

Progress in Process Simulation for Submicron MOSFETs

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SUMMARY

A unified model for impurity codiffusion in silicon is proposed. The basic mechanism employed here is the point-impurity pair diffusion as presented by Mulvaney and Richardson in a generalized description of the impurity-interstitial model by Morehead and Lever. The model consists of coupled equations for the impurities and point defects, in which all species including structural effects - a major new process variable - are treated on the same footing. Among other things, this model accounts for point defect perturbations due to high concentration diffusion and for long range, point defect mediated, enhancement or retardation of the diffusion. The ability of the approach allowing for the first time a consistent analysis and exploration of the diffusion phenomena step by step on various levels of complexity is demonstrated by numerical examples and comparison with the experiment. Finally the present equations are compared with extant models, in particular those adopted in SUPREM IV, and the pertinent differences are discussed.

I) INTRODUCTION

The scaling of vertical and lateral dimensions in both MOS and bipolar technologies requires a tight control of the diffusion processes in the silicon. It should be remembered that after all the very structure of dopant profiles determines the operating characteristics of the integrated circuits. Slight variations in the final impurity distribution often have a profound impact on device performance and on device reliability. Nowadays, the prediction and simulation of dopant profiles in one, two and - a fortiori - in three dimensions in a modern IC manufacturing process is no longer feasible through empiricism and intuition; it requires a modelling on a sound physical basis. The integrated circuit process engineer must be able today to anticipate the effects of hundreds of process variables on device performance, instead of relying on time consuming and costly experience based on trial and error. The current capabilities to achieve the desired device performance by an optimization of the process sequence and process parameters are marred by deficiencies in process models, by the inflexible structure of the simulation programs impeding the implementation of a new model, by the inefficiency of the numerical algorithms, and by lacking training in the application of modern software tools within an integrated simulation to the technological needs. The

principal aim of the process simulation is firstly a dramatic reduction of experiments required in a process development, and secondly to provide an insight into the mechanisms of the processes to harness purposely these effects to achieve superior device performance.

Submicron technologies entail extremely sensitive dependence of the dopant diffusivities on the point defect dynamics, on crystal damage produced during ion implantation or resulting from incomplete recrystallization of preamorphized silicon layers, on short-time cycles of rapid thermal annealing, on the treatment of the surface, such as oxidation or nitridation - to mention just a few. It is a grave fallacy to entertain the opinion that these new technologies can be described by extrapolations of existing process models, by simple adjustment of the model parameters until superficial agreement with the available data is achieved. The misery facing the process engineer is that he cannot be certain whether all his effort will be useful for the next process variation that he considers. In view of largely expanded parameter space and of enhanced sensitivity of the diffusion coefficients on a variety of processes the final shapes of the dopant profiles are almost impossible to assess without reliable simulation. In this context an additional circumstance has to be considered: The measurements on "blanket wafers" of 1D dopant profiles are inadequate to grasp the reality in two and three dimensions of the impurity distributions in submicron devices. The present state-of-the-art measurement techniques (except for few approaches of limited applicability known to the author [1,2,3]) are not yet capable of precise determination of lateral 1D dopant profile, let alone 2D distributions. Thus simulation of 2D profiles is not only desirable, but plainly necessary.

The answer to the question which now naturally arises, namely, how can we trust the results of 2D simulations, is comprised within the provision of correct and accurate physical models applicable over a broad range of process conditions. In this article I present the results of a recent effort to address the shortcomings and lack of sophistication in available process models.

The paper is organized as follows: In Section II a new theoretical framework for impurity diffusion in silicon will be presented. It consists of coupled equations for the impurities and for the interstitials and vacancies. The dynamics and the interaction between impurities, point defects, structural defects and boundary conditions is described democratically on the same footing. The essential feature of the present formalism are new equations for interstitials and vacancies which provide the major coupling between the impurities apart from extant and well known couplings, such as via the Fermi level for example. The advantage of the formalism is its consistence allowing for the first time to describe situations of various complexity by one single model. In section III we present some numerical examples and comparison with experiment, where it is coherent or where the experimental data are available. In section IV the proposed formalism is compared with extant models, in particular with the advanced models used in SUPREM IV [4], which is one of the first point-defect based process simulators.

II) NEW MODEL EQUATIONS FOR PROCESS SIMULATION

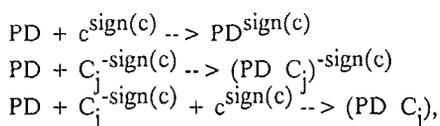
It has been realized for some time [5-8] that only adequate description of the dynamics of interstitials and vacancies can provide a proper theoretical basis for a successful simulation of the impurity diffusion in silicon. This circumstance is well known from such phenomena as, for example, the emitter push effect, high surface concentration phosphorus diffusion, enhanced and retarded diffusion due to the oxidation or to the nitridation. Unfortunately, until now the diffusion of the respective impurity has been modelled more or less independently of other impurities, except for the field

enhancement and the Fermi-level effect [4,9]. However, following the established wisdom that the impurities diffuse via interstitials and vacancies, it is clear that, with regard to these species, there exists sharp competition between the impurities among each other on the one hand, and them and structural crystal defects - such as stacking faults or dislocation loops and boundary conditions, such as point defects injection or annihilation at the surfaces - on the other hand. In addition, it is also known that, while the impurities compete locally in some region of the silicon crystal they can also provide point defects in excess for dopants distributed over completely different regions of the crystal.

As a consequence of this competition among the diffusion species for point defects, each competitor can influence dramatically the behaviour of the extant impurities not only locally but over large distances. Clearly, this situation has to be reflected in the equations describing the dynamics of interstitials and vacancies and, further, the resulting spatial and transient distributions of the point defects must enter in turn the diffusion equations for the impurities. The formalism proposed here accomplishes these objectives. For the diffusion of only one impurity, like phosphorus or boron together with interstitials, but discarding the dynamics of the vacancies and all of the source terms, the set of equations given below reduces to the equation given by Mulvaney and Richardson [10].

Morehead and Lever [11] have developed a model to explain the tail diffusion of boron and phosphorus. They assume that the interstitials combine with the impurity, and the interstitial-impurity pair diffuses. When the impurity becomes substitutional, the interstitial is released and may diffuse into the crystal. In their model they assume that at any point in the crystal, the flux of impurity-interstitial pairs into the bulk is equal to the flux of interstitials towards the surface. In principle, their approach allows either vacancies or interstitials to play the same role. Note that the interstitial-impurity pair diffusion is conceptually a different approach as the "interstitialcy" mechanism, in which an impurity atom makes an elementary movement in two steps. In the first step it is pushed from a substitutional position into an interstitial position by a neighbouring selfinterstitial, and next, in the second step, it takes over a new substitutional site by pushing one of its neighbouring lattice atoms into an interstitial site. At this point the "interstitialcy" mechanism ought not to be confounded with the interstitial diffusion, in which an impurity atom moves from one interstitial site to another without involving point defects. Mulvaney and Richardson in generalizing the latter model include dynamic effects, and relax its assumption of the equality of the impurity-interstitial pair flux and the interstitial flux.

In this approach we allow to diffuse all impurities partly via interstitials and partly via vacancies. The vacancy-impurity pair is meant to be a bound state between these two species. We also relax the boundary condition for interstitials and vacancies for high surface concentration effects in the bulk by assuming that all impurities generate interstitials above the solubility limit [12]. Thus there is an asymmetry in the equations for vacancies and interstitials. The most important points of this theory are the new diffusion equations for interstitials and vacancies, which provide the essential coupling between the impurities. In complete analogy to the approach by Morehead and Lever, we have considered the following reactions:



where PD (point defects) stand either for I (interstitials) or for V (vacancy), c for holes or electron, $\text{sign}(c)$ is the sign of the elementary charge, and C_j denotes the electric active volume concentration of the impurity j (= phosphorus, boron, arsenic, antimony etc.). Of course, additional reactions for example, additional charge states of the point defects, can be implemented into the set of equations given below. However, it is economical to confine oneself to conceptually most simple mechanisms. The equations for the impurity j (phosphorus, boron, arsenic, antimony,...N) are given in eqs. (1-2).

$$\begin{aligned} \frac{\partial C_j}{\partial t} = \nabla \left[\left(D_I f_j \frac{C_I}{C_I^{\text{eq}}} + D_V \bar{f}_j \frac{C_V}{C_V^{\text{eq}}} \right) \nabla C_j + D_j C_j \frac{f_j}{C_I^{\text{eq}}} \nabla C_I + \right. \\ \left. + D_j \bar{f}_j \frac{C_j}{C_V^{\text{eq}}} \nabla C_V + Z_j C_j D_j \frac{q}{kT} \left(f_j \frac{C_I}{C_I^{\text{eq}}} + \bar{f}_j \frac{C_V}{C_V^{\text{eq}}} \right) \nabla \Psi \right] \\ - k_{\text{cl}}^j C_j^m c^k + k_{\text{D}}^j C_j^{\text{clust}} \end{aligned} \quad (1)$$

$$\frac{\partial C_j^{\text{clust}}}{\partial t} = \frac{1}{m_j} [k_{\text{cl}}^j C_j^m c^k - k_{\text{D}}^j C_j^{\text{clust}}] \quad (2)$$

Here D_j is the diffusivity of the impurity j dependent on the Fermi-level, f_j is the fractional interstitially diffusion component of the impurity j , \bar{f}_j the corresponding fractional vacancy diffusion component, C_I^{eq} and C_V^{eq} denote the equilibrium concentration of interstitials and vacancies, respectively; C_j^{clust} is the concentration of the clustered impurity j in contrast to the electric active concentration C_j . The dynamics between C_j^{clust} and C_j is here described by a simple cluster model with clustering coefficient k_{cl}^j and de-clustering coefficient k_{D}^j , but can be substituted by any reasonable model describing clustering or precipitation; and its form is not essential here. The formation of clusters or the precipitation is assumed to lead to a decrease in diffusivity for increasing concentration above a certain value for the concentration. In the case of arsenic, for instance, it has been observed (Matano analysis) that the diffusivity shows a peak at about $3 \cdot 4 \cdot 10^{20} \text{cm}^{-3}$ and then decreases with the further increase of arsenic concentration. Another feature of the clustering phenomena will be discussed below in conjunction with the equations for the point defects.

Ψ denotes the electric field and Z_j is the charge state for the impurity j . The rigour of this formalism would suggest $f_j + \bar{f}_j = 1$. However, this strict complementarity may be traded off against such effects as the gradual filling of the traps by point defects [13] or direct coupling between the impurities [14] for example.

The crucial equations of this model are the equations for interstitials and vacancies given in eqs. (3-4).

$$\begin{aligned} \frac{\partial C_I}{\partial t} = \nabla \left[\left(D_I + \sum_{j=1}^N f_j D_j \frac{C_j}{C_I^{\text{eq}}} \right) \nabla C_I + \sum_{j=1}^N f_j D_j \frac{C_I}{C_I^{\text{eq}}} \nabla C_j + \right. \\ \left. + \sum_{j=1}^N Z_j f_j D_j C_j \frac{C_I}{C_I^{\text{eq}}} \frac{q}{kT} \nabla \Psi \right] + k (C_I C_V - C_I^{\text{eq}} C_V^{\text{eq}}) + \\ + \alpha D_I C_I g(x) - \beta_j \sum_{j=1}^N \frac{\partial C_j^{\text{clust}}}{\partial t} \end{aligned} \quad (3)$$

$$\frac{\partial C_v}{\partial t} = \nabla \left[\left(D_v + \sum_{j=1}^N \bar{f}_j D_j \frac{C_j}{C_v^{eq}} \right) \nabla C_v + \sum_{j=1}^N \bar{f}_j D_j \frac{C_v}{C_v^{eq}} \nabla C_j + \sum_{j=1}^N Z_j \bar{f}_j D_j \frac{C_v}{C_v^{eq}} C_j \frac{q}{kT} \nabla \psi \right] + k (C_I C_v - C_I^{eq} C_v^{eq}) \quad (4)$$

Here k describes the bulk recombination velocity between interstitials and vacancies, α the sink efficiency of dislocation loop distribution $g(x)$, as induced by a preamorphization procedure [15], β_j the strength of interstitial generation in regions where the impurity concentration exceeds the solubility limit, $\beta_j = \beta_j(m_j, k_{cl}^j, k_D^j)$. The growth of dislocation loops can be straightforwardly described by an additional equation not given here (see for example [16]). Also the decoration of the dislocation loops by interstitial boron and phosphorus atoms (electrically inactive) can be taken into account by analogous terms as in the equation for interstitials, eq.(3) ($\propto D_I C_I g(x)$).

The equations have a remarkably high degree of symmetry. Note that all non-diagonal diffusion coefficients are factorial hybrids of the diagonal ones. Even more remarkably is the circumstance that the only parameters of this theory are $D_I, C_I^{eq}, D_V, C_V^{eq}$, the sink efficiency α in presence of dislocation loops or other structural defects, recombination velocity k , and the interstitial generation rates β_j for impurities above the solubility limits. Moreover these parameters seem to reflect directly the physical complexity and not merely to mock it. The diffusion coefficients D_j are taken from conventional models (as used in SUPREM III, [9]), which guarantees that for all so-called intrinsic cases eqs. (1-4) reproduce the standard and successful models. In this sense eqs. (1-4) represent the unified framework for the description of diffusion phenomena in silicon.

To complete the formal part of the model the boundary conditions for interstitial and vacancies must be emphasized. Oxidation or nitridation of the silicon surface implies injection of interstitials or of vacancies, respectively. Also the surface recombination velocities at various interfaces are to be considered in the well known manner. This can be handled in complete analogy to the prescriptions given in Refs. [4-7].

III) EXAMPLES OF THE MODEL PREDICTIONS AND COMPARISON WITH THE EXPERIMENT

In our first example the effects of the preamorphization highlight the importance of the point defect dynamics for the impurity diffusion in submicron devices. The amorphization of the top layer (thickness ca. 0.2 μm) of the silicon crystal is performed by a blanket high dose Si implant prior to source/drain implantation. The critical damage density - the number of vacancies per unit volume in the silicon crystal C_V - to amorphize the Si-crystal is $C_V^{crit} = 1.55 \cdot 10^{22} \text{cm}^{-3}$. During the subsequent drive-in the amorphized layer recrystallizes very quickly, but there remains residual damage layer in a depth x_{dis} (0.2 μm) corresponding to C_V^{crit} such that $C_V(x_{dis}) = C_V^{crit}$. The width w_{dis} of the damaged layer corresponds to the gradient [17] $\partial C_V(x) / \partial x|_{x=x_{dis}}$ and can directly be read off from TEM pictures ($w_{dis} = 30 - 50 \text{nm}$). The residual layer acts as an effective sink for the interstitials during the subsequent drive-in. The efficiency to absorb the interstitials has been determined from our diffusion simulations. In Fig. 1, the phosphorus and buried boron profile are simulated with and without the effect of

preamorphization. It can be seen, that phosphorus diffusion produces interstitials in supersaturation and that the dislocation loops in the damaged layer - a remnant of the amorphization - lower effectively the interstitial supersaturation concentration in the bulk. The agreement for the phosphorus diffusion with and without preamorphization is excellent. Fitting the phosphorus SIMS profile after a drive-in at 900 °C for 40 min the interstitial diffusivity D_I , and the equilibrium interstitial concentration C_I^{eq} estimated by Tan and Gösele [16] turned out to be most reasonable. The impurity profiles are very sensitive to these values and to the boundary condition for the interstitials at the surface. The increase of D_I leads to the formation of the characteristic diffusion tail at higher impurity concentrations. The increase of C_I^{eq} results in a shorter and steeper diffusion tail. The exact magnitude of these quantities cannot be ascertained on this level. Small variations in D_I and C_I^{eq} can be traded off against clustering effects of the phosphorus, the phosphorus diffusivity, against the characteristics of the vacancy dynamics and against the values assigned to the fractional interstitial and vacancy diffusion components f_i and f_v , respectively. However, the interstitial supersaturation can be probed by the diffusion of the buried layer beyond the layer of dislocation loops. The inclusion of buried boron layer constitutes the next level of complexity described by the same model in a natural way, allowing to narrow or to pin down the parameter for the interstitial dynamics. As can be seen from Fig. 1 in the case of preamorphization the buried boron layer displays a retarded emitter push effect (in absence of phosphorus implant the boron profile after the same drive-in is steeper than the boron profile indicated by the dashed line in Fig. 1). A corresponding experiment with the buried boron layer is presently under way. The phosphorus and boron profile with preamorphization have been obtained simply by activating the sink term $\propto D_I C_I g(x)$ using the values for x_{dis} and w_{dis} provided by the TEM pictures and adjusting the sink efficiency α . It could be surmised, that the sink efficiency α can be traded against the width of the damaged layer, since both parameters together determine the overall sink efficiency. However, it turned out that the shape of the impurity profile with preamorphization is more sensitive to α and w_{dis} than the reduction of the interstitial concentration in the bulk which depends on an overall sink efficiency and on the location of the damaged layer with respect to the silicon surface. The experimental value w_{dis} with adjusted sink efficiency has provided the best fit to the experiment.

In Fig. 2 a prediction is made which constitutes a crucial test for the mechanism of impurity-interstitial pair diffusion invoked by Morehead and Lever [11]. Shifting the damaged zone deeper into the bulk but keeping the same sink efficiency α as in Fig. 1 we observe a local minimum in interstitial concentration leading via the pairing mechanism to a local maximum of the phosphorus concentration within the tail region. The experimental data for deep amorphization implants show indeed the additional hump in the phosphorus profile at the location of the dislocation loop layer. However, it must be still clarified whether this hump is merely an aggregation of phosphorus atoms decorating the dislocation loops effectuated by a conventional diffusion mechanism and by the subsequent capture of the passing phosphorus atoms at the damaged layer. The effect in Fig. 2 can be easily understood. It should be remembered that the Morehead-Lever-mechanism assumes that at any point the flux of the phosphorus-interstitial pairs into the crystal is balanced by an opposite interstitial flux. Although in this formulation (see Ref. [10]) the assumption of the equality of the impurity-interstitial pair flux and the interstitial flux is relaxed, the argument is based primarily on the circumstance that the pertinent fluxes go in opposite direction - an intrinsic property of the pair diffusion. In Fig. 1, the interstitial flux given by the sign of $\partial C_I / \partial x$ is oriented all the time towards the surface. In Fig. 2, the gradient between 0.35 μm and 0.50 μm is directed towards the bulk because of the negative slope in this region caused by the absorption of the interstitials in the damaged zone. In contrast to the situation given in Fig. 1, the

absorption of the interstitials in Fig. 2 results in a local minimum of the interstitial concentration because in $0.5 \mu\text{m}$ depth the phosphorus concentration is too low to build up the interstitial concentration and the absorption is entirely uncompensated. As a consequence, the phosphorus flux in the interval $0.35 - 0.50 \mu\text{m}$ is directed towards the bulk, which means that the phosphorus atoms in this region are swept back leading to the local hump in the phosphorus distribution.

Our second example is illustrated in Fig. 3 where the simultaneous diffusion at 900°C for 100 min of high concentration phosphorus and boron and medium concentration of antimony is shown together with the distribution of interstitials and vacancies. The simultaneous diffusion of the three impurities is compared with the diffusion of each impurity in absence of the other. This example shows how the competition between the impurities with respect to the point defects constitutes mutual diffusion coupling between the respective species. It can be seen that phosphorus diffusion is not changed by the presence of antimony and boron. Boron displays the expected emitter push effect, while the diffusion of antimony is slightly retarded by the presence of high phosphorus concentration. It should be noted that the diffusion of all five species in Fig. 3 is described by one consistent model. It is remarkable that the computing time for this example is comparable to the computing time for examples in Fig. 1 and Fig. 2 (smaller than 120 sec CPU) due to the symmetry of the equations. It should be noted that the results in Fig. 1 - 3 have been obtained in a natural way from one consistent model given in eqs. (1-4). This equations have been coded in one dimension using the process simulator ZOMBIE [18] which turned out to be an extremely valuable tool in developing and understanding of this formalism. For two-dimensional problems essentially the same moduls containing the structure of the eqs. (1-4) can be transferred to the 2-D process simulator PROMIS [19], which has the same structure and philosophy as ZOMBIE [18].

IV) COMPARISON OF THE PRESENT MODEL WITH EXTANT DIFFUSION MODELS

Nobody can nowadays seriously contest that the most important mechanism by which dopants diffuse is via interactions with point defects. Therefore a reliable calculation of impurity distribution requires (whenever possible) physical models which couple the local dopant diffusivity. The crucial point here is not whether or not to couple impurity dynamics with the dynamics of the point defects, but *how* to couple them. This implies naturally the next question: What are the origin and basic mechanisms of transient inhomogeneities of the point defect distributions? What kind of equations can account for them?

The thermodynamic source for point defects which introduces some degree of entropy into the crystal lattice in order to minimize the free energy above 0°K is reflected by the equilibrium concentration values for interstitials and vacancies, C_I^{eq} and C_V^{eq} , respectively. Of higher interest and of more practical importance are the extrinsic sources of point defects. Almost any surface treatment is apt to act as a source or a sink of point defects. The oxidation or nitridation with the resulting enhanced and retarded diffusion are well-known examples of injection of interstitials or vacancies into bulk silicon. A non-oxidizing $\text{SiO}_2\text{-Si}$ interface may suffice here as an example for a quite efficient interstitial sink. These effects have been studied extensively by the Stanford group [20] and also by others and considered by suitable boundary conditions for point defects.

However, as seen from Fig. 1 there are also dynamic effects giving rise to redistribution of the interstitials by the impurity diffusion itself and that the interstitial sinks caused by crystal damage constitute a major new process variable. There has been

hitherto no formalism which addressed these effects on various levels of process complexity in a consistent way. Rather, until now the dopant diffusivity of an impurity j at each point in space has been coupled to the local point-defect concentration according to eq. (5) [4,7],

$$D_j^{\text{eff}} = D_j (f_j C_I / C_I^{\text{eq}} + \bar{f}_j C_V / C_V^{\text{eq}}) \quad (5)$$

This particular form of the coupling implemented in SUPREM IV consists of first calculating the point defect distribution and *then* using the local point defect concentration to modify the local dopant diffusivity. The total flux for the impurity j , apart from the trivial field term, is given by $F_j = D_j^{\text{eff}} \nabla C_j$. This flux corresponds to the first term in eq. (1). The fluxes proportional to the gradients of point defect concentrations, ∇C_I and ∇C_V (see eqs. (1-2)), are altogether neglected. The point defect dynamics on the other hand were believed [4, 7, 20] to obey the following continuity equations.

$$\frac{\partial C_I}{\partial t} = \nabla (D_I \nabla C_I) + k (C_I C_V - C_I^{\text{eq}} C_V^{\text{eq}}) \quad (6)$$

$$\frac{\partial C_V}{\partial t} = \nabla (D_V \nabla C_V) + k (C_I C_V - C_I^{\text{eq}} C_V^{\text{eq}}) \quad (7)$$

Comparing eqs. (6-7) with eqs. (3-4) it is seen that the former constitute only one term of the latter. Thus the present eqs. (1-4) contain and reproduce eqs. (5-7) but go considerably beyond them.

It is of major interest to assess under which circumstances the additional terms are important for correct simulation. Although this issue will be explored in a separate study [21], some preliminary findings can be stated beforehand. The fluxes proportional to ∇C_I and ∇C_V in eq. (1) are for most realistic applications of minor relevance, because $\nabla C_I, \nabla C_V$ and impurity concentrations C_j are seldom simultaneously sufficiently large at the same position. However, they will become important for lower temperatures than 900 °C or in such a situation as shown in Fig. 2.

More serious are the deficiencies in the eqs. (6-7) for the point defects. For high concentration impurity diffusion the fluxes given by the sums over the impurities present in the silicon (see eqs. (3-4)) are of paramount importance, since they determine the point defect distribution as dramatically as the sinks and sources at the surface. When the diffusion of an impurity produces excess point defects, the point defect concentration will no longer be a unique function of the local impurity concentration. In a reasonable model the generation of excess point defects is related to the flux of the impurity from the high concentration region, and consequently must be time dependent. These terms account also for long range effects such as the emitter push effect illustrated in Fig. 1. Clearly, these terms must not be omitted.

The principal deficiency of models like that in eqs. [5-7] has been already pointed out by Hu [22] almost twenty years ago, that even simple systems need, in

general, to be formulated using a complete set of equations of irreversible thermodynamics, including cross terms from all constituents. The flux equations have to be written in the form

$$J_i = \sum_j L_{ij} F_j \quad (8)$$

with as many terms as there are constituents, where F_j is the thermodynamical driving force. A simple Fick's law is no longer applicable, as in the case of pair diffusion. The diffusion flux is not just given by one term associated with the gradient of the respective species, but is also contributed by cross terms which may in some cases actually dominate. The problem of eq. (8) is, of course, to determine the matrix elements L_{ij} . Their specific functional form cannot be simply found from Onsager reciprocal relation, the Gibbs-Duhem relation, or the conservation of lattice sites, because these relations are devoid of the intrinsic features of the codiffusion dynamics. The model proposed here shows that L_{ij} emerge naturally from the generalized mechanism by Morehead and Lever [11].

In summary we wish to stress that within the selfconsistent formalism presented here, based on the impurity-point defect pair diffusion - the equations for point defects, in particular - constitute an indispensable generalization of the extant models to deal successfully with the process simulation of submicron structures.

ACKNOWLEDGEMENT

The author profited greatly from the interactions with Dr. Neppi and his group while supporting their effort in designing the submicron logic.

REFERENCES

- [1] W. Rösner, W. Hänsch, B. Moore, M. Orlowski, A. Spitzer and C. Werner, "Determination of Lateral Drain Profiles from Gate-Drain Overlap Capacitances", VLSI-Symp. Dig. 1988 p. 9
- [2] M. Orlowski, C. Mazure and F. Lau, "Submicron Short Channel Effects due to Gate Reoxidation Induced Lateral Interstitial Diffusion", IEDM-Proceedings 1987, p. 632
- [3] P. Reutman, I. Albers and D.R. Myers, "An Investigation of the Two-Dimensional Shape of Ion Implanted Regions", I. Appl. Phys. 55, 1984, p. 4436
- [4] I. D. Plummer and R. W. Dutton, Computer Code SUPREM IV (Integrated Circuits Laboratory Stanford University 1986), see for example
M. E. Law "Two Dimensional Numerical Simulation of Impurity Diffusion in Silicon", PhD dissertation, Department of Electrical Engineering, Stanford University, January 1988
- [5] U. Gösele, "Diffusion in Semiconductors", in Semiconductor Silicon, eds. H. R. Ruff and T. Abe, Electrochem. Soc., Pennington, N. J. 1986, p. 541
- [6] R. B. Fair, "Concentration Profiles of Diffused Dopants in Silicon", in Impurity Doping Processes in Silicon, ed. F. F. Y. Kang, North-Holland, New York, 1981 p. 315
- [7] P. M. Fahey, "Point Defects and Dopant Diffusion in Silicon" PhD dissertation, Department of Electrical Engineering, Stanford University, June 1985
- [8] S. M. Hu, "Modelling Diffusion in Silicon: Accomplishments and Challenges" in 3rd Int. Symposium on VLSI Science and Technology, ed. W. M. Bulks, Electrochem. Soc., 1985
- [9] C. P. Ho, I. D. Plummer, S. E. Hansen and R. W. Dutton, "VLSI Process Modelling-SUPREM III, IEEE ED 30 No. 11, 1983, p. 1438
- [10] B. I. Mulvancy and W. B. Richardson, "Model for Defect-Impurity Pair Diffusion in Silicon", Appl. Phys. Lett. 51, 1987, p. 1439

- [11] F. F. Morehead and R. F. Lever, "Enhanced Tail Diffusion of Phosphorus and Boron in Silicon: Self-Interstitial Phenomena", *Appl. Phys. Lett.* 48, 1986, p. 151
- [12] I. C. C. Tsai, D. G. Schimmel, R. B. Fair, and W. Maszara, "Point Defect Generation During Phosphorus Diffusion in Silicon", *J. Electrochem. Soc.* 134, 1987, p. 1508 u. 2348
- [13] P. B. Griffin, S. T. Ahn, W. A. Tiller and I. D. Plummer, "Model for Bulk Effects on Si Interstitial Diffusivity in Silicon", *Appl. Phys. Lett.* 51, 1987, p. 115
- [14] M. Orlowski, to be published
- [15] C. Mazure, I. Winnerl and F. Nepl, "Impact of S/D Preamorphization on CMOS Performance", *Proceedings of the ESSDERC '87 Conference, Bologna, 1987*, p. 585
- [16] T. Y. Tan and U. Gösele, "Kinetics of Silicon Stacking Fault Growth/Shrinkage in an Oxidizing Ambient Containing a Chlorine Compound", *J. Appl. Phys.* 53, 1982, p. 4767
- [17] M. Orlowski, C. Mazure and L. Mader, "Simulation of Source/Drain Structures for Submicron MOSFETs with and without Preamorphization", to be published in the *Proceedings of the ESSDERC '88 Conference, Montpellier, 1988*
- [18] W. Jüngling, P. Pichler, S. Selberherr, E. Guerrero and H. W. Pötzl, "Simulation of Critical IC-Fabrication Processes Using Advanced Physical and Numerical Methods", *IEEE ED 32*, 1985, p. 156
- [19] P. Pichler, W. Jüngling, S. Selberherr, E. Guerrero and H. W. Pötzl, "Simulation of Critical IC-Fabrication Steps", *IEEE ED 32*, 1985, p. 1940
- [20] Stanford Research Reports 1985, 1986, 1987, Integrated Circuits Laboratory, Stanford University
- [21] M. Orlowski, in preparation
- [22] S. M. Hu, *Physical Review* 180, 1969, p. 773

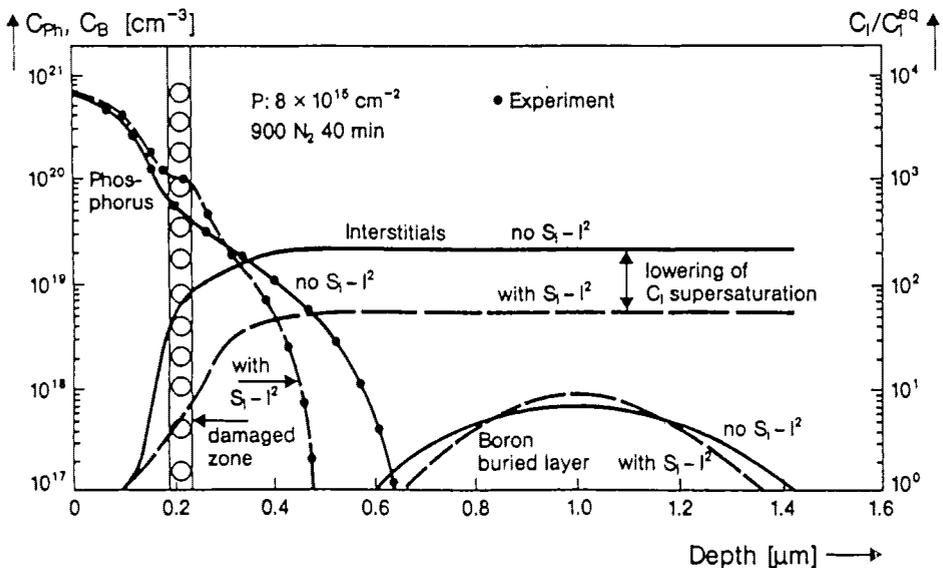


FIG. 1: High concentration phosphorus diffusion and the emitter push effect on buried boron layer after 900°C , 40 min drive-in with and without preamorphization. The concentration of the vacancies has been suppressed for clarity.

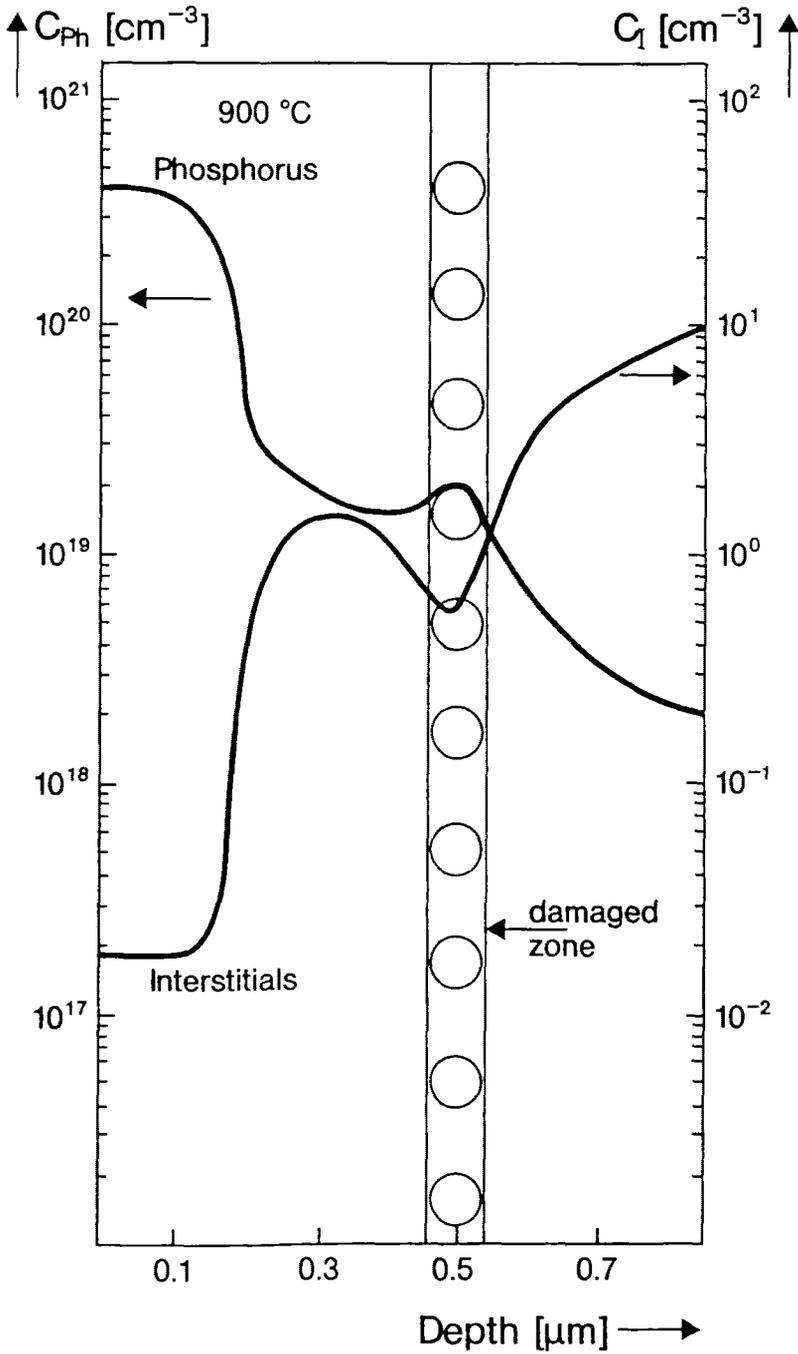


Fig. 2: Prediction of a local maximum in the phosphorus tail for deep amorphization.

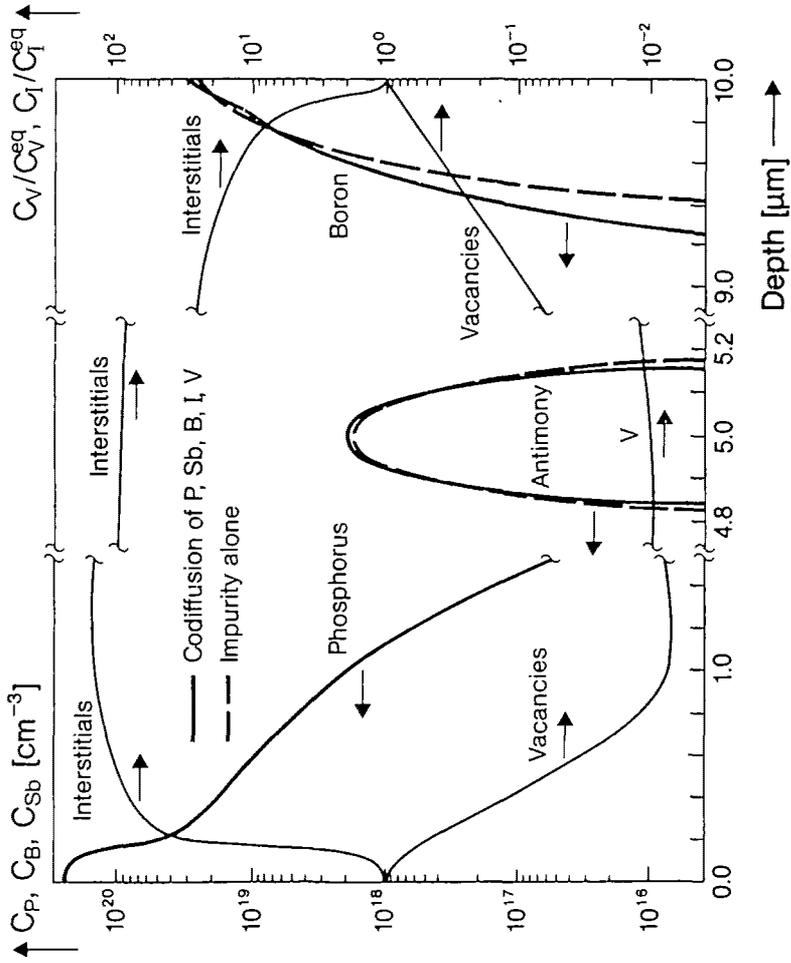


Fig. 3: Coupled phosphorus-antimony-boron-interstitial-vacancy diffusion after 900 °C 100 min.