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Mathematical Modeling of the AMCs Cross-Contamination Removal in the FOUPs: Finite Element Formulation and Application in FOUP's Decontamination

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Abstract**—**Nowadays, with the increasing of the wafer's size and the decreasing of critical size of integrated circuit manufacturing in modern high-tech, microelectronics industry needs a maximum attention to challenge the contamination control. The move to 300 [mm] is accompanied by the use of Front Opening Unified Pods for wafer and his storage. In these pods an airborne cross contamination may occur between wafers and the pods. A predictive approach using modeling and computational methods is very powerful method to understand and qualify the AMCs cross contamination processes. This work investigates the required numerical tools which are employed in order to study the AMCs cross-contamination transfer phenomena between wafers and FOUPs. Numerical optimization and finite element formulation in transient analysis were established. Analytical solution of one dimensional problem was developed and the calibration process of physical constants was performed. The least square distance between the model (analytical 1D solution) and the experimental data are minimized. The behavior of the AMCs intransient analysis was determined. The model framework preserves the classical forms of the diffusion and convection-diffusion equations and yields to consistent form of the Fick's law. The adsorption process and the surface roughness effect were also traduced as a boundary condition using the switch condition Dirichlet to Neumann and the interface condition. The methodology is applied, first using the optimization methods with analytical solution to define physical constants, and second using finite element method including adsorption kinetic and the switch of Dirichlet to Neumann condition.

Keywords**—**AMCs, FOUP, cross-contamination, adsorption, diffusion, numerical analysis, wafers, Dirichlet to Neumann, finite elements methods, Fick's law, optimization.

I. Introduction

A watchful attention is required to challenge the contamination control during the manufacture of integrated circuit (I.C) in high-tech microelectronics engineering. Integrated circuits are manufactured from a monocristallin silicium plates (wafer) [1]. Minutiarization of the I.C is designed with the 45, 32, 22 [nm], in fact, the wafer's surface is very sensitive to contamination. In the semiconductor manufacturing, particle, bacterial, metallic and molecular contaminations of the wafer are critical subjects, which can potentially cause defect on the use and have impacts in the device performance [1]-[3]. In this work, we keep more attention in molecular contamination that can damage and induce a significant impact in manufacturing yields. The wafer carrier and storage plays a significant role for contamination control [4]. The use of the Front Unified Pods (FOUPs) to transport from tool to tool 25 wafers in the 300 [mm] are necessary to protect the wafer against contamination mainly the Airborne Molecular Contamination. This container may contain a lot of contaminant including, there so called AMCs or Airborne Molecular Contaminants and can still contain a significant amount of contamination with the potential to damage the wafer. This enclosed mini-environment is made of porous polymers, mainly in PC, COP, PP, PEEK and PEI [1]-[3], [5], [6].

These materials are known with their adsorption and outgas properties. They are also able to absorb volatile compounds present in the atmosphere coming from the connection to equipment or from the fresh assembly of wafers just processed (post processed wafers). During the storage, these wafers may outgas the chemicals used with during the process. As results, a reversible and an irreversible outgassing of contaminant previously trapped in polymer is possible. In fact a contemned FOUP already itself may be a source of contamination because it already adsorbs the contaminant from the wafers. This cross-contamination scheme was clearly evidenced for volatile acids in presence. Many works have been published which deal with experiment measurement method to quantify and to investigate this phenomena for each types of material [1]-[3].

Generally, when one object becomes contaminated by either direct or indirect contact with another object which is already contaminated, we talk about cross contamination. In microelectronics industry, this process generally takes place at FOUPs which contain the wafers before and after production. The main object sources of the contamination in microelectronic factory are the wafer, air, FOUP by which a new wafer may be contamined before the manufacturing processes.

Some manufacture processes such as dry engraving (plasma), depot and photolithography are the source of

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contamination, when the wafer is already processed its surface is contamined by the volatile acids [4], [5]. After this manufacturing process, these wafers will be stored in the FOUP. Then, the wafer is exposed to the FOUPs atmosphere and an acid pollution may happen from wafer to FOUP by the intermediate air (atmosphere). As outlined before, the FOUP material can absorb the contaminant in it's around, an adsorption phenomenon from air to the internal surface of the FOUP followed by diffusion in volume happens. When the wafer moved or the FOUP is opened, the air in the FOUP atmosphere changes and desorption phenomena takes place, a cross contamination from FOUP to new wafer may happen i.e. contamination of the new wafer stored by the FOUP already contamined by the volatile acid.

Indeed, in order to successfully ensure the miniaturization the integrated circuits manufacturing, we have mainly through the advent of 300[mm] wafer manufacturing technologies new methods that are required for facing this challenge. To endeavor a systematic analysis and control of the underlying system, numerical simulation should help to mimic the process behaviors. Modeling and computational method are worth method to predict and to quantify physical phenomenon such as AMCs cross contamination within FOUP.

Motivated by the above phenomena, this work describes and develops the finite element formulation devoted to AMCs cross contamination in order to investigate the effect of the contaminant to its close environment. We propose new strong numerical tools for AMCs cross-contamination able to qualify and to quantify the residual contamination in the FOUP. The model validation method is based on correlation of the observed data and the direct method together.

II. Model Settings

Modeling the adsorption of AMCs cross contamination between wafer and FOUPs is based on adsorption phenomena. In general two concepts of adsorption, physical and chemistry adsorption models will be considered. A detailed review of various adsorption kinetics (adsorption, desorption) models was given in [6], [7]. In this model the transport towards the surface is purely diffusive and we investigate the concentration in the internal area of FOUPs by using the thermodynamics laws. These thermodynamics laws are traduced by the Henry constant in order to connect the concentration of the contaminant at the FOUPs atmosphere and the concentration at the internal surface of the FOUPs.

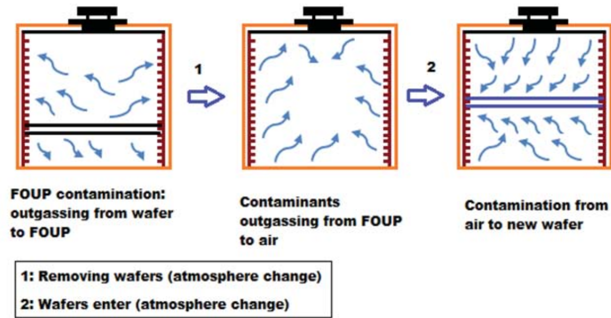

Fig. 1 Schematic illustration for the three main cross contamination processes steps

The mathematical model of diffusion process in these two domains is based on Fick's second law of diffusion. At the interface of that domain a kinetics law will be established. According to Fick's first and second law, also known as the diffusion equation [8], [9], is defined in the first part of (1).

Where here *i: =s, g*. The AMCs cross contamination is governed by diffusion time dependent process in which the rate of diffusion is a fraction of time. In this process, the contaminant moves from a region of high concentration (wafer) to one of low concentration (internal surface of FOUP) [10]. In the outgassing phenomenon, the contaminant moves from FOUP to the wafer. We assume that, on, we have the wafer area in which the source of contamination takes place during the contamination time. We assume that the advection and reaction time scales are slow compared to the diffusive time scales. The equation for transient contaminant transfer between the wafer and the internal part of the FOUP is given by (1).

$$\begin{cases} \dfrac{\partial C^s}{\partial t} = \nabla.(\mathbf{D}_s \nabla C^s) + \mathbf{q} \quad \text{in } (\Omega_s \times [0,\mathrm{T}]) \\ \mathbf{B.C}\begin{cases} C^s.\mathbf{n} = h_0 C^g \text{on } (\Gamma_\mathrm{N}) \\ -\mathbf{D}_s \nabla C^s.\mathbf{n} = 0 \text{ on } (\partial\Omega_s - \Gamma_\mathrm{N}) \end{cases} \\ \mathbf{I.C}, C^s(0,.).\mathbf{n} = 0 \text{in } (\Omega_s \times [0,\mathrm{T}]) \\ \dfrac{\partial C^g}{\partial t} = \nabla.\left(\mathbf{D}_g \nabla C^g\right) - \nabla.(\mathbf{u}C^g) \quad \text{in } (\Omega_g \times [0,\mathrm{T}]) \\ \mathbf{B.C}\begin{cases} -(\mathbf{D}_g \nabla C^g - \mathbf{u}C^g).\mathbf{n} = N_0^g + k_c[C_0 H(t-\varepsilon) - C^g] \text{on } (\Gamma_\mathrm{D}) \\ C^g.\mathbf{n} = \dfrac{C^s}{h_0} \text{on } (\Gamma_\mathrm{N}) \\ -(\mathbf{D}_g \nabla C^g - \mathbf{u}C^g).\mathbf{n} = 0 \text{on } (\partial\Omega_g - (\Gamma_\mathrm{N} \cup \Gamma_\mathrm{D})) \end{cases} \\ \mathbf{I.C}, C^g(0,.).\mathbf{n} = 0 \quad \text{in } (\Omega_g \times [0,\mathrm{T}]) \end{cases} \tag{1}$$

The initial conditions are defined; it consists to consider that at the initial time $t := 0$the FOUP and its atmosphere are not yet contamined i.e. $C^s(t=0) := 0$at $C^g(t=0) := 0$. Practically, these studies have done with a new FOUP for a first use. In the model, $\mathbf{D}_g$ and $\mathbf{D}_s$ are the gas diffusion coefficient in gas and solid medium, which has no connection with the spatial location and no variation in time, [m^2/s]. The unknown of the problem are C^g and C^swhich are respectively the concentration of the contaminant and the concentration at the internal FOUP's surface $H(t-\varepsilon)$is the Heaviside function, C_0 is the initial concentration in FOUP's atmosphere when the wafers have been finished to outgassing the contaminant, h_0 is

the Henry constant and $\mathbf{n}$ is the outer unit normal vector, $T$is the final time and $\mathbf{q}$ is the source.

Because the wall concentration C^s depends on the concentration C^gwe assume the following boundary condition: on Γ_Da prescribed inflow concentration is imposed and at the interface the two concentrations will be balanced by the Henry constant. We start by developing some analytical solutions for the diffusion equation with uniform diffusivities in an unbounded domain and for very simple boundary conditions as determined by J. Crank in [10]. Then we solve the more general equation using finite element method, a numerical technique of optimization, for any type of boundary conditions. In this approach, we use the assumptions below. We suppose that, the FOUP and the membrane are homogenous and isotropic. Adsorption resolution of the contaminant is balanced at the surface. The surface roughness of the internal surface of the FOUP or the membrane is neglected but we take into account of this parameter when we use the Henry law at the surface. Then the diffusion coefficient is weakly function of the concentration.

$$-(\mathbf{D}_g\nabla C^g + \mathbf{u}C^g).\mathbf{n} = N_0^g + k_c[C_0 H(t-\varepsilon) - C^g] \quad (2)$$

Firstly we assume that there is no inner flux N_0^g (no initial flux) and we assume that we have a transient boundary conditions with a laminar gas flow on this boundary ($\mathbf{u}$ =0). When k_c is sufficiently large, we have the Dirichlet condition i.e $C^g \simeq C_0 H(t-\varepsilon)$and if k_c we have the Neumann's boundary condition (for the neutral area of the wafer), i.e.$(-\mathbf{D}_g\nabla C^g + \mathbf{u}C^g).\mathbf{n} = 0$. To conditionning $C_0$and $k_c$we need a parametric study was made to ensure the stability.

We have,

$$\text{if}\begin{cases} k_c \geq 1 \Rightarrow C^g \simeq C_0 H(t-\varepsilon) \text{if } 0 < t \leq (\mathrm{t_c} + \mathrm{t_p}) \\ k_c = 0 \Rightarrow (-\mathbf{D}_g\nabla C^g + \mathbf{u}C^g).\mathbf{n} = N_0^g \text{if } \mathrm{t} > (\mathrm{t_c} + \mathrm{t_p}) \end{cases} \quad (3)$$

where the computed quantity is obtained by the analytical solution, such that the concentration at the internal surface is $\mathbf{Q}_\infty$ and there is no initial distribution in the polymer membrane. The diffusion coefficient $\mathbf{D}_g$ is the unknown; it is obtained by using the optimization method [11].

A. Finite Elements Discretization

We use the Galerkin finite element formulation for numerical solutions of the problem given by (1). It is obtained by multiplying the governing equation by an appropriate test function respectively ϕ and ψ for the concentration C^s and C^g respectively, and by integrating over the computational domain. In this case, we have

$$\begin{cases} \int_{\Omega_s} \frac{\partial C^s}{\partial t}\phi dV = \int_{\Omega_s} \nabla.(\mathbf{D}_s\nabla C^s)\phi dV + \int_{\Omega_s} \mathbf{q}\phi dV \\ \int_{\Omega_g} \frac{\partial C^g}{\partial t}\psi dV = \int_{\Omega_g} \nabla.(\mathbf{D}_g\nabla C^g)\psi dV + \int_{\Omega_g} \nabla(\mathbf{u}C^g)\psi dV \end{cases} \quad (4)$$

For that, let us consider first the functional $H^1(\Omega_s)$ and $H^1(\Omega_g)$ in which we search the solution in accordance with regularity $H_s^1 = \{\phi \in H^1(\Omega_s) | \phi = s\forall x \in \Gamma_s\}$ and $H_s^1 = \{\psi \in H^1(\Omega_s) | \psi = s\forall x \in \Gamma_g\}$ where$H_s^1(\Omega_s)$ and $H_s^1(\Omega_g)$ are a Sobolev space, classically defined as $H_s^1(\Omega_s) = \{\phi \in L^2(\Omega_s), \| \nabla\phi \| \in L^2(\Omega_s)\}andH_s^1(\Omega_g) = \{\psi \in L^2(\Omega_g), \| \nabla\psi \| \in L^2(\Omega_g)\}$. Where $L^2(\Omega_s)$ and $L^2(\Omega_g)$ are the Hilbert vector space of the functions respectively on (Ω_s) and (Ω_g). Therefore, $L^2(\Omega_s) = \{\phi(x) | \int_{\Omega_s} |\phi(x)|^2 dx < \infty\}$ and $L^2(\Omega_g) = L^2(\Omega_g) = \left\{\psi(x) \middle| \int_{\Omega_g} |\phi(x)|^2 dx < \infty\right\}$ are considered.

By using Green's theorem [12], integration by parts leads to,

$$\begin{cases} \int_{\Omega_s} \frac{\partial C^s}{\partial t}\phi dV = -\int_{\Omega_s} \nabla.(\mathbf{D}_s\nabla C^s).\nabla\phi dV + \int_{\Omega_s} (\mathbf{D}_s\nabla C^s).\mathbf{n}\phi dV \\ \qquad + \int_{\Omega_s} \mathbf{q}\phi dV \\ \int_{\Omega_g} \frac{\partial C^g}{\partial t}\psi dV = -\int_{\Omega_g} \nabla.(\mathbf{D}_g\nabla C^g).\nabla\psi dV + \int_{\Omega_g} (\mathbf{D}_g\nabla C^g).\mathbf{n}\psi dV \\ \qquad - \int_{\Omega_g} \nabla(\mathbf{u}C^g)\psi dV \end{cases} \quad (5)$$

By applying the Galerkin's weighted residual method and the Green's theorem mentioned above, the variational formulation corresponding the AMCs cross contamination is given by (4). Consequently the weak formulation of the AMCs model should be introduced:

We find $C^s \in H^1(\Omega_s)$ and $C^g \in H^1(\Omega_g)$ such that,

$$\begin{cases} a_1\left(\frac{\partial C^s}{\partial t}, \phi\right) + b_1(C^s, \phi) = L_1(\phi)\ \forall\phi \in H^1(\Omega_s) \\ a_2\left(\frac{\partial C^g}{\partial t}, \psi\right) + b_2(C^g, \psi) = L_2(\psi)\ \forall\psi \in H^1(\Omega_g) \end{cases} \quad (6)$$

$$L_1(\phi) = \int_{\Omega_s} \mathbf{q}\phi dV$$

$$L_2(\phi) = \int_{\Omega_g} N_0^g \psi dV$$

$$a_1\left(\frac{\partial C^s}{\partial t}, \phi\right) = \int_{\Omega_s} \frac{\partial C^s}{\partial t}\phi dV$$

$$a_2\left(\frac{\partial C^g}{\partial t}, \psi\right) = \int_{\Omega_g} \frac{\partial C^g}{\partial t}\psi dV$$

$$b_1(C^s, \phi) = \int_{\Omega_s} \mathbf{D}_s\nabla C^s.\nabla\phi dV$$

$$b_2(C^g, \phi) = \int_{\Omega_s} \mathbf{D}_g\nabla C^g.\nabla\psi dV - \int_{\Omega_g} \nabla.(\mathbf{u}C^g)\psi dV + \int_{\Gamma_D} k_c(C_0 H(t-\varepsilon) - C^g)\psi dS$$

Notice that the domain $\Omega_s$and $\Omega_g$are decomposed into finite subdomains Ω_s^e and Ω_g^e for each elements. Similarly, boundary $\partial\Omega_s$ and $\partial\Omega_g$ are decomposed in $\partial\Omega_s^e$ and$\partial\Omega_g^e$. Finally, the time interval is subdivided by n subintervals.

For the spatial discretization, we consider the finite element partition $\mathcal{T}_h^s$ and $\mathcal{T}_h^s$ of Ω_s and $\Omega_g$respectively into tetrahedral

elements. Again for simplicity, we will consider that the finite element partition associated to $\mathcal{T}_h^s$ and $\mathcal{T}_h^s$ are uniform, h is the size of the element domains. Let us C_h^s and C_h^g are the approximations solutions of C^s and C^g respectively.

We find $C_h^s \in H^{1h}(\Omega_s)$ and $C_h^g \in H^{1h}(\Omega_g)$

$$\begin{cases} a_1\left(\frac{\partial C_h^s}{\partial t}, \phi_h\right) + b_1(C_h^s, \phi_h) = L_1(\phi_h)\ \forall \phi_h \in H^{1h}(\Omega_s) \\ a_2\left(\frac{\partial C_h^g}{\partial t}, \psi_h\right) + b_2(C_h^g, \psi_h) = L_2(\psi_h)\ \forall \psi_h \in H^{1h}(\Omega_g) \end{cases} \quad (7)$$

Finally, we obtain a system of first order differential equations and using the matricial notation, we have

$$\begin{bmatrix} \mathbb{M}^s & 0 \\ 0 & \mathbb{M}^g \end{bmatrix} \begin{pmatrix} \dot{\mathbf{C}}^s \\ \dot{\mathbf{C}}^g \end{pmatrix} + \begin{bmatrix} \mathbb{D}^s & h_0 \\ h_0^{-1} & \mathbb{D}^g \end{bmatrix} \begin{pmatrix} \mathbf{C}^s \\ \mathbf{C}^g \end{pmatrix} = \begin{pmatrix} \mathbb{F}^s \\ \mathbb{F}^g \end{pmatrix} \quad (8)$$

where $\mathbf{C}^s$ and $\mathbf{C}^g$ are the vectors of nodal unknown concentrations, $\mathbb{M}^s$ and $\mathbb{M}^g$ are the time constant matrices, $\mathbb{F}^s$ and $\mathbb{F}^g$ are the source and external flux vector. The system of ordinary differential equations above has to be integrated in time. Using the finite difference approximations, explicit Euler scheme, and system (8) can be written at time $t + \Delta t$ as:

$$\begin{bmatrix} \mathbb{M}^s & 0 \\ 0 & \mathbb{M}^g \end{bmatrix}^e \begin{pmatrix} \mathbf{C}_{n+1}^s - \mathbf{C}_n^s \\ \mathbf{C}_{n+1}^g - \mathbf{C}_n^g \end{pmatrix}^e + \Delta t \begin{bmatrix} \mathbb{D}^s & h_0 \\ h_0^{-1} & \mathbb{D}^g \end{bmatrix}^e \begin{pmatrix} \mathbf{C}_n^s \\ \mathbf{C}^g \end{pmatrix}^e = \Delta t \begin{pmatrix} \mathbb{F}_n^s \\ \mathbb{F}_n^g \end{pmatrix}^e \quad (9)$$

where,

$$\mathbb{F}_n^s = \int_{\Omega_s^e} \mathbf{q}\mathbf{N} dV$$

$$\mathbb{F}_n^g = \int_{\Omega_g^e} \mathbf{q} N_0^{\mathbf{g}} \mathbf{N} dV$$

$$\mathbb{M}^s = \int_{\Omega_s^e} \mathbf{N}^{\mathbf{T}} \mathbf{N} dV$$

$$\mathbb{M}^g = \int_{\Omega_g^e} \mathbf{N}^{\mathbf{T}} \mathbf{N} dV$$

$$\mathbb{D}^s = \int_{\Omega_s^e} \mathbf{D_s} \nabla \mathbf{N}^{\mathbf{T}}.\mathbf{N} dV$$

$$\mathbb{D}^g = \int_{\Omega_g^e} \mathbf{D_g} \nabla \mathbf{N}^{\mathbf{T}}.\mathbf{N} dV + \int_{\Omega_g^e} \nabla.(\mathbf{u}\mathbf{N}^{\mathbf{T}}) dV \quad + \int_{\Gamma_D} k_c(C_0 H(t-\varepsilon) - \mathbf{N}^{\mathbf{T}}) \mathbf{N} dS$$

and **N**denote the linear interpolation function at each bode. By using the assembly theory for all subdomains, we have:

$$\mathsf{U}_{e=1}^m \begin{bmatrix} \widetilde{\mathbb{M}}^s & 0 \\ 0 & \widetilde{\mathbb{M}}^g \end{bmatrix}^e \begin{pmatrix} \mathbf{C}_{n+1}^s - \mathbf{C}_n^s \\ \mathbf{C}_{n+1}^g - \mathbf{C}_n^g \end{pmatrix}^e + \mathsf{U}_{e=1}^m \Delta t \begin{bmatrix} \widetilde{\mathbb{D}}^s & h_0 \\ h_0^{-1} & \widetilde{\mathbb{D}}^g \end{bmatrix}^e \begin{pmatrix} \mathbf{C}_n^s \\ \mathbf{C}^g \end{pmatrix}^e = \mathsf{U}_{e=1}^m \Delta t \begin{pmatrix} \widetilde{\mathbb{F}}_n^s \\ \widetilde{\mathbb{F}}_n^g \end{pmatrix}^e \quad (10)$$

where

$$\widetilde{\mathbb{M}}_{ij}^{s,g} = \sum_{ij}^{p_nodes} \mathbb{M}_{ij}^{s,g}, \widetilde{\mathbb{D}}_{ij}^{s,g} = \sum_{ij}^{p_{nodes}} \mathbb{D}_{ij}^{s,g}, \widetilde{\mathbb{F}}_j^{s,g} = \sum_{j}^{p_nodes} \mathbb{F}_j^{s,g}$$

By considering this switch conditions, the matrix components in (10), can be written:

$$\mathbb{F}_n^s = \int_{\Omega_s^e} \mathbf{q}\mathbf{N} dV$$

$$\mathbb{F}_n^g = \int_{\Omega_g^e} \mathbf{q} N_0^{\mathbf{g}} \mathbf{N} dV$$

$$\mathbb{M}^s = \int_{\Omega_s^e} \mathbf{N}^{\mathbf{T}} \mathbf{N} dV$$

$$\mathbb{M}^g = \int_{\Omega_g^e} \mathbf{N}^{\mathbf{T}} \mathbf{N} dV$$

$$\mathbb{D}^s = \int_{\Omega_s^e} \mathbf{D_s} \nabla \mathbf{N}^{\mathbf{T}}.\mathbf{N} dV$$

$$\mathbb{D}^g = \int_{\Omega_g^e} \mathbf{D_g} \nabla \mathbf{N}^{\mathbf{T}}.\mathbf{N} dV + \int_{\Omega_g^e} \nabla.(\mathbf{u}\mathbf{N}^{\mathbf{T}}) dV + \int_{\Gamma_D} k_c \mathbf{N}^{\mathbf{T}} \mathbf{N} dS$$

III. Some Results and Discussions

This section presents the validation of the model with experiment data. We provide a thorough illustration and discussion of the model results corresponding to the application in industrial conditions. The industrial condition of AMCs cross contamination needs to switch the boundary condition Dirichlet-Neumann. In practice, this method is defined as the contaminant concentration increase to the maximum value during the contamination time, and when the contamination time is finished, the wafer area is considered as a neutral area.

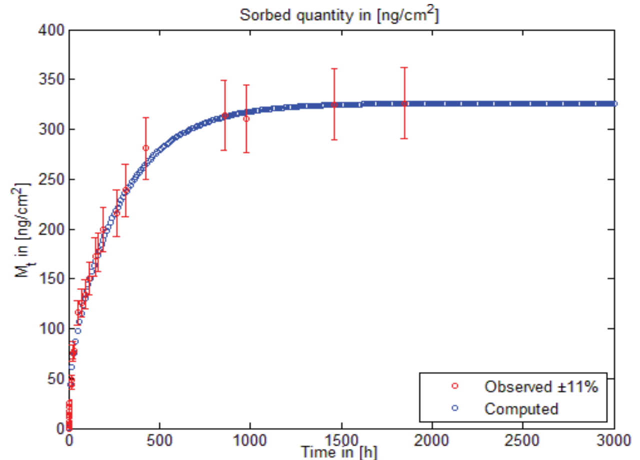

Fig. 2 Sorbed quantity for the contaminant XC1: validation of the model with the experiment data

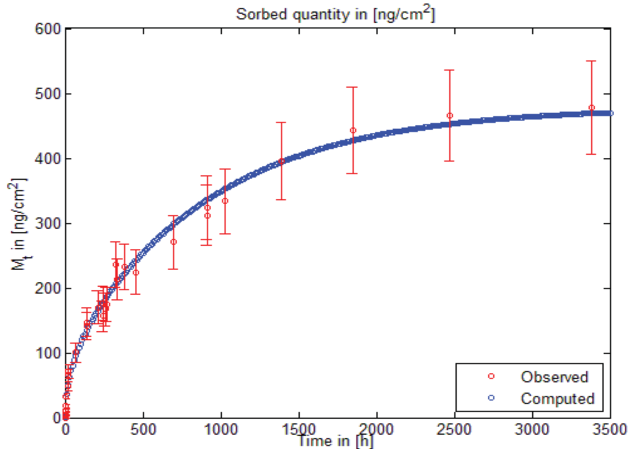

Fig. 3 Sorbed quantity for the contaminant XC2: validation of the model with the experiment data

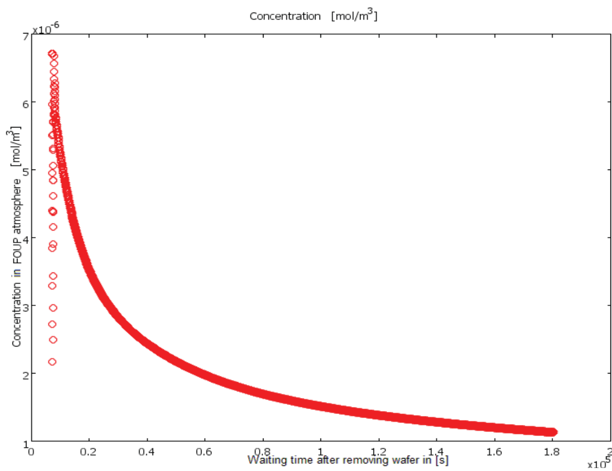

Fig. 4 Outgassing process after removing FOUP, contaminant moves from FOUP's surface to atmosphere

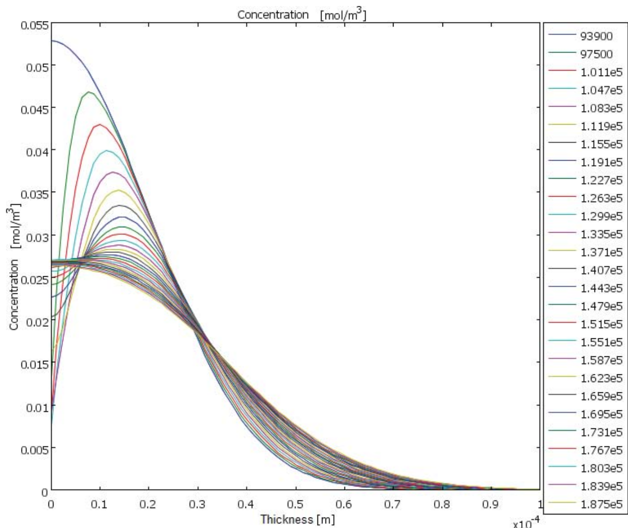

Fig. 5 Outgassing process after removing wafer, cleaning effect after purging FOUP with an inert gas

IV. Conclusions

A general numerical tool illustrates a mathematical model of the AMCs cross contamination between wafers post processed and the FOUP has been developed. The basic model is obtained by the convection diffusion and diffusion equations. An interface condition is established to connect the concentration in air (at the FOUP's atmosphere) and the concentration at the internal surface of the FOUP (polymer). This interface condition is developed according to the Henry law, in order to takes into account of the surface topography and the kinetic law at the interface. Analytical solution is presented for a simple model. Numerical formulation is developed for the AMC, stability and convergence study are detailed and parameter sensibility analysis. The coupled partial differential equations together with the appropriate boundary conditions are numerically solved with Comsol multiphysics software.

We have proposed a simplified model for AMCs cross contamination and discuss some results and its correlation with experimental data. The diffusion coefficient is fitted with the experimental data. We observe good correlation between theoretical results and observed data.

It reveals that the sorbed quantity in the thin membrane (measurement obtained by using the reactor) of the polymer fits the purely diffusive model already established by [10]. In such case, the kinetic law and the solubility are not yet taken into account. For some material and some contaminant, the simple model remains valuable and gives a good correlation, but for other contaminant such is not the case. Our AMCs model can give general solution for the behavior of each contaminant; because we take into account the main parameter with may induce a significant change in the solutions (surface topography and kinetic law). Then for each contaminant responsible of the AMCs cross contamination, we have a powerful model; the first one is to evaluate the diffusion coefficient by optimization method, and the second one is to qualify the dynamics of the AMC cross contamination between wafer and FOUP. The model is calibrated for each polymer and for many level of the contamination.

The model has been tested by 17 cases for the couple (contaminant/polymer), and 90% of the behavior has a good correlation between the model (theoretical solutions) and the data (experiment measurement). The rest of the test i.e. 10\% has no appropriate correlation, and by using the model an optimum diffusion coefficient has been obtained for many data. We have shown that we have good information of the adsorption capacity for each polymer. Many polymer adsorbs easily and desorbs easily too, but it depends on the type of the contaminant. A brief study which simulate the reversible desorption has been performed in order to determine the critical time needed to desorbs the contaminant already sorbed.

This model remains reliable and we can use it with industrial conditions of the utilization of the FOUP. The entire model has been solved numerically by Comsol multiphysics (software able to solve a coupled partial differential equation). The temperature effect is not yet taken into account in this

model. The exploitation of the boundary condition switching from Neumann to Dirichlet and the quantification of the reversible and irreversible diffusions will be developed in the AMCs cross contamination applications.

Now we are able to fit and to determine the diffusion coefficient of each contaminant responsible of the AMC characterization with a reliable model. For the two mainly contaminants (XC1 and XC2) responsible of the AMCs in general in microelectronic industry, a simple model has been proposed. The model is stable and has been tested with many cases for utilization in order to valid his performance. The general model still consistent in FOUP scale but it needs the value of the velocity during the purge and the decontamination steps. As classical finite element method, a minimum size of the mesh is needed in order to ensure the stability, because the diffusion coefficient of the contaminant is very small.

It should be mentioned that the present simple model have its limitations, this model is not appropriate to describe the adsorption of the particular case, and then we need to add the interface condition to take into account the surface topography and the kinetic law.

There are also important questions that must be addressed through testing, including how often and at what points during the transport process FOUPs are needed to be purged to maximize their effectiveness at preventing contamination. A cooperative effort between suppliers of FOUPs, process tools, and automated material-handling systems are needed in order to adopt and benefit from this proposed design feature.

NOMENCLATURE

$\nabla.$: Divergence operator
∇ : Gradient operator
h_0 : Henry constant
$\mathbf{u}$: Contaminant velocity
$\mathbf{q}$: Source
$\mathbf{D}_s$: Diffusion coefficient in polymer
$\mathbf{D}_g$: Diffusion coefficient in internal FOUPs atmosphere
$\mathbf{Q}^{the}$: Experimental sorbed quantity of the contaminant in polymer
$\mathbf{Q}^{exp}$: Computed quantity of the contaminant in polymer
C^s : Concentration in polymer
C^g : Concentration in internal FOUPs atmosphere
C_0 : Concentration on the wafer area
$\mathbf{n}$: Outer unit normal vector
N_0^g : Inlet concentration ux
$H(t-\varepsilon)$: Heaviside function with delay ε
Ω_s : Polymer domain
Ω_g : Contaminant domain
AMCs : Airborne Cross contamination
FOUP : Front Opening Unified Pod
B.C : Boundary Condition
I.C : Initial Condition
AFM : Atomic Force Microscopy
REV : Representative Elementary Volume

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