A COMPUTATIONAL FRAMEWORK FOR MULTISCALE MODELING IN CHEMICAL VAPOR DEPOSITION PROCESSES

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Abstract. A methodology for coupling multiple length scales in chemical vapor deposition (CVD) processes is presented. A reactor scale model (RSM), used for the description of the macro-scale in the bulk, is coupled with a feature scale model (FSM), used for the description of the topography evolution of the micro-scale features on the wafer. The RSM is implemented with a commercial software for computational fluid dynamics, namely FLUENT, and the FSM combines a ballistic model for the species' transport inside features (e.g. trenches), a surface chemistry model, and a profile evolution algorithm based on the level set method. The coupling of the RSM with the FSM is performed through the correction of the boundary condition for the species consumption along the wafer. The coupling methodology implements flow of information in both directions, i.e. from the RSM to the FSM and backwards. Tungsten deposition inside a predefined micro-topography of trenches on the wafer in a CVD vertical reactor is the case studied. The effect of the density (number) of trenches as well as their aspect ratio (depth/width) on the species' consumption and the average growth rate are investigated. The increase of the density and/or the aspect ratio of the trenches yields to an increase of the species' consumption and to a decrease of the average growth rate. The latter is due to the loading phenomenon, i.e. the depletion of reactants due to their increased consumption on the micro-topography on the wafer. The effect of the micro-topography on the Arrhenius plot is also investigated: It is predicted that the existence of the micro-topography can induce a shift of the transition and diffusion limited regimes to lower temperatures.

1 INTRODUCTION

Chemical Vapor Deposition (CVD) is one of the most widely used processes for the production of thin solid films. CVD processes have the ability to produce a large variety of films and coatings of metals, semiconductors, and inorganic as well as organic compounds. The specifications include film thickness, film uniformity, surface morphology, and purity [1], vary with the application and material, and they strongly depend on the application of the fabricated device: From micro- or nano-electro-mechanical systems (MEMS or NEMS), micro- and nano-electronic devices, to protein microarrays and chips [2].

Since the size of the fabricated devices shrinks to lower scales, the specifications refer currently to properties in micro- or nano-scale. The primary manipulation of the events at the micro- and nano-scale, such as the filling of a micro-trench or the nano-roughness growth of a coating, occurs at the macro-scale, so there is a strong motivation for multiscale modeling [3, 4, 5] in order to predict and control the micro- phenomena in terms of macro-parameters.

A detailed coverage of all types of models joining multiscale modeling of CVD processes as well as progress and challenges in the field can be found in previous reviews [6, 7]. In this work, multiscale modeling is accomplished by coupling a model for the description of the reactor bulk phase – termed as Reactor Scale Model (RSM) – with a model describing the evolution of the film growth in a micro-topography on the wafer, termed as Feature (e.g. trench or hole) Scale Model (FSM) [see Fig. 1].

Regarding RSM, the partial differential equations describing the transport phenomena have to be solved numerically for the velocity field, the distribution of pressure, temperature, and species concentration along with the mechanisms describing the chemical reactions in the bulk phase [8, 9]. The wide variety of CVD processes is treated effectively with commercial codes, such as FLUENT [10], PHOENICS [11] and COMSOL[12]. In this work, FLUENT is used.

The FSM consists of three sub-models [13, 14]: A ballistic model for the species' transport inside features [15, 16], a surface chemistry model, and a profile evolution algorithm based on the level set method [17, 18].

The coupling between RSM and FSM is implemented by a correction of the boundary condition for the consumption of species on the wafer, i.e. by imposing an effective (apparent) consumption on the wafer which takes into account the existence of the micro-topography. Computational information "flows" from the macro- scale to the micro-scale, and vice versa, in the course of the simulation [19].

The coupling methodology described in this work combines aspects of both two approaches reported previously on coupling RSM with FSM. We use a continuum ballistic model for the transport calculations inside features, which was adapted mainly by Cale and co-workers [20, 21, 22]. We use the notion of the effective consumption of species on the wafer, which is close to the notion of the effective reactivity calculated by Monte Carlo methods by Jensen and Rodgers [23].

Tungsten (W) deposition by a surface reaction between Tungsten hexafluoride (WF₆) and Hydrogen (H₂) on a patterned wafer with trenches (of uniform density on the wafer) is the case studied. The aim is to study the effect of the trench density (number) on the wafer and the trench aspect ratio (depth/width) on the species consumption and the growth rate and to investigate if the existence of trenches on the wafer affects the Arrhenius plot.

The Arrhenius plot shows the mean growth rate on the wafer versus the inverse of the deposition temperature. Three regimes can be observed in an Arrhenius plot: The diffusion or transport regime (at high temperatures), where the growth is controlled by the diffusion of the reactants to the wafer, the reaction limited regime (at low temperatures) where the growth is controlled by the surface reaction, and the transition regime (at intermediate temperatures, between diffusion and reaction limited regimes) where both diffusion and surface reaction affect the growth. The growth rate is an important factor to produce films with specific properties. Knowledge of the underlying mechanism during deposition, allows the design and the control of the operating parameters (temperature and consequently pressure and inflow velocity) of the CVD reactor. For example when the specification is the film uniformity, it is desirable to work in the reaction limited regime.

The rest of the paper is structured as follows: In the next two sections a description of the RSM and FSM is included. The fourth section is a detailed presentation of the proposed coupling methodology followed by the case study. The paper ends up with the results and the conclusions.

2 REACTOR SCALE MODEL. MODELING THE MACRO-SCALE

The governing equations describing the physical problem in the macro-scale are: the continuity, the momentum, the energy and the species transport equation [24, 25]. In steady state and in vector notation the above set of equations is:

a) Continuity equation

$$\nabla \cdot (\rho \mathbf{u}) = 0 \tag{1}$$

where ρ is the mass density of the mixture and **u** the velocity.

b) Momentum equation

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \left[\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}}) - \mu \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right] + \rho \mathbf{g}$$
(2)

where P is the pressure, μ the viscosity, I the unit tensor, and g is the gravity acceleration.

c) Energy equation

$$C_{p}\nabla\cdot\left(\rho\mathbf{u}T\right) = \nabla\cdot\left(\lambda\nabla T\right) - \sum_{i=1}^{N}\mathbf{j}_{i}\cdot\frac{\nabla H_{i}}{M_{i}} - \sum_{i=1}^{N}\sum_{k=1}^{N_{r}}H_{i}\gamma_{ik}r_{k}^{g}$$
(3)

where C_p is the specific heat of the mixture, T the temperature, λ the thermal conductivity, \mathbf{j}_i the diffusive mass flux of species i, H_i the enthalpy of formation of species i, M_i the molecular weight of species i, γ_{ik} the stoichiometric coefficient of species i in reaction k, N the number of species in the gas phase, N_r the number of volumetric reactions, and r_k^g is the molar rate of volumetric reaction k.

d) Species transport equation

$$\nabla \cdot \left(\rho \mathbf{u} \omega_i\right) = -\nabla \cdot \mathbf{j}_i + M_i \sum_{k=1}^{N_r} \gamma_{ik} r_k^g \quad i = 1, \dots, N-1$$
(4)

where ω_i is the mass fraction of species *i*. The system of equations closes with the ideal gas law. The appropriate boundary conditions for the case study are mentioned in Section 5.1.

The computational fluid dynamics (CFD) problem in the macro-scale is solved in steady state numerically with FLUENT where the finite volume method [25, 26] is used.

No features on the wafer surface are included in the computational domain of the macro-scale; FLUENT cannot treat the physical phenomena inside features, since the Knudsen number inside features is greater than 1 and the continuum hypothesis is invalid.

3 FEATURE SCALE MODEL. MODELING THE MICRO- SCALE

The FSM [13] consists of a a ballistic model [15, 16] for the species' transport inside features (e.g. trenches), a surface chemistry model, and a profile evolution algorithm.

The ballistic model is used for the calculation of the local fluxes of each reactant inside the features (trenches). In particular, the local fluxes are calculated by solving the system of nonlinear integral equations which reads [27]

$$\Gamma_{i}(\mathbf{x}) = \Gamma_{direct,i}(\mathbf{x}) + \iint_{A_{f}} \left\{ 1 - S_{E,i} \left[\Gamma_{I}(\mathbf{x}'), \Gamma_{2}(\mathbf{x}'), ..., \Gamma_{N}(\mathbf{x}') \right] \right\} Q_{i}(\mathbf{x}, \mathbf{x}') \ \Gamma_{i}(\mathbf{x}') dA' \quad (5)$$
$$i = I, N$$

where $\Gamma_i(\mathbf{x})$ is the local flux and $\Gamma_{direct,i}(\mathbf{x})$ is the direct flux, i.e. the flux coming directly from the bulk, of species *i* at an elementary surface of the feature at position \mathbf{x} . Note that both $\Gamma_i(\mathbf{x})$ and $\Gamma_{direct,i}(\mathbf{x})$ are scalar (and not vectors) as they are the result of the inner product of the flux vector with the normal vector of the surface the flux arrives at. The integral in the right hand side of Eq. (5) stands for the flux arriving at \mathbf{x} from all other elementary surfaces of the feature. A_f is the surface area of the feature. $S_{E,i}$ is the effective sticking coefficient of species *i* and represents the effective net loss (if $S_{E,i}>0$) or creation (if $S_{E,i}<0$) of species *i* on the surface. $S_{E,i}$ varies locally from surface to surface inside the feature and surface reaction kinetics is used for its calculation. $Q_i(\mathbf{x}, \mathbf{x}')$ is the differential transmission probability from \mathbf{x}' to \mathbf{x} which incorporates geometric characteristics (orientation, visibility and distance of the elementary surfaces at \mathbf{x} and \mathbf{x}') as well as the reemission mechanism of species *i* [16, 27].

The direct flux at a surface at **x** depends on a) the solid angle $\Omega(\mathbf{x})$, through which the surface is visible to the bulk phase of the reactor, b) the orientation of the surface which is defined by the unit normal vector at **x**, $\mathbf{n}(\mathbf{x})$, and c) the flux distribution of the species in the bulk phase and above the patterned wafer, $\Gamma_{bulk,i}(\theta, \varphi)$. The direct flux reads [27]

$$\Gamma_{direct,i}(\mathbf{x}) = \int_{\Omega(\mathbf{x})} \Gamma_{bulk,i}(\theta, \varphi) d\Omega' \cdot \mathbf{n}(\mathbf{x})$$
(6)

The calculation of the solid angle can be simplified [27, 28, 29] in cases of features with specific geometric characteristics (infinite length trenches or axisymmetric holes). For this type of features the surface integral of Eq. (6) can be reduced [15, 27, 30] to a line integral. In this work, we use the reduced expressions for infinite length trenches [27].

The *surface chemistry model* describes the surface processes and essentially quantifies the effect of local partial pressures (or concentrations or fluxes) on the local deposition rate. In addition, it is used for the calculation of the local effective sticking coefficients of the species.

If we consider that the deposition is the result of a single surface reaction, the local surface reaction rate at a surface at \mathbf{x} inside a feature is

$$r^{s}(\mathbf{x}) = k_{0} \exp\left(\frac{-E_{a}}{RT}\right) f\left[P_{1}(\mathbf{x}), P_{2}(\mathbf{x}), \dots, P_{N}(\mathbf{x})\right]$$
(7)

where k_0 is the pre-exponential factor, E_a the activation energy, and R is the ideal gas constant. The function $f[P_1(\mathbf{x}), P_2(\mathbf{x}), \dots, P_N(\mathbf{x})]$ expresses the dependency of the surface reaction rate on the local partial pressures of the species.

The local effective sticking coefficient of species *i* inside a feature depends on the local surface reaction rate and the local flux of species *i*, $\Gamma_i(\mathbf{x})$, according to the relation

$$S_{E,i}(\mathbf{x}) = \frac{\gamma_i r^s(\mathbf{x}) N_A}{\Gamma_i(\mathbf{x})}$$
(8)

where γ_i is the stoichiometric coefficient of species *i* in the surface reaction and N_A is the Avogardo's number. According to the kinetic theory of gases, the formula linking the partial pressure of species *i* with the flux of species *i* is

$$P_i(\mathbf{x}) = \frac{4\Gamma_i(\mathbf{x})}{u_i} k_B T$$
(9)

where k_B is the Boltzmann constant and u_i is the mean speed [31] of species *i*.

By using Eq. (9) the rate can be expressed in terms of species' fluxes and the system of integral equations [Eq. (5)] reads

$$\Gamma_{i}(\mathbf{x}) = \Gamma_{direct,i}(\mathbf{x}) + \int_{A_{f}} \left\{ 1 - \frac{N_{A}\gamma_{i}k_{0}\exp\left(\frac{-E_{a}}{RT}\right)g\left[\Gamma_{1}(\mathbf{x}'),\Gamma_{2}(\mathbf{x}'),\dots,\Gamma_{N}(\mathbf{x}')\right]}{\Gamma_{i}(\mathbf{x}')} \right\} \mathcal{Q}_{i}(\mathbf{x},\mathbf{x}') \ \Gamma_{i}(\mathbf{x}')dA' \quad (10)$$

$$i = 1,\dots,N$$

The function $g[\Gamma_1(\mathbf{x}'), \Gamma_2(\mathbf{x}'), ..., \Gamma_N(\mathbf{x}')]$ expresses the dependency of the surface reaction rate on the local fluxes of the species. The latter system of nonlinear integral equations is solved by an iterative procedure [27].

The local deposition velocities are calculated by multiplying the local deposition rates with the ratio M_i / ρ_{film} (*i* refers to the depositing species, ρ_{film} is the density of the deposited film) and then are fed to the *profile evolution algorithm, namely the level set method* [17, 18]. The central mathematical idea of the level set method lies in the consideration that the moving boundary is embedded in the level set function Φ , and represents a specific contour of Φ . The basic equation of the method describing the evolution of the level set function is the initial value problem

$$\boldsymbol{\Phi}_t + F \mid \nabla \boldsymbol{\Phi} \mid = 0, \ \boldsymbol{\Phi}(\mathbf{x}, \ t = 0) = q(\mathbf{x}) \tag{11}$$

where $q(\mathbf{x})$ is the initial condition, and F at \mathbf{x} is the component of the velocity in the normal direction of the contour of Φ passing through \mathbf{x} . More details for the implementation on profile evolution under deposition or etching conditions can be found elsewhere [13, 19].

4 COUPLING METHODOLOGY

In order to couple the physical phenomena in the two scales, the boundary condition [Eq.(12)] for solving the species equation [Eq. (4)], and more specifically the consumption rate of each species *i* on the wafer is being modified in order to take into account the existence of the micro-features on the wafer, without the features be

"visible" by macro-scale. *The coupling is performed through an iterative procedure where the flow information is in both directions: From macro- to micro-scale and vice versa.* The proposed methodology for coupling the two scales, or RSM with FSM, can be seen schematically in Fig. 1.



Figure 1: The schematic of the coupling methodology. A) Macro-scale: CVD reactor. B) The "interface" between RSM (macro-scale) and FSM (micro-scale): A boundary cell at the top of a cluster of features. A is the total surface of the features in the cluster. \overline{A} is the surface of the boundary cell through which information is transferred from the macro- to the micro-scale and vice versa. Boundary condition for the consumption of species is imposed on \overline{A} which belongs to the boundary of the computational domain of the macro-scale. ω_i , ρ , and T are fed to micro-scale and \overline{R}_i^s is returned back to the macro-scale. C) A

profile (cross section) of a single feature (trench) on the wafer. A_f is the surface of the feature. Calculations of the local deposition velocities are done in a single wafer for every cluster (corresponding to a boundary cell) of features on the wafer.

The coupling methodology starts with the numerical solution of the equations in the macro-scale [Fig. 1(a)], i.e. Eqs. (1)–(4), with FLUENT. *The, necessary for the solution, boundary condition for the species equation is calculated by considering corrected deposition kinetics which allow to take into account the micro-topography on the wafer without including it in the computational domain of the RSM. In particular, the effect of micro-topography on the deposition kinetics is expressed by a correction of the pre-exponential factor; instead of using the real pre-exponential factor, an effective value is used (k_{0,eff}). In the case of a single surface reaction (no bulk phase reactions are consider), the boundary condition for the species equation [Eq. 4] is*

$$\rho D_i \frac{\partial \omega_i}{\partial \mathbf{n}^s} = \gamma_i M_i r_{eff}^s(\mathbf{x}) = \gamma_i M_i k_{0,eff} \exp\left(\frac{-E_a}{RT}\right) f\left[P_1(\mathbf{x}), P_2(\mathbf{x}), \dots, P_N(\mathbf{x})\right]$$
(12)

where D_i is the diffusion coefficient of species *i* [see Section 5.1], \mathbf{n}^s the unit normal vector to the surface of the wafer and $r_{eff}^s(\mathbf{x})$ is the *effective rate* of the surface reaction. For the starting solution of the equations in the macro-scale, $k_{0,eff} = k_0$ [see Eq. (7)].

After the solution, the mass density, ρ , the temperature, T, and the mass fractions, ω_i , of species at surface \overline{A} of each boundary cell j [Fig. 1(b)] are fed into the micro-scale. We consider that these properties are constant for the cluster of features corresponding to a boundary cell. As a consequence, to avoid duplicate calculations, FSM is applied to a single feature for each boundary cell [Fig. 1(c)].

P, *T*, and ω_i are used for the calculation of $|\Gamma_{bulk,i}(\theta, \varphi)|$ [Eq. (6)] which, for a neutral species *i* and according to the kinetic theory of gases, equals to

$$|\Gamma_{bulk,i}(\theta,\varphi)| = |\Gamma_{bulk,i}| = \frac{1}{4}n_iu_i$$
(13)

Note that there is no effect of θ , φ on $|\Gamma_{bulk,i}|$ if the species involved in the reaction are neutral; the angular distribution of a neutral species is isotropic. n_i is the number density of species *i*,

$$n_i = \omega_i \frac{N_A}{M_i} \rho \tag{14}$$

The mean speed of species i, u_i , is calculated by the kinetic theory of gases

$$u_i = \left(\frac{8k_BT}{\pi m_i}\right)^{1/2} \tag{15}$$

where m_i is the mass of a molecule of species *i*.

After the calculation of $|\Gamma_{bulk,i}|$ [Eq. (13)], the local fluxes or the local partial pressures [Eq. (9)] are calculated by coupling of the surface model with the ballistic model for the local flux calculation. Then, the local surface reaction rate is calculated by Eq. (7). The local consumption rate of species *i* inside the features is

$$R_i^s(\boldsymbol{x}) = M_i \gamma_i r^s(\boldsymbol{x}) \tag{16}$$

Integration of Eq. (16) over the total surface of the feature cluster corresponding to the boundary cell [surface A in Fig. 1(b)] yields the effective consumption rate of species *i* at the features' cluster,

$$\overline{R}_{i}^{s} = \frac{1}{\overline{A}} \int_{A} R_{i}^{s}(x') dA'$$
(17)

The calculation of \overline{R}_i^s is performed at every boundary cell *j* (on the wafer) of the computational domain of the macro-scale. \overline{R}_i^s takes into account the micro-topography on the patterned wafer. The pre-exponential factor of Eq. (12) is then corrected according to the equation

$$k_{0,eff}^{(n+1)} = k_{0,eff}^{(n)} \frac{\overline{R}_i^{s,(n+1)}}{\overline{R}_i^{s,(n)}}$$
(18)

modifying the boundary condition [Eq. (12)] for the species equation of RSM [Eq. (4)]. The superscripts (n+1) and (n) correspond to two successive steps of the iterative procedure.

The numerical solution in the macro-scale is repeated with the new boundary condition on the wafer, i.e. new values for $k_{0,eff,j}$ (the added index *j* corresponds to the boundary cell *j*). The iterative procedure stops when convergence on all $\overline{R}_{i,j}^s$ is achieved. After convergence the local deposition rate for each feature at each boundary cell is fed

to the profile evolution algorithm. The profile evolution is performed for a time step Δt . Δt satisfies the stability criterion for the profile evolution calculations [17]. We consider that during Δt the change in the topography is negligible in affecting the consumption of species on the wafer surface. The new profiles of the features at each boundary cell are stored and are used for the calculations at the next time step.

The procedure described above is repeated at every time step. For the results presented in this work the number of the required iterations for the convergence on all $\overline{R}_{i,i}^{s}$ and at each time step is less than 4.

5 CASE STUDY

The case studied in this work is CVD of W. The deposition occurs by a surface reaction between WF_6 and H_2 on a patterned wafer with trenches. Details of the implementation are described in the next sections.

5.1 Conditions in the macro-scale

CVD of W occurs in a axisymmetric vertical CVD reactor [32] [Fig. 1(a)]. The carrier gas is Argon (Ar) and the precursor is WF₆. Along with the carrier and the precursor, H₂ is inserted in the reactor. There are no reactions in the bulk phase of the reactor. The momentum equations along with the continuity, energy, and species equations, i.e. Eqs. (1) – (4), are discretized and solved in cylindrical co-ordinates with FLUENT which implements the finite volume method. The pressure-based solver is used along with the SIMPLE algorithm [26, 33]. The computational domain is discretized in 7143 cells with the mesh generator program GAMBIT [34]. Additional computations were performed in meshes up to 35000 cells. The error between the mesh used in our computations and the fine mesh of 35000 cells was less than 3%.

The Stefan – Maxwell equations are used for calculating the diffusive flux of each species [33, 35]. The thermal diffusion coefficients are calculated by an empirical relation built in FLUENT accounting for the Soret effect which causes heavy molecules to diffuse less rapidly towards a heated surface than light molecules. For the binary diffusion coefficients, the viscosity, and the thermal conductivity, Chapman-Enskog formulas [24, 33] are used; the Lennard-Jones parameters are taken from [36]. Regarding the mixture properties, mass weighted mixing rules are used for calculating the viscosity and thermal conductivity. The operating pressure of the reactor is 133 Pa.

For the boundary conditions: Two different inlet configurations are considered: a) 1 sccm of WF₆, 199 sccm of Ar and 1000 sccm of H₂ and b) 100 sccm of WF₆, 100 sccm of Ar, and 1000 sccm of H₂. No-slip boundary conditions are imposed on the walls of the reactor.

The temperature at the inlet and on the walls of the reactor is 298 K. On the wafer the temperature range is 473 K to 1073 K [see Section 6]. The walls, where the wafer is supported, are adiabatic.

The flux of all species on the reactor walls is zero with an exception on the wafer where the surface reaction (deposition) takes place [see Eq. (12)]. Outflow boundary conditions [34] are imposed at the outlet of the reactor.

5.2 Conditions in the micro-scale

The patterned wafer includes a series of similar trenches and its diameter is 6 cm. The density of trenches is considered uniform along the wafer and its range is from 1 to 16 trenches per 32 μ m. The aspect ratio (AR) of the trenches for the cases studied is 1.5, 3 and 5 with initial width 1 μ m.

The profile (cross section) of the trenches is identical along the direction normal to the paper [Fig. 1(c)]. Thus, the integral of Eq. (5) [or Eq. (10)] is simplified to a line integral and the local flux is calculated along the arclength of the trench profiles. By exploiting the symmetry of the initial trench profile, the solution is performed at the half of the trench profile.

Concerning the discretization of the computational domain for the profile evolution by the level set method, and for the results presented in the following section, $\Delta x = \Delta y =$ 0.025 µm. The time step (Δt) for the profile evolution is dictated by the stability criterion and depends on the local deposition velocity. It is set to 125 s for the first inlet configuration and 8 s for the second.

5.3 Deposition kinetics

The surface reaction taking place on the wafer is

$$WF_6 + 3H_2 \rightarrow W_{(s)} + 6HF$$

The pertinent surface reaction rate is [37]

$$r = 20000 \frac{P_{H_2}^{0.5} P_{WF_6}}{1 + 1000 P_{WF_6}} \exp\left(-\frac{8300}{T}\right)$$
(19)

where P_{H_2} and P_{WF_6} are the partial pressures (in Torr) of H₂ and WF₆. *T* is the temperature (in K) on the wafer.

6 RESULTS AND DISCUSSION

The coupling methodology described in Section 4 is applied. Results for the first inlet configuration (1 sccm of WF₆ at the inlet) are shown in Fig. 2. Fig. 2(a) demonstrates film growth profiles at different time instances for a trench of a cluster of trenches extending from 0.045 m to 0.05 m from the center of the wafer. Fig. 2(b) shows the average (over the wafer) consumption rate of WF₆ versus deposition time. WF₆ consumption is computed according to the formula

$$\left\langle \overline{R}_{WF_{6}}^{s} \right\rangle_{\sum \overline{A}_{j}} = \frac{\sum_{j=1}^{N_{b,w}} \overline{A}_{j} \overline{R}_{WF_{6},j}^{s}}{\sum_{j=1}^{N_{b,w}} \overline{A}_{j}}$$
(20)

where the index *j* corresponds to the boundary cell *j* [Fig. 1(b)]. $N_{b,w}$ is the number of boundary cells with one face on the wafer. Note that all surfaces \overline{A}_j of Eq. (20) remain constant during deposition as they belong to the boundary of the computational domain of the macro-scale [Fig. 1(b)].

The existence of the trenches (at t = 0 s the trenches are empty) increases the effective surface where W can be deposited and for that the consumption rate of WF₆ increases. As time evolves the trenches are filling [Fig. 2(a)] and the effective surface approaches a flat surface (wafer surface without micro-topography). It is considered that a trench is filled up, either compactly or by forming a void, when a point of the trench profile crosses the symmetry line. The trench of Fig. 2(a) fills up at 16750 s; then, the

consumption rate of WF_6 approaches the one computed without taking into account the existence of the trenches on the wafer [see curves at 20000 s in Fig. 2(b)].

In Fig. 3 the same results as in Fig. 2 are shown for 100 sccm of WF_6 at the inlet. As in the case of 1 sccm, the average consumption rate decreases monotonically to approach the value without micro-topography [Figs. 3(b)]. In this case, the decrease is steeper compared to Fig. 2(b) because the deposition rate is greater and the trench fills faster.



Figure 2: Trench profiles and WF₆ consumption on the wafer vs deposition time when 1 sccm of WF₆ enter the reactor. Wafer temperature is 673 K. The density of features on the wafer is 8 trenches per 32 μ m. a) Trench profile evolution at the cluster of trenches extending from 0.045 m to 0.05 m from the center of the wafer. The profiles are at equidistant time spaces (2500 s). b) Average consumption rate of WF₆ on the wafer.

By comparing the trench profile evolution in the two cases of WF_6 inflows [Figs. 2(a) and 3(a)] one could observe that in the case of low inflow of WF_6 (1 sccm) the deposition is anisotropic (non conformal) and a void is formed inside the trench. On the other hand, in high inflow of WF_6 (100 sccm) the deposition is isotropic (conformal).

The difference of the trench profiles in the two cases of inflow of WF₆ are attributed to differences of the effective sticking coefficient of WF₆, S_{E,WF_6} . In the case of 1 sccm, the local S_{E,WF_6} ranges from 10⁻² to 10⁻³ and in the case of 100 sccm it ranges from 10⁻⁵ to 10⁻⁶. In the case of 100 sccm, due to the very low value of S_{E,WF_6} (very low probability for WF₆ sticking), the number of reemissions – and consequently the redistribution of flux inside the trench – is high. As a result, the flux is almost the same for every elementary surface of the trench and the deposition is isotropic. The redistribution is not so effective in the case of 1 sccm where S_{E,WF_6} is higher.



Figure 3: Trench profiles and WF₆ consumption on the wafer vs deposition time when 100 sccm of WF₆ enter the reactor. Wafer temperature is 673 K The density of features on the wafer is 8 trenches per 32 μ m. a) Trench profile evolution at the cluster of trenches extending from 0.045 m to 0.05 m from the center of the wafer. The profiles are at equidistant time spaces (160 s). b) Average consumption rate of WF₆ on the wafer.

The area of the trench sidewall close to the top where the deformation can be seen [Fig. 2(a)] is the most exposed area to the bulk, i.e. receives the greater direct flux. This is the reason for the high deposition rates at this area and the anisotropic deposition.



Figure 4: WF₆ consumption on the wafer, average growth rate on the wafer and Arrhenius plots when
 1 sccm of WF₆ enter the reactor. a) WF₆ consumption and average growth rate on the wafer for different trench densities and AR. The temperature on the wafer is 673 K. b) Arrhenius plots without micro-topography, 8 trenches / 32 μm, AR=1.5 and for 16 trenches / 32 μm, AR=3.

Fig. 4(a) demonstrates WF_6 consumption at the wafer for different trenches' densities and AR, for the case of 1 sccm WF_6 at the inlet. The results are presented at t = 0 s when the WF_6 consumption is maximum [see Fig. (2b)]. The increase of both the trench density and AR yields to an increase of the average consumption rate of WF_6 . This is expected as the effective surface on the wafer increases as feature density and AR increase.

The average growth rate, also shown in Fig. 4(a), is defined as

$$\left\langle \overline{GR}^{s}_{WF_{6}} \right\rangle_{\sum A_{j}} \approx \frac{\sum_{j=1}^{N_{b,w}} \overline{A}_{j} \frac{M_{W} R^{s}_{WF_{6},j}}{M_{WF_{6}} \rho^{s}_{W}}}{\sum_{j=1}^{N_{b,w}} A_{j}}$$
(21)

where ρ_w^s is the mass density of the solid W and M_W , M_{WF_6} are the molecular weights of W and WF₆ respectively. Eq. (21) is the growth rate reduced to the actual microtopography on the wafer. Note that the surfaces A_j of Eq. (21) change during deposition – in contrast to Eq. (20) – as they comprise the evolving profile of the trenches Fig. 1(b)].

Whereas the average consumption rate of WF_6 increases with the increase of the trench density or the AR of the trenches, the average growth rate decreases. The latter is due to the loading phenomenon [38] observed in diffusion or transport limited regime. The loading phenomenon in CVD processes is commonly met in horizontal, thermal wall reactors [2, 39]. A depletion of WF_6 occurs due to its increased consumption on the increased effective surface.

Fig. 4(b) shows the Arrhenius plot without micro- topography in the wafer (uncoupled case), for trench density 8 trenches every 32 μ m of AR 1.5, and for trench density 16 trenches every 32 μ m of AR 3 (coupled cases). At low temperatures, the values of the Arrhenius plot correspond to the reaction limited regime; the deposition rate is controlled by the reaction mechanism. At high temperatures, the values of the Arrhenius plot correspond to the diffusion or transport limited regime; the deposition rate is controlled by the diffusion or transport mechanism. The region where the curve changes slope is referred to as transition regime and in that region both of the above mechanisms are important in the deposition of the film.

The Arrhenius plot is affected from the existence of the micro-topography in the regions where the diffusion phenomena are important, namely the transition regime and the diffusion or transport limited regime. This is due to the loading phenomenon. As it can be seen in Fig. 4(b), for the coupled cases, at high temperatures the average growth rate decreases, but in low temperatures, where it is controlled by the reaction mechanism, it is constant. Moreover, the transition and diffusion limited regimes are shifted to lower temperatures [see Fig. 4(b)].



Figure 5: WF₆ consumption on the wafer, average growth rate on the wafer and Arrhenius plot when 100 sccm of WF₆ enter the reactor. a) WF₆ consumption and average growth rate on the wafer for different trench densities and AR. The temperature on the wafer is 673 K. b) Arrhenius plots without micro-topography, 8 trenches / 32 µm, AR=1.5 and for 16 trenches / 32 µm, AR=3.

In Fig. 5 the same results as in Fig. 4 are presented for 100 sccm of WF₆ at the inlet. Fig. 5(a) shows the WF₆ consumption and the average growth rate. For the case of AR=1.5, the slope for both the WF₆ consumption and the average growth rate, with respect to the trench density, is not so steep compared to the results in Fig. 4(a). The effective surface is increased but not enough for the diffusion phenomena – and consequently the loading phenomenon – to be important. Moreover, a shift to lower temperatures of the transition and diffusion limited regimes in the Arrhenius plot is not observed [see Fig. 5(b)]; the diffusion mechanisms are not important and the growth rate is controlled by the reaction. For higher values of AR, as in the case of AR=3, the transition diffusion limited regimes are slightly shifted at lower temperatures as it is shown in Fig. 5(b) and the average growth rate decreases as the AR of the trenches increases [see Fig. 5(a)]. Note that even thought in the case of 100 sccm the average growth rate is reduced from 450 A/min to 360 A/min (16 trenches / 32 μ m, AR=3), the reduction is ~20%, in contrast to the 1 sccm case where the corresponding reduction is ~86%.

7 CONCLUSIONS

A computational framework for coupling of the macro- with the micro-scale in a CVD reactor is described. In particular a RSM is coupled with a FSM and the bridge between the two scales is the boundary condition for the species consumption along the wafer. The RSM is implemented with the commercial package FLUENT which performs the solution of continuity, momentum, energy and species equations. The FSM consists of a continuum ballistic model for the transport calculations inside the features, a surface chemistry, and a profile evolution algorithm.

The deposition of W inside micro-trenches of different AR by the surface reaction of WF_6 with H_2 is investigated. The calculations show that the existence of the trenches increases the effective surface where W can be deposited and for that the consumption rate of WF_6 increases. On the other hand, this increase of the effective surface causes the decrease of the average growth rate due to loading phenomenon and can shift the transition and diffusion limited regimes of the Arrhenius plot to lower temperatures.

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