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PROCESS MODELING

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This contribution is intended to review the international state of the art in process modeling with particular emphasis on doping. Representative results for ion implantation into two- and three-dimensional structures are presented. Redistribution of dopants, interstitials and vacancies with fully coupled models are discussed. Local oxidation simulations of LOCOS structures and trench sidewalls demonstrate the inherent power of process simulation. Some remarks on the computational requirements are given.

1. INTRODUCTION

In the development of miniaturized devices for integrated circuits and particularly their technology, the demand for models being capable to predict the various processing steps of device fabrication is growing dramatically due to the tight coupling of electrical device effects with the doping profile. The utilization of computer aided simulation tools has proven to be invaluable in the development of new and/or improved processes due to their enormous complexity since modern processes for integrated circuits contain several hundred individual steps [17], [21], [26].

Device fabrication processes can be principally categorized into two groups. Lithographical processes which serve patterning purposes and doping processes which determine for a given structure the electrical properties of the intended semiconductor device. The first group consists of deposition and etching with spatial selectivity in order to enable structuring. It may be viewed as a fixed process which provides flexibility in layout. The second group is composed of ion implantation, annealing, diffusion, thermal oxidation and epitaxy. This contribution is intended to review the state of the art of some of the most relevant topics in process modeling. Particular emphasis is put on doping. Section 2 is primarily devoted to the simulation of Ion-Implantation. In Section 3 the diffusion of dopants is dealt with. In Section 4 some of the various details of the oxidation of silicon are discussed.

2. ION-IMPLANTATION

Ion-Implantation has developed into the most important doping technique for integrated circuits. To describe ion-implantation profiles methods based on distribution functions together with spatial moments have been used widely in the last two decades. The principle of these methods is to assume a functional type for the distribution function and to calculate its free parameters from its spatial moments [34]. These moments may be obtained either by experiments [31] or by theory [9], [20] [41].

The above sketched methods suffer in accuracy for complex targets [33]. Particularly for two and three-dimensional applications realistic range and damage results cannot be obtained. As reviews on these problems [32], [36] can be recommended. To overcome these shortages more accurate transport models based on the Boltzmann transport equation [10], [37] or Monte Carlo methods have to be applied where the individual ion trajectory is followed explicitly [3], [23]. Thereby an exact consideration of surface and interface shapes and a rigorous treatment of elastic scattering is possible. Furthermore they yield the full distribution function rather than a few moments of the distribution. The Monte Carlo method can also be extended to include the simulation of recoil cascades [24] and defect production [13], [39]. The only but major limitation of this method is its inherent demand on computational resources.

However, recent investigations,e.g. [12], show promising progress in algorithmic details to establish the Monte Carlo method for ion-implantation in industrial applications. Fig.1 shows the ion concentration normalized with respect to the implantation dose below a vertical mask edge for a 200keV boron implant into silicon obtained with a classical model based on the Pearson IV distribution function in depth direction and a convolution with a Gaussian distribution function using a constant lateral standard deviation in lateral direction. Fig.2 shows the same result obtained with a full Monte Carlo simulation. Fig.3 shows what one can obtain by enhancing the convolution in lateral direction with depth dependent lateral standard deviation and depth dependent lateral kurtosis. The agreement between Fig.3 and Fig.2 is remarkable. The difference in demands on computational resources is orders of magnitude in favor of the enhanced convolution [12].

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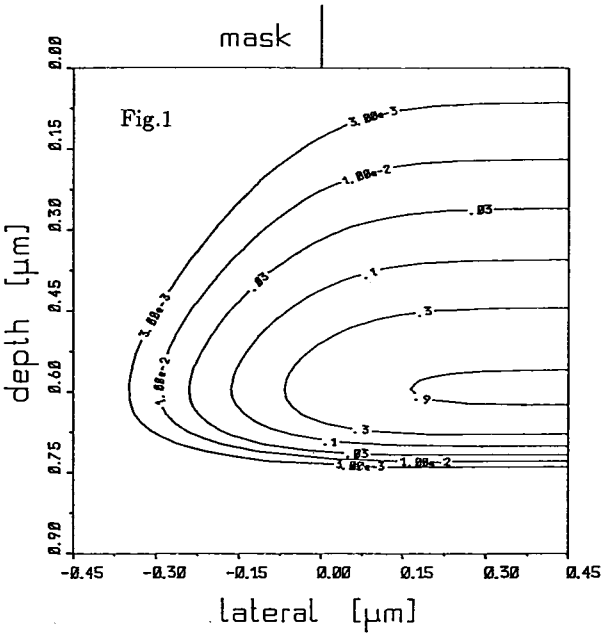
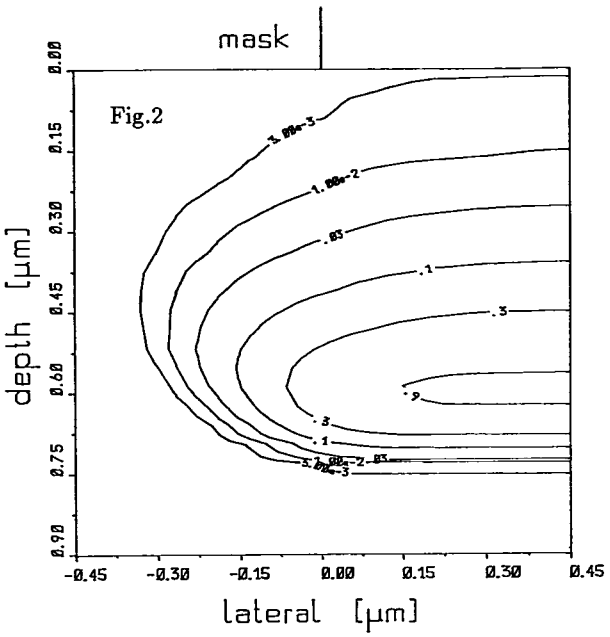




3. DIFFUSION

Diffusion is the physical mechanism which is responsible for the redistribution of impurity atoms. By means of diffusion processes one can obtain a desired shape of the distribution of dopants incorporated into the semiconductor by, e.g., ion implantation. As review on the problem [2] can be recommended. The diffusion of dopants in semiconductors is always treated by the two laws of Fick:

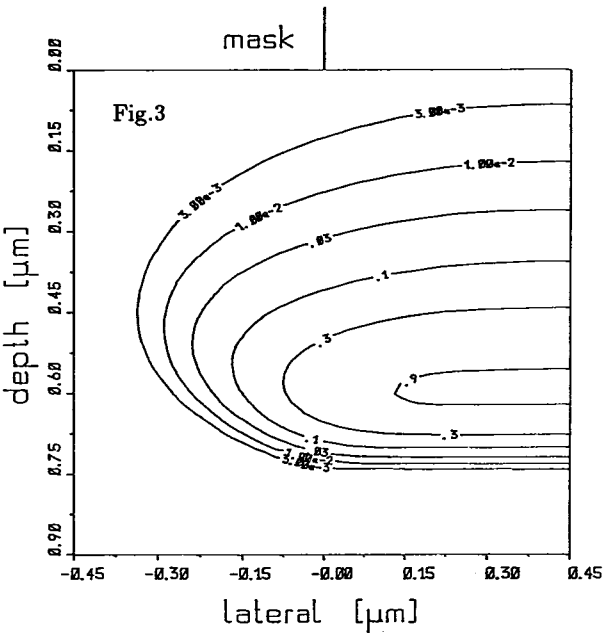
$$\vec{J}_i = -D_i \cdot (\operatorname{grad} Ct_i - Z_i \cdot \frac{q}{k \cdot T} \cdot Ce_i \cdot \operatorname{grad} \psi) \quad (1)$$

$$\frac{\partial Ct_i}{\partial t} + \operatorname{div} \vec{J}_i = 0 \quad (2)$$

For the i-th dopant Ct_i is the total concentration; Ce_i is the electrically active part of the concentration; Z_i is the charge state and ψ is the electrostatic potential.

All work in modeling has been involved in determining the nature of the effective diffusivity D_i. It can be assumed that dopants in silicon diffuse by interaction with point defects (vacancies, interstitials). Therefore it is of paramount importance to understand how these defect concentrations interact with the doping concentration and surface conditions.

The first model being established quite well for modeling the effective diffusivity has been proposed by Fair [7]. The effective diffusivity is broken up into a sum of diffusivities each of which is caused by the interaction between the dopants and the lattice vacancies with a specific charge state.



$$D_i = D_i^o + D_i^- \cdot CV^- + D_i^= \cdot CV^= + D_i^+ \cdot CV^+ \quad (3)$$

CV^x is the with respect to the neutral vacancy concentration normalized vacancy concentration with charge state x; superscript o stands for neutral, $-$ for singly negative charged, $=$ for doubly negative charged and $+$ for singly positive charged. The existence of vacancies with just these four charge states has been shown by Watkins [40]. The individual diffusivities in (3) are modeled temperature dependent with Arrhenius laws.

The normalized vacancy concentration can be estimated using the relative population statistics by Shockley and Last [35].

$$CV^{-} = \frac{n}{n_i}, \qquad CV^{=} = \left(\frac{n}{n_i}\right)^2, \qquad CV^{+} = \frac{p}{n_i} \quad (4)$$

The electrostatic potential ψ has to be obtained through a solution to the Poisson equation where in almost all cased the zero space charge approximation can be applied [15]. The electrically active part Ce_i of the concentration must be either estimated by static relations [11] or the solution of appropriate differential equations for the electrically active concentration [15].

Unfortunately does model (3) have difficulty when anomalous diffusion effects associated with surface injection of defects is considered. Of practical interest is the effect of the surface treatment on the distribution of point defects. Oxidation, nitridation and oxynitridation are all known to perturb the defect concentrations and therefore the dopant diffusivities. One of the best known phenomena is oxidation enhanced/retarded diffusion (OED/ORD) where silicon injected interstitials cause increased/decreased diffusion. Early attempts to account for OED/ORD where based on empirical corrections of the effective diffusivities by, e.g., a constant multiplier or an additive term [8], [38].

The present state of the art procedure for modeling effective diffusivities makes also use of an empirical relation.

$$D_i = D_i^o \cdot \left(f_I \cdot \frac{CI}{CI_{eq}} + f_V \cdot \frac{CV}{CV_{eq}}\right) \quad (5)$$

CI and CV denote the interstitial and vacancy concentration, respectively. It is assumed here that just vacancies of one specific charge state are relevant and the superscript has been dropped. The subscript eq indicates equilibrium values. f_I and f_V are simple fudge constants from the interval [0,1]. The problem has now been transferred to obtaining the interstitial and vacancy concentrations. These concentrations are believed to obey a standard continuity equation of the following form:

$$\frac{\partial CI}{\partial t} = \operatorname{div}(D_I \cdot (\operatorname{grad} CI) - R \quad (6)$$

$$\frac{\partial CV}{\partial t} = \operatorname{div}(D_V \cdot (\operatorname{grad} CV) - R \quad (7)$$

D_I and D_V are the diffusivities of interstitials and vacancies, respectively. They are usually modeled just temperature dependent with an Arrhenius law. R is the vacancy/interstitial recombination rate which is usually modeled very simply with (8) where K denotes a fit factor identified as bulk recombination parameter.

$$R = K \cdot (CI \cdot CV - CI_{eq} \cdot CV_{eq}) \quad (8)$$

Solutions to the differential equations (6) and (7) with appropriate boundary and initial conditions have now to be seeked. This can be accomplished by analytical approximations, e.g. [19], or fully numerically, e.g. [4], [5], [18], [28]. However, with some distant view to the problem one has to admit that there remain many open questions regarding the numerical values and the temperature dependence of the many coefficients and the appropriate formulation of the boundary conditions. A challenging alternative regarding the many problems associated with coupled point defect and impurity diffusion could be based on Monte Carlo methods simulating the motion of the respective point defects, i.e. vacancies and interstitials, together with the motion of the dopants. Some first attempts into this direction of research have been started with [1].

It is easily said to "solve" a system of partial differential equations in eventually two or three space dimensions. Practical implementation of such simulation programs, however, requires treatment of many subtle details. One particular problem is the appropriate discretization of the space and time domain. Fig.4 shows a simple simulation example, namely four snapshots of a coupled diffusion of a shallow arsenic implant and a deep boron implant. On the top of the figure the spatial mesh at the four snapshot times is drawn. This mesh is obtained with a fully adaptive procedure which equilibrates in a minimizing manner the local truncation error introduced through the transformation of a differential equation into a system of discrete equations.

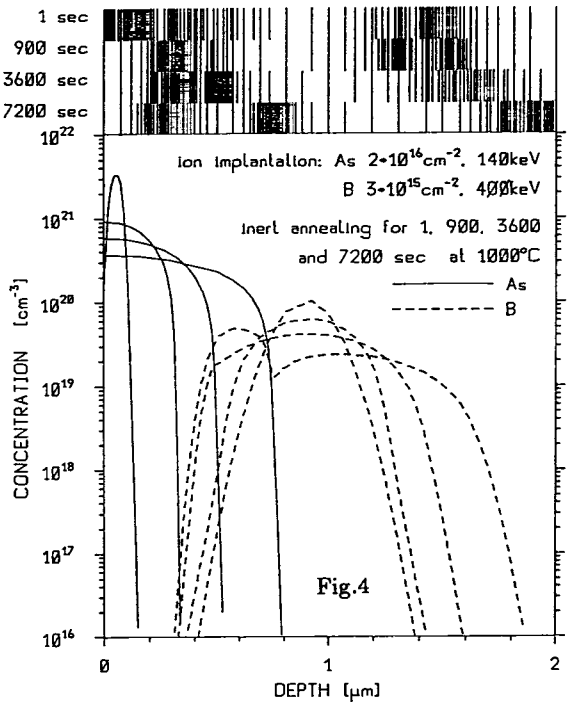


Fig.4

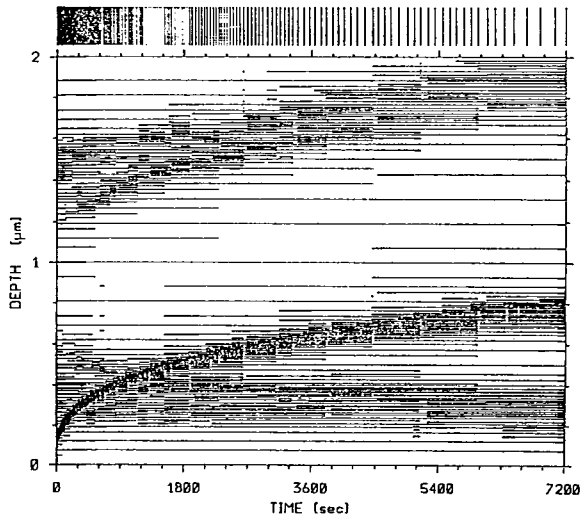


Fig.5

Fig.5 shows the evolution of the spatial mesh in time. It is necessary to follow the "gradients" of the profile to achieve an accurate solution. Taking an a priori mesh which is fine enough in the whole desired simulation time interval to guarantee an acceptably accurate solution would increase the demand on computer resources to indisputable values. The implementation of the adaptation procedure, however, requires brilliant people and regarding my personal experience lots of hours of cumbersome programming.

4. OXIDATION

In thermal oxidation oxidant from the gas phase diffuses in the form of O_2 molecules in the SiO_2 network toward the interface to form new SiO_2 material. This "growth" is convoyed by a significant volume change. At sufficiently high temperatures the reaction is assisted by visco-elastic flow of the oxide film toward the surface. As review on the whole subject [29] can be recommended.

The major problem associated with oxidation is the modeling of the SiO_2 growth rate. It can be obtained in case of one-dimensional problems by integrating the oxygen flux which diffuses through an SiO_2 layer of thickness d_{ox} to react at the surface.

$$d_{ox}^2(t) + A \cdot d_{ox}(t) = B \cdot (t + \tau) \qquad (9)$$

B and B/A are the parabolic and linear reaction constants, respectively; τ accounts for an eventually existing initial oxide thickness. Some refinement of (9) is required for very thin oxide thicknesses, cf. [22].

In one space dimension oxidation simulation can be stated to have been successful. However, for two- and three-dimensional oxidation no well established theory is available today, e.g. [16]. Typical examples for non-satisfactorily solved problems are the lateral oxidation near a mask edge giving rise to the bird's beak phenomenon, cf. Fig.6, and the oxidation of a trench, cf. Fig.7. The figures are very nice simulation examples obtained with the SMART program [25].

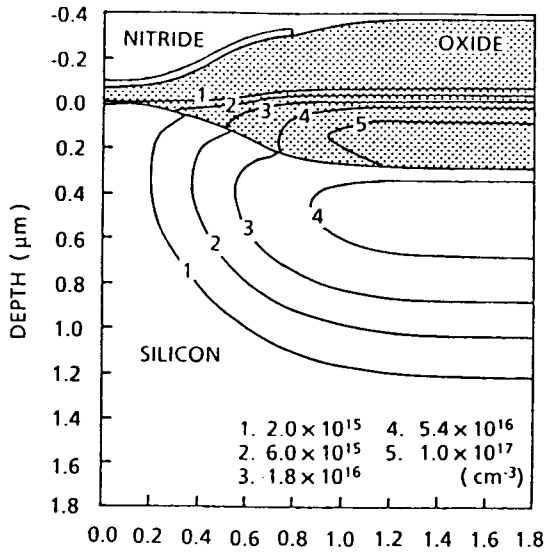


Fig.6

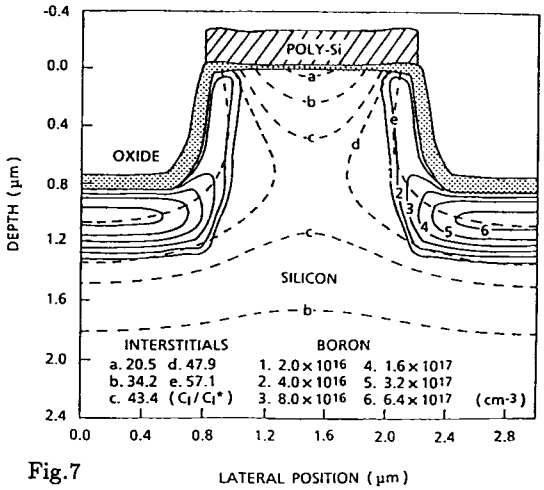


Fig.7

Various models have been developed which allow approximate solutions to the oxidation problem in two space dimensions. The first successful attempt to simulate the bird's beak problem dates back to Penumalli [27]. In this approach the diffusion equation and the associated boundary conditions are transferred by means of a coordinate transformation to a coordinate system where the moving boundary remains stationary. With this approach the solution domain is simplified at the expense of complicating the underlying equations. The benefit is the applicability of straightforward numerical solution methods. The serious bottleneck of this method is that the movement of the silicon interface must be known a-priori in a parametric form.

More realistic models account for the moving Si-SiO_2 interface with explicitly solving the equations of motion for the visco-elastic flow of the oxide, e.g. [14], [30]. This is indeed a very burdensome task and extensively demanding in computer resources. Therefore simplifying assumptions to the equations of motion obviously aid any solution procedure. For high temperatures, say above 950°C, flow of oxidant is primarily viscous which allows to reduce the hydrodynamic equations to the creeping flow equations.

$$\mu \cdot \operatorname{div} \operatorname{grad} \vec{v} = \operatorname{grad} P, \qquad \operatorname{div} \vec{v} = 0 \qquad (10)$$

$\vec{v}$ is the velocity of the oxidant, μ and P are viscosity and pressure, respectively. Successful applications of this model can be found in, e.g. [16], [25].

Further studies are definitely needed to clarify in sufficient detail the physics underlying oxidation. Distinctive emphasis will have to be put on the influence of pressure and tension on the kinetic parameters of oxidation, the implication of the viscoelasticity of the oxide and the interaction of oxide growth with diffusion of dopants and point defects. A particular problem is constituted by models for the interface conditions which describe the point defect generation and recombination to account in a quantitative manner for oxidation enhanced/retarded diffusion. New experiments will have to be cleverly designed in order to isolate overlapping and compensating effects, cf. [4]. Last not least, significant progress regarding numerical algorithms has to be achieved in order to make the demands on computational resources for a simulation program acceptable, cf. [25].

5. CONCLUSION

The use of computer simulation in the development of new process generations has become a widely accepted technique to reduce the high costs and long turn around times of experiments, cf. [6]. Process simulation programs are widely distributed in industrial and academic sites. In the future we can expect increased sophistication of computer programs combined with a better understanding of the physical processes to have an even stronger impact in the design of new technologies and device structures. The increase in performance of new computer systems will aid this development.

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