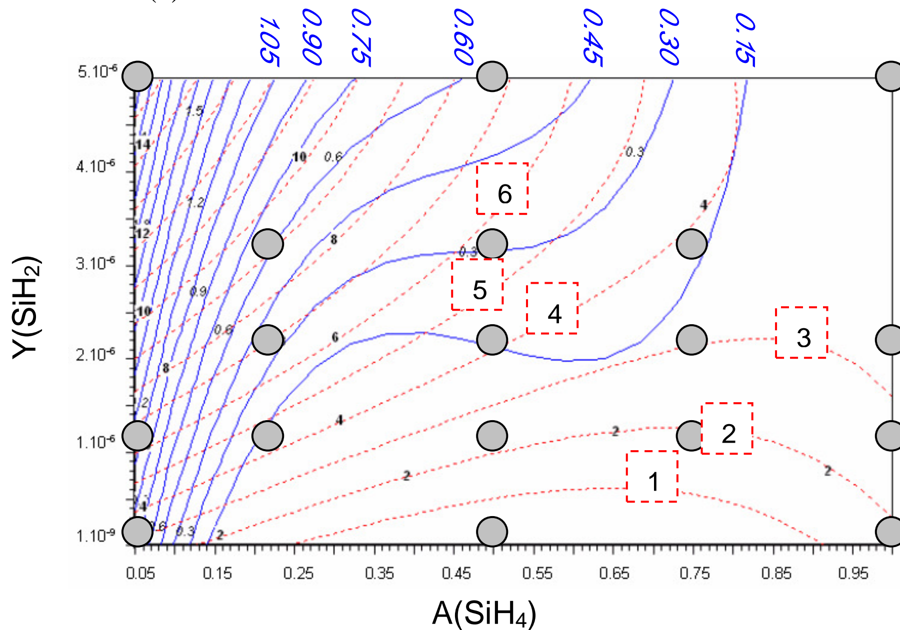


Figure 4: Relative difference (%) between BTRM SC predictions and those obtained with the continuum model at y=-0.5 µm (– – – value) plotted from interpolation of the SC results performed with the 18 simulated combinations of $Y(SiH_2)$ and $A(SiH_4)$ values (○) $R(SiH_2)/R(SiH_4)$ (—— *value*)

In Figure 3, some thickness profiles predictions at the bottom and top parts of the trench, obtained with both BTRM and our continuum model are given for several non-conformable cases. The corresponding plots of thickness profiles do not appear in Figure 3 in order to not overload it but note that the SC predictions of the two models was in perfect agreement for very conformable deposits. A good agreement for non-conformable deposits is revealed at depths greater than 2µm. But for depths lower than 2 µm a disagreement between SC predictions of the two models appears when the deposition moves away from conformable conditions as it is shown in Figure 3. However, the maximum relative difference observed has been limited, since it is equal to 16% for respectively $Y(SiH_2)$ and $A(SiH_4)$ of $5.10^{-6}$ and 0.05 which corresponds to unrealistic conditions in an industrial tubular horizontal hot-wall furnace.

Figure 4 summarizes results of the relative difference (%) in SC predictions between the BTRM approach and our continuum model, at 0.5 µm of the trench inlet, in the zone where the disagreement is the most important. These results are superposed to the corresponding variations of the $R(SiH_2)/R(SiH_4)$ ratio calculated on the wafer plane surface. This relative difference logically increases with the $R(SiH_2)/R(SiH_4)$ ratio. However it is worth noting that these values show a satisfactory agreement for all real industrial cases, since they are systematically lower than 5%.

## CONCLUSIONS

On the basis of a continuum approach, a reactor scale then a trench scale model including an original dynamic mesh procedure, have been developed. This package allows simulating both high AR trenches presenting important etching defects such as bowings, and lowly conformed LPCVD silicon-based films. The level of resolution of the trench model, 100 nm at present time, could be easily increased. A satisfactory agreement has been obtained with the BTRM *EVOLVE* code, even for extreme non conformal films, proving the validity of the present work. An important advantage of our continuum models is that the computations times are up to three times lower than those of BTRM implemented in *EVOLVE*. Additional works are now in progress aiming first to better interconnect the reactor and trench scale models, then to validate the results by comparison with experimental thickness and composition profiles, for pure polysilicon and *in-situ* boron-doped silicon LPCVD films, along deep submicronic trenches of interest for microelectronic power components.

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