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Abstract—It is considered the mathematical models design of clean rooms. It is defined the structure of mathematical models and suggested the algorithm of pollution dynamics modeling on based of finite elements method.

Index Terms—Clean rooms; mathematical models; finite elements method.

I. INTRODUCTION

In semiconductor manufacture among all processes included in a wafer processing it is required the most rigid control of air purity at the workplace.

Since the main contribution to the pollution of the environment in clean room manufacture (CRM) is accounted for the operator and process equipment, there is a necessity of local clean volumes, free from human presence. Thus the major air pollutant becomes an atmospheric aerosol which was missed by the high purity filter, i.e. the fraction of submicron aerosol.

Only hygroscopic (hydrophilic) particles are able to increase its size with increasing relative humidity ϕ . Therefore it is important to analyze the nature of aerosol particles which are present in clean rooms, their origin, as well as their impact on the quality of microelectronic products.

The particles, formed by mechanical friction, can remain after the grinding of silicon wafers. The micro particles are formed in air guide networks because of erosion of the inner pipe surface as well as the air flow may comprise solid particles of salts formed in the irrigation chamber at the contact of air with water [1]. Minor decrease of density in fine air filters can greatly reduce their effectiveness. Powerful source of technologically very dangerous aerosol are leaking exhaust system oil.

Intensity of oil mist generation consisting of droplets ranging in size from 0.01 to several microns, is very high. Generators of aerosol particles are all moving and friction knots, joints, control elements, a places subjected to thermal shock and vibration. The main source of aerosol particles is a human. The micro particles in 60 % of cases are the cause of defect, of which the share accounted for man is 40 %.

As impurities in the air of the room may present different gases in the residual amount, as well as a

pairs of chemicals and organic solvents. Large molecules of gases such as NO₂, H₂S also cause contamination during wafer processing. At a concentration of oxidant about 10⁻⁵ % on unexposed areas during photolithography process photo resist areas are observed. This is the result that in a negative resist and unexposed areas the cross-linking reaction is also developed.

Depending on the chemical properties of the micro particles a serious impediment can be both large and ultrafine particles. The required purity of the air, corresponding to a given class CRM exists only at a certain height from the final filter to the place of wafer processing. During the dust generation indoors large particles fall down, and small scatter in different directions and, if not picked up by the flow of conditioned air, are accumulates in stagnant zones of CRM.

Water micro droplets presented in air can absorb soluble gases (SO₂, NO) and the oxidant (H₂O₂ ozone) which react in a liquid phase with the production volatile substances.

II. THEORY OF CONDENSATION GROWTH OF AEROSOL PARTICLES UNDER SATURATION CONDITIONS

Solutions of condensation droplet growth problem are studied in [2] – [4] and many others [5] – [14].

The system of equations describing the transport of heat, steam and drops growth, or droplet with $r < 30$ micron evaporation can be represented as:

$$\frac{\partial \rho}{\partial t} = D_n \Delta \rho; \quad \frac{\partial T_i}{\partial t} = \chi_i \Delta T_i;$$

$$\frac{\partial m}{\partial t} = 4\pi r^2 D_n \left. \frac{d\rho}{dr} \right|_{r=R},$$

where ρ , D_n are the density and the diffusion coefficient of the pair respectively; T_i , χ_i are temperature,

thermal diffusivity of air ($i = 1$) and of liquid ($i = 2$); m is the mass of the droplet surface.

Equation must be solved under the following conditions:

$$\begin{aligned} \rho &= \rho_\infty, T_1 = T_\infty \quad \text{at } r \rightarrow \infty; \\ \rho &= \rho_0, T_1 = T_2 = T \quad \text{at } r = R; \\ \left(LD_n \frac{\partial \rho}{\partial r} + k_1 \frac{\partial T_1}{\partial r} + k_2 \frac{\partial T_2}{\partial r} \right) \Big|_{r=R} &= 0, \end{aligned}$$

where L is the heat of condensation; k_1 and k_2 are the coefficients of thermal conductivities of air and

water, respectively; $\chi = \frac{k}{\rho c_p}$, where c_p is specific heat of a substance.

However, this system also in practical calculations leads to a rather complex mathematical calculation. Further simplification can be done if the external conditions (temperature, pressure) are changing very slowly, using the so-called quasi-stationary approximation.

The drop growth in the atmosphere can be considered quasi-stationary approximation, not taking into account the internal and external convection and taking into account as an amendment temperature jump at the drop surface and concentration jump.

In this case, the equation of droplet growth can be presented in the following form:

$$\frac{\partial R}{\partial t} = \frac{D_n}{\rho_2 R} f_1(R, l) [\rho_\infty - \rho_0(R, T, c)],$$

where c is the concentration of the solution; f_1 is amendment to the kinetic regime.

Decreasing of the vapor pressure is caused by the presence of the solute in the droplet.

Saturated vapor pressure above the drop of the solution can be represented as:

$$\begin{aligned} p_0(R, T, c) &= p_0(R, T) [1 - \Phi(c)] = \\ &= p_0(T_n) [1 - \Phi(c)] \exp \left[\frac{L}{R_n T_\infty} + 2 \frac{\sigma}{\rho_3 R_n T R} \right], \end{aligned}$$

where c is the concentration of the solute; $\Phi(c)$ is function characterizing the pressure decrease.

$$\sigma = \sigma_0 \left(1 + \frac{a}{R^3} \right),$$

σ is the surface tension of the solute; σ_0 is surface tension of pure water; a is a certain coefficient.

Define $\Delta T = T - T_\infty$.

This factor can be regarded as a not very significant and confine account $\Phi(c)$.

The quantity $\Phi(c)$ taking into account electrolytic dissociation subject can be written as follows:

$$\Phi(c) = \frac{im_c M}{\left(\frac{4}{3} \pi \rho_p R^3 - m_c \right) M_c} = \frac{iM_c}{(\rho_p - c) M_c},$$

where m_c and M_c are weight and the molecular weight of the solute; M is molecular vapor weight; c is the concentration of the solute substance, g/sm³; ρ_p is a density of the solution; i is Van't Hoff factor characterizing the degree of dissociation of the solute, which depends on the concentration and temperature.

For dilute solutions of the Van't Hoff factor taken equal to a constant value, which is determined by the number of ions formed by the dissociation of one molecule (for NaCl – $i = 2$, for CaCl₂ – $i = 3$ etc.). As condensation nucleus contain a mixture of solutes, B. Meyson [4] suggests that for all nucleus we can take the number $1 = 2.22$.

In [9], the following empirical formula for $\Phi(c)$ is determined:

$$\Phi(c) = \frac{a}{\frac{R^3}{R_0^3} - b} = \frac{ac}{\rho_c - bc},$$

where ρ_c – the density of the salt; R_0 – radius drops of a saturated solution; a and b – some constants.

In [13], a numerical solution of the problem. In it, unlike the previous work accounted Kelvin effect, the latent heat of condensation and dissolution effects. The method does not account for the coagulation, sedimentation and the presence of sources. Solution of the system of differential equations is obtained by “moving section”. Domain size of aerosol particles is divided into n classes, each of which can move with time. The results of calculations performed for the same conditions as in the previous case.

It is clear that within thousandths of a second from the beginning of the process (i.e., almost instantaneously) a dramatic increase in the smallest fraction of the aerosol (more than an order of magnitude), then it is as if the redistribution of moisture due to the capture cross a larger particle size. This shows the danger of sharp fluctuations in humidity, which can cause immediate sharp rise in some of the aerosol particles.

To determine the droplet growth with reasonable accuracy in practical calculations using the Langmuir equation:

$$t = \frac{\rho RT (d^2 - d_0^2)}{8DM(\rho_\infty - \rho_0)} = \frac{\rho RT (d^2 - d_0^2)}{8DM\rho_\infty(1 - \delta)}, \quad (1)$$

where δ is the degree of supersaturating; D is diffusion coefficient; M is molecular weight of the solute in gram moles.

Taking into account the clarification given by Fuchs [2], (1) can be written as:

$$t = \frac{\rho RT}{DM\rho_\infty} \left[\frac{d^2}{8} + \frac{dD}{2\alpha v_x} - \frac{\Delta}{2}d + \Delta^2 \ln \left(\frac{d + 2\Delta}{2\Delta} \right) \right],$$

where Δ is the distance that the evaporating molecule must pass before its collision with a gas molecule

$$\Delta = \lambda \left(\frac{m_1 + m_2}{m_1} \right)^{\frac{1}{2}},$$

α (water) = 0.034; m_1 and m_2 are the mass of the gas molecules and vapor, respectively; λ is the

mean free path of the gas molecules; $v_x = \left(\frac{kT}{2\pi m_2} \right)^{\frac{1}{2}}$.

The estimate of the characteristic time of establishing equilibrium between the drop of the solution to the equilibrium radius and its environment given in [13]. It showed, for not very low super saturation or under saturation $|\delta|$:

$$\tau = 0,4k_3 \frac{r^2}{|\delta|};$$

$$k_3 = \frac{D_v \rho_v}{\left[1 + \frac{D_v \rho_v L_v}{\chi T} \left(\frac{L_v}{R_v T} - 1 \right) \right] \rho_f},$$

where D_v – a vapor diffusion coefficient; ρ_v – a vapor density; L_v – the heat of vapor condensation of vapor; R_v – vapor gas constant; χ – the thermal diffusivity of air; T – air temperature; ρ_f – density of the fluid is formed by condensation of vapor.

It is defined, that $k_3 = 10^{-6} \text{cm}^2 \cdot \text{c}^{-1}$ for water vapor under normal conditions. For these conditions, the ratio becomes:

$$\tau = 4 \cdot 10^{-5} r^2 / |\delta|.$$

In an atmosphere with a relative humidity values of the temperature change processes; and hence the humidity, occur slowly enough. Therefore, the study

of submicron particles with sizes of atmospheric aerosol sprays can always be considered in equilibrium.

III. MATHEMATICAL DESCRIPTION OF HEAT AND MASS TRANSFER PROCESSES

As shown above, the condensing increasing of particles is connected with changes in relative humidity. This change can be observed not only in the air entering the clean room from the outside, but a certain gradient of relative humidity change takes place in the room due to the changes of temperature fields, pressure, partial pressure of vapor in the presence of air flow.

All the pattern of distribution of heat and humidity fields in the room can be described by the following system of differential equations:

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + \frac{1}{\rho} \frac{\partial p}{\partial x} &= 0; \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} - \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + \frac{1}{\rho} \frac{\partial p}{\partial y} &= 0; \end{aligned} \quad (2)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0;$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} - a \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) = \frac{I_q}{c_p \rho};$$

$$\frac{\partial p_{10}}{\partial t} + \frac{\partial p_{10}}{\partial x} + v \frac{\partial p_{10}}{\partial y} - D_{10} \left(\frac{\partial^2 p_{10}}{\partial x^2} + \frac{\partial^2 p_{10}}{\partial y^2} \right) = I_0,$$

here u and v – the velocity components along x and y ; p – a pressure; T – a temperature; $p_{10} = p_1/p$ – a relative partial pressure of vapor; ρ – a density of the air; ν – a kinematic viscosity of air; a – a thermal diffusivity of air; D_{10} – a diffusion coefficient of water vapor; c_p – a heat capacity; I_q and I_0 – sources.

First equations (Navier-Stokes equations) describe the motion of a viscous incompressible medium in the space (and the continuity equation of conservation of momentum). The last two characterize the distribution of temperature and relative partial vapor pressure, i.e. thermohygrometric field clean room.

The first three equations uniquely determine the velocity and pressure and can be considered as a separate system. Thus when determining the pressure it is arose some difficulties that can be avoided by applying the algorithm Poisson for pressure.

In solving of this equations system is convenient to execute the following transformations. Differen-

tial members in the system are transformed by summation of first two equations into equalities

$$\frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) = 0; \quad \frac{\partial}{\partial y} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) = 0.$$

Then we obtain the system:

$$\frac{\partial u}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial u}{\partial y} - \nu \left(2 \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 v}{\partial x \partial y} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial x}; \quad (3)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} - \nu \left(\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial x^2} + 2 \frac{\partial^2 v}{\partial x^2} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial y}. \quad (4)$$

Differentiating with respect to x and y and adding the resulting expression, we obtain for the pressure Poisson equation of the form

$$\frac{1}{\rho} \nabla^2 p = - \left[W^2 + U \frac{\partial w}{\partial x} + V \frac{\partial v}{\partial y} + 2 \left(\frac{\partial v}{\partial x} \frac{\partial u}{\partial y} - \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} \right) \right] + 2\nu \nabla^2 W - \frac{\partial w}{\partial t},$$

where

$$W = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}$$

members

$$w^2 + u \frac{\partial v}{\partial x} + v \frac{\partial u}{\partial y} \text{ and } 2\nu \nabla^2 w,$$

can be neglected and write the equation in the form

$$\nabla^2 p = - \left[\frac{\partial w}{\partial t} + 2 \left(\frac{\partial v}{\partial x} \frac{\partial u}{\partial y} - \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} \right) \right]. \quad (5)$$

Equations (3), (4), (5) together allow us to determine the unknown.

Analytical solutions of such a system does not exist, so there are different numerical methods for solving systems of differential equations (finite difference or finite element).

In this paper, the solution of this problem is obtained using the finite element method.

IV. ALGORITHM FOR SOLVING THE PROBLEM OF HEAT AND MASS FINITE ELEMENT METHOD

The finite element method is that any continuous value can be approximated by a discrete model, which is based on the set of piecewise continuous functions defined on a finite set of subdomains or elements.

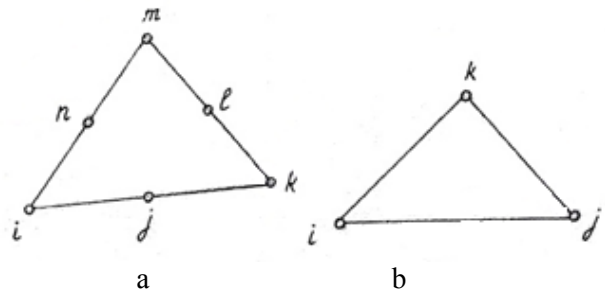
Sequence of construction of the discrete model is as follows:

1. The area under consideration is fixed in a finite number of points (nodes). Meaning uninterrupted value at each node is considered variable.

2. Continuous domain of values is partitioned into a finite number of subdomains that have common nodes and collectively approximate the shape of the region.

3. Continuous value is approximated by a polynomial on each element of which is determined by the nodal values of this quantity. For each item, its polynomial chosen so as to maintain continuity of values along the boundary.

Since we solve the planar problem, as adopted by the finite element second-order triangular element having six nodes (Figure, a).



Triangular finite element: a is the quadratic; b is linear

Nodal values of a scalar φ is denoted $\Phi_i, \Phi_j, \dots, \Phi_n$ and the coordinates of these nodes – $(X_i, Y_i), (X_j, Y_j) \dots (X_n, Y_n)$.

Interpolating the polynomial for a quadratic triangle has view:

$$\varphi = a_1 + a_2x + a_3y + a_4x^2 + a_5y^2 + a_6xy. \quad (6)$$

The nodes of the following conditions:

$$\begin{aligned} \varphi &= \Phi_1 \text{ at } x = X_1, y = Y_1; \\ &\dots\dots\dots; \\ \varphi &= \Phi_n \text{ at } x = X_n, y = Y_n. \end{aligned}$$

Substituting (2) into (3) leads to a system of six equations with unknowns $a_1 \dots a_6$. Solving the system and substituting the resulting values in (6), we write the polynomial in the form:

$$\varphi = N_i \Phi_i + N_j \Phi_j + \dots + N_n \Phi_n,$$

where N_1, N_2, N_n are some algebraic function of x and y , called shape functions of this element. In matrix for mexpression canbewrittenasfollows:

$$\varphi = [N] \{\Phi\}.$$

Derived from φ to x and y have the form:

$$\frac{\partial \varphi}{\partial x} = \frac{\partial N_i}{\partial x} \Phi_i + \frac{\partial N_j}{\partial x} \Phi_j + \dots + \frac{\partial N_n}{\partial x} \Phi_n;$$

$$\frac{\partial \varphi}{\partial y} = \frac{\partial N_i}{\partial y} \Phi_i + \frac{\partial N_j}{\partial y} \Phi_j + \dots + \frac{\partial N_n}{\partial y} \Phi_n.$$

Orinmatrixform:

$$\frac{\partial \varphi}{\partial x} = \frac{\partial [N]}{\partial x} \{\Phi\},$$

$$\frac{\partial \varphi}{\partial y} = \frac{\partial [N]}{\partial y} \{\Phi\}.$$

Interpolation relations conveniently written in the coordinate system associated with the element. For the triangular element is the most common local coordinate system defined by three relative coordinates L_1, L_2, L_3 . Each coordinate is the ratio of the distance from the selected point of the triangle to one of its sides to the height, pubescent on this side of the opposite vertex. The values of these coordinates vary from "0" to "1". Obviously these coordinates are not independent, they satisfy

$$L_1 + L_2 + L_3 = 1.$$

Shape functions for the quadratic elements have the form:

$$N_i = L_1(2L_1 - 1);$$

$$N_j = 4L_1L_2;$$

$$N_k = L_2(2L_2 - 1);$$

$$N_l = 4L_2L_3;$$

$$N_m = L_3(2L_3 - 1);$$

$$N_n = 4L_1L_3.$$

To compute the partial derivatives of

$$\frac{\partial N_\beta}{\partial x} \quad u \quad \frac{\partial N_\beta}{\partial y} \quad (\beta = i, j \dots n).$$

Use the Jacobi matrix coordinate transformation. Jacobi matrix has the form:

$$[I] = \begin{bmatrix} \frac{\partial x}{\partial L_1} & \frac{\partial y}{\partial L_1} \\ \frac{\partial x}{\partial L_2} & \frac{\partial y}{\partial L_2} \end{bmatrix},$$

Then

$$\begin{Bmatrix} \frac{\partial N_\beta}{\partial L_1} \\ \frac{\partial N_\beta}{\partial L_2} \end{Bmatrix} = [I] \begin{Bmatrix} \frac{\partial N_\beta}{\partial x} \\ \frac{\partial N_\beta}{\partial y} \end{Bmatrix},$$

Thus, to obtain the derivatives:

$$\begin{Bmatrix} \frac{\partial N_\beta}{\partial x} \\ \frac{\partial N_\beta}{\partial y} \end{Bmatrix} = [I] \begin{Bmatrix} \frac{\partial N_\beta}{\partial L_1} \\ \frac{\partial N_\beta}{\partial L_2} \end{Bmatrix},$$

For the pressure p as the final element uses a linear simplex element with three nodes (Figure, b). Interpolating polynomial for it have the form:

$$\varphi = a_1 + a_2x + a_3y.$$

Shape function, in contrast to the quadratic element, expressed in terms of L is coordinates presented expressions:

$$M_i = L_1; \quad M_j = L_2; \quad M_n = L_3.$$

Derivative forms of the functions of x and y are determined by the same procedure as for the quadratic element.

V. CONCLUSION

Improved integration of VLSI imposes more stringent requirements for air quality (number of dust, temperature and humidity) in clean rooms. Transition to clean local volumes, allowing to exclude contamination introduced by the operator and the equipment, leads to the fact that the main source of atmospheric aerosol pollution becomes. Mathematical modeling of the internal environment of the clean room, conducted using a known system of differential equations of heat and mass, allows the characterization of the velocity distribution of the air temperature. Relative partial pressure of water vapor in the room.

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В. М. Синєглазов, В. М. Федосенко, К. М. Радько. Побудова математичних моделей динаміки забруднень в «чистому приміщенні»

Розглянуто побудову математичних моделей забруднень в «чистому приміщенні». Визначено структуру математичних моделей і запропонований алгоритм моделювання динаміки забруднень на основі методу кінцевих елементів.

Ключові слова: чисті приміщення; математичні моделі; метод кінцевих елементів.

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В.М. Синеглазов, В.Н. Федосенко, Е.Н. Радько. Построение математических моделей динамики загрязнений в «чистом помещении»

Рассмотрено построение математических моделей загрязнений в «чистом помещении». Определена структура математических моделей и предложен алгоритм моделирования динамики загрязнений на основе метода конечных элементов.

Ключевые слова: чистые помещения; математические модели; метод конечных элементов.

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