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MODELING OF CONCENTRATION PROFILE OF CHARGE CARRIERS IN INHOMOGENEOUS EPITAXIAL LAYERS

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The new approach to the construction of the microtechnology physical-technological models is proposed in the present work. This approach allows us to analyse the processes of the IC and hybride IC epitaxial, resistive and conductive structures growth and formation of their electrophysical and mechanical parameters. We elaborated the model describing charge carriers concentration profile of inhomogeneous epitaxial structures that were grown under different technological conditions.

INTRODUCTION

In IC and semiconductor devices production which based on epitaxial layers it is necessary to make defined charge carriers concentration profiles in the semiconductor structure. It is particularly important in heteroepitaxial system growth. The use of physical-technological models which adequately describe charge carriers concentration profile being formed during film growth gives a possibility to predict many important parameters.

Simultaneously with the development of the traditional searching methods to guarantee the characteristics of the integrated circuits film layers, for example, methods of the search for the mathematical theory of the experiment, the methods of the film layers synthesys, based on the mechanisms and regularity of the charge transfer in the formalize multiphase heterogeneous and amorphous systems, representing idealize film structure models, are receiving wide spreading. This methods are based on the physical-technological models of the technological processes, connecting the integrated circuit electrophysical characteristics with materials properties, technological regimes and constructive parameters of the IC elements.

MODEL OF EPITAXIAL STRUCTURE GAS PHASE GROWTH

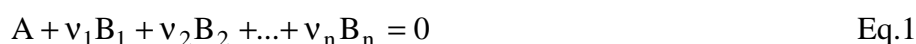
Epitaxial layers for microelectronics must be characterized by definite set of electrophysical parameters formed in the film growth process. At present there are many works dedicated to the growth processes of epitaxial films, but a general theory, allowing to model their properties adequatly and to operate the growth processes, is not yet developed. It is limited by both varied materials and technological processes, which are used for epitaxial growth, particularly, thermal and cathod vacuum deposition, molecular-beam epitaxy, gas phase deposition and solution and melting crystallization.

The elaborated physical-technological model of the growing of the epitaxial structures allows us to examine the gas phase growing processes of epitaxial and resistive films deposition in common methodological approach. This approach is based on creation of the data base of the technological processes, film and substrate materials, critical technological parameters system employment, with help of which working parameters of processes are standardized.

Epitaxial film is looked as layered structure and layers properties change in time gradually during the forming process and depend on external technological factors.

The transferring velocity of depositive material from reactor space to the substrate is dependent on the process type, reactor construction and dynamics of the equilibrium mixture motion in reactor. This process essence is in the diffusion mechanism of the components motion through boundary layer and it is described by diffusion kinetics. The diffusion to substrate take place simultaneously with the desorbed materials diffusion through the boundary layer from surface to the reactor space. Therefore, both these processes must be described within framework of the general diffusion task. Boundary layer thickness depends both from the velocity and character of the gas mixture transferring over the substrate and the gas viscosity.

The Curtis-Girschfelder diffusion differential equations system is solved for multy-components gas mixtures, accounting the diffusion coefficients changing for the great temperature gradients and various temperature profiles. Heterogeneous reaction on the substrate surface with thermodynamical equilibrium can be written in general form



Hereby, A is depositive component, B_i base gas components and ν_i - stoichiometric coefficients.

We assumed the exponential temperature distribution in the boundary layer which described by relation

$$T = T_0 \cdot e^{-ax} \quad \text{Eq. 2}$$

and for one-dimension task for gas components flows density follow expression was obtained

$$Q_k = \frac{\nu_k Q(\gamma - 1)}{R \cdot T \cdot [e^{(\gamma-1) \cdot a \cdot l} - 1]} \cdot \left[\frac{\nu_k}{m_k} + \sum_i^n \frac{\nu_i}{m_{ki}} \right] \ln \frac{P_{kl} \sum_i^n \frac{\nu_i}{m_{ki}} - \nu_k \sum_i^n \frac{P_{il}}{m_{ki}}}{P_{kl} \sum_i^n \frac{\nu_i}{m_{ki}} - \nu_k \sum_i^n \frac{P_{i0}}{m_{ki}}} \quad \text{Eq. 3}$$

where l - boundary layer thickness; T_0 - substrate temperature, K; R - gas constant; ν_i - binary gas coefficients at T_0 ; P_i - gas components partial pressure; n - number of gas components; $1.7 \leq \gamma \leq 2$.

Indexes 0,1 apply to substrate and boundary layer limit, correspondingly. Sums are solved for all $i \neq k$, and

$$m_k = \frac{1}{n-1} \cdot \sum_i^n \frac{1}{m_{ki}} \quad \text{Eq. 4}$$

Under these conditions film deposition velocity is regulated by diffusion flows in gas phase.

Surface processes at real conditions are realized followly, and, practically, may be looked as the first order heterogeneous reaction type



where K_1 , K_2 - velocity constants of the etching and crystallization reactions, correspondingly, $\nu_0' = 1/\nu_1$ and $\nu_2' = \nu_2/\nu_1$.

Therefore, accounting the surface reactions, velocity of growth or etching

$$V = \frac{M \cdot v_0'}{\rho} \cdot Q_{B_1} \quad \text{Eq. 6}$$

where M, ρ - molecular weight and depositive matter density, Q_{B_1} - flow of the base component B_1 to surface or in opposite direction, which is determined from Equation (3). Normal structure growth velocity can be written in form

$$V = \frac{M \cdot v_0'}{\rho} \cdot C_{B_1} \cdot k \cdot F \cdot e^{-\frac{W}{RT}} \quad \text{Eq. 7}$$

Hereby, C_{B_1} is concentration of base component B_1 near surface, W, k, F constants, which depend on process realization conditions.

ELECTROCONDUCTIVITY MODEL OF EPITAXIAL STRUCTURES

Electroconductivity is chosen as a modeled parameter because of the most informative characteristics of the epitaxial structure.

During the model development the coordinate system is chosen so that X -axis coincides with the direction of film growth and the beginning of the coordinate coincides with the lower wafer plane. Assume, that in optimal growth conditions the presence of microinhomogeneity of the film properties can be ignored.

Epitaxial layer has physically inhomogeneous structure and it may be conditionally layered on several regions - surface space charge region, epitaxial layer thickness with inhomogeneous impurity distribution directly and the region bordering with the wafer (transition layer). The latter is connected with analogous wafer region bordering with the epitaxial layer. This division for homoepitaxy is conventional but it reflects the process of structure formation. Analogous division may be realized for heteroepitaxial structures (such as GaAlAs/GaAs etc.). The homoepitaxial structure is monolithic, therefore the limit values for adjacent layers are identical, but for heteroepitaxial structure it is necessary to account influence of uncorrespondence lattices parameters d on limit conditions

$$d = \frac{a_i - b_i}{a_i} \quad i = 1, 2 \quad \text{Eq. 8}$$

where a_i, b_i - lattice parameters in coincides layers in i -direction.

Specific electroconductivity of a homogeneous substrate may be assumed to be dependent on temperature only and at constant conditions

$$\sigma_1 = \sigma_{01} \frac{y}{z} \left(H - \frac{1}{2} \right) \quad \text{Eq. 9}$$

where H - substrate thickness, l - transition layer thickness, σ_{01} - substrate specific electroconductivity.

Specific electroconductivity of the transition layer during constant doping level out of gas phase in the film growing process is determined by redistribution of impurities concentration at the expense of diffusion processes between the growing film and substrate, autodoping and numbers of initiating defects in crystal lattice. In the overwhelming majority of cases the transition layer conductivity is determined by the distribution of the dominant impurities in it, that is expressed as

$$\sigma_2 = q_x \int_{H-\frac{1}{2}}^{H+\frac{1}{2}} [N_1(x) + N_2(x)] \mu_n(x) dx \quad \text{Eq. 10}$$

where $N_1(x)$ - concentration function, described by the diffusion; $N_2(x)$ - concentration function, described by autodoping; $\mu(x)$ - function, which describe the charge carriers mobility in transition layer.

Charge carriers mobility depends not only from $N(x)$, but also from the structure defectivity. Epitaxial film specific conductivity external to transition layer is assumed as coordinates independent. If this assumption is not real, then epitaxial film may always be divided into layers, in which this interpretation is allowed, and the film conductivity may be considered as a sum of isolated layers conductivities

$$\sigma_3 = A \int_{H+L/2}^{H+h-1} \sigma_{03} dx \quad \text{Eq. 11}$$

where σ_{03} - epitaxial layer specific conductivity; L - thickness of layer, which is determined by the surface conductivity; H, h - thicknesses of substrate and epitaxial film.

For the L determination we use expression

$$L = B \cdot L_d \quad \text{Eq. 12}$$

where $B=4\div 5$ - coefficient, which allow to take into account the influence of surface conductivity on structure parameters and

$$L_d = \left(\frac{\varepsilon \varepsilon_0 kT}{q^2 n_i} \right)^{\frac{1}{2}} \quad \text{Eq. 13}$$

Here ε - relative dielectric material constant; ε_0 - vacuum dielectric constant; n_i - charge carriers concentration, determined by intrinsic conductivity.

Layer conductivity, connected with the space surface charge presence, is determined from the following expression

$$\sigma_4 = A \int_{H+h-1}^{H+h} \sigma_{04}(x) dx \quad \text{Eq. 14}$$

where $\sigma_{04}(x)$ - surface layer conductivity.

Value σ_{04} is determined by simultaneous solution of adiabatic equation and carriers distribution in surface charge field

$$\frac{\partial^2 \varphi}{\partial x^2} = - \frac{\rho_{ch}}{\varepsilon \cdot \varepsilon_0} \quad \text{Eq. 15}$$

at corresponding boundary conditions

$$\varphi(x = -0) = \varphi(x = +0) = \varphi_s > 0 \quad \text{Eq. 16}$$

$$\varepsilon_s \frac{\partial \varphi}{\partial x}(x = +0) - \varepsilon_p \frac{\partial \varphi}{\partial x}(x = -0) = qn_t \quad \text{Eq. 17}$$

$$\varepsilon_s \frac{\partial \varphi}{\partial x}(x = h) = qn \quad \text{Eq. 18}$$

$$\varphi(x \rightarrow \infty) = 0; \quad \text{Eq. 19}$$

where

$$\rho_{\text{ch}} = q((n - n(x)) - (p - p(x)) - N_a + N_d). \quad \text{Eq. 20}$$

Hereby, φ_s is surface potential; n_t - surface traps concentration and $\varepsilon_s = 11.9 \cdot \varepsilon_0$ i $\varepsilon_p = 3.9 \cdot \varepsilon_0$ dielectric constants of silicon and its oxid.

In Fig. 1 experimental and calculated by model charge carriers distribution profiles in transition layer of Si:P epitaxial structure are shown.

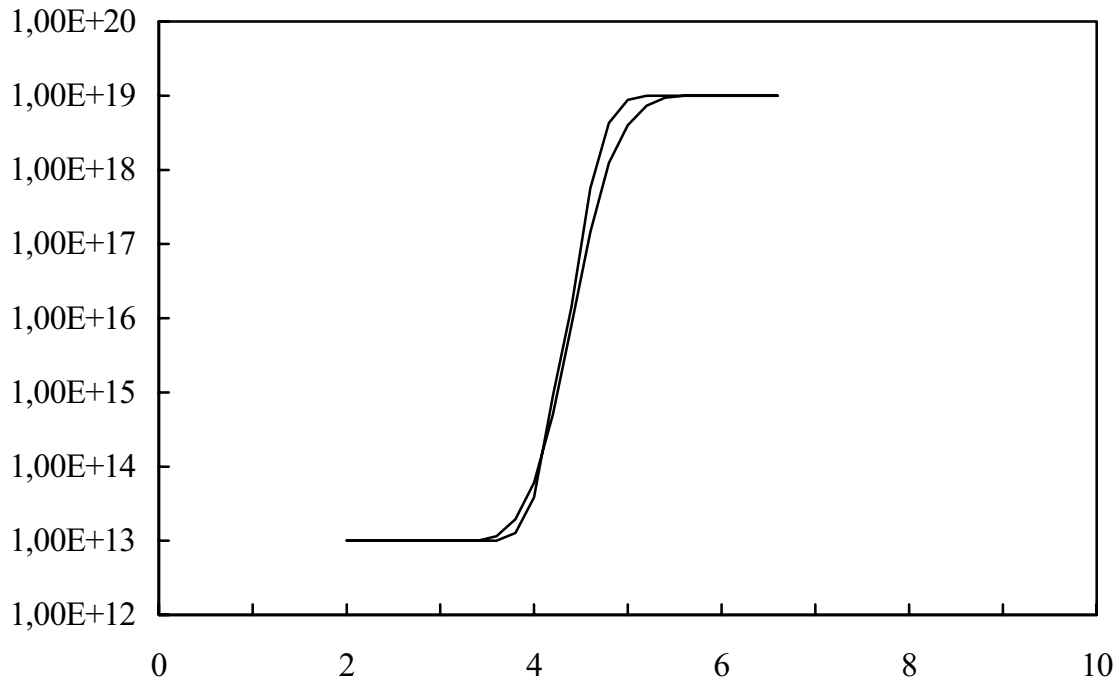


Fig. 1. Comparison between experimental and theoretical concentration profiles in Si:P structure: 1 - calculated by model; 2 - experimental

CONCLUSION

The physical-technological models of the IC thin-film layers fabrication and its characteristics, based on approach that film is looked as layered structure and layers properties change in time gradually during the forming process and depend on external technological factors, were developed.

This approach allows to analyse the processes of the IC and hybride IC epitaxial, resistive and conductive structures growth and formation of their electrophysical and mechanical parameters.

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