NEW THREE-PHASE MODEL FOR SEGREGATION AND OUTDIFFUSION PHENOMENA

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A new three-phase model describing dopant redistribution at an interface that separates two adjacent bulk phases is proposed. In this model the interface (layer) is considered as a third phase (3) of finite thickness in its own right, which mediates the dopant redistribution between the adjacent bulk phases (1) and (2). The dynamics of the redistribution is formulated in terms of the following rate equations, see Fig.1:

$$\frac{\partial C_1}{\partial t} = -a_{13}C_1 + e_{31}C_3 \qquad \frac{\partial C_3}{\partial t} = a_{13}C_1 - e_{31}C_3 + a_{23}C_2 - e_{32}C_3 \qquad \frac{\partial C_2}{\partial t} = -a_{23}C_2 + e_{32}C_3 \qquad (1)$$

where C_i denotes the dopant concentration in the respective phase (i), the coefficients a_{13} and a_{23} denote the absorption rates of the dopant in the interface layer from the bulk phases (1) and (2), and correspondingly, the coefficients e_{31} and e_{32} describe the emission rates of the dopant from the inter-phase (3) into the bulk phases (1) and (2), respectively. As an interface layer of finite thickness can accept only a finite dose of the dopant, it is clear that some maximum concentration $C_{3,max}$ within the inter-phase (3) cannot be exceeded. The absorption coefficients a_{13} and a_{23} must therefore exhibit a saturation behavior at high concentrations close to $C_{3,max}$ in the interphase (3). Therefore

$$a_{13} = a_{13}^0(C_{3,max} - C_3) \qquad a_{23} = a_{23}^0(C_{3,max} - C_3) \qquad (2)$$

For stationary case, i.e. $t \to \infty$ eqs.(1,2) with the initial concentrations C_1^0, C_2^0, and C_3^0 can be solved analytically. It can be seen that the stationary solutions depend only on the total initial concentration $C_{tot}^0 = C_1^0 + C_2^0 + C_3^0$ and on the two ratios of emission and absorption coefficients, e_{31}/a_{13}^0 and e_{32}/a_{23}^0. Inserting eq.(2) into eq.(1) and assuming equilibrium case, i.e. $\partial C_3/\partial x = 0$ one obtains $N_3 = N_{3,max}(C_1 + \alpha C_2)/(C_1 + \alpha C_2 + \beta)$ where $\alpha = a_{23}^0/a_{13}^0$ and $\beta = (e_{31} + e_{32})/a_{13}^0$ with $N_3 = C_3 W$ and $N_{3,max} = C_{3,max} W$, W being the width of the interface layer. The latter equation relates the total dopant dose in the interface layer (N_3) to the concentrations C_1 and C_2 at both sides of the interface in good agreement with the data for the interface and bulk segregation of phosphorus [1,2,3].

It can be demonstrated [1,4] that this model if applied to a single homogeneous phase reduces to an ordinary diffusion equation. This demonstrates that the transition phenomena related to redistribution at the interface and the diffusion dynamics found a common theoretic description. The immediate advantage of this formulation is that the coupling between the interface dynamics and the diffusion in the adjacent bulk phases can be described in a new, consistent, and unambiguous way derived from first principles [1,4]. The resulting equations are from the beginning in discretized form and can be cast into one single equation describing multiphase difusion by means of new finite difference operators [4].

From these equations a workable dynamic segregation model coupled to the diffusion dynamics in bulk phases and being compatible with existing simulation tools is easily derived, see Fig.2; the result of such derivation is:

$$\frac{\partial C_1}{\partial t} = -a_{13}^0(C_{3,max} - C_3)C_1 + e_{31}C_3 - \kappa_1 F_1 \qquad (3)$$

$$\frac{\partial C_3}{\partial t} = a_{13}^0(C_{3,max} - C_3)C_1 - e_{31}C_3 + a_{23}^0(C_{3,max} - C_3)C_2 - e_{32}C_3 \qquad (4)$$

$$\frac{\partial C_2}{\partial t} = -a_{23}^0(C_{3,max} - C_3)C_2 + e_{32}C_3 - \kappa_2 F_2 \qquad (5)$$

$$\frac{\partial \bar{C}_1}{\partial t} = D_1 \frac{\partial^2 \bar{C}_1}{\partial^2 x} \qquad and \qquad \frac{\partial \bar{C}_2}{\partial t} = D_2 \frac{\partial^2 \bar{C}_2}{\partial^2 x} \qquad (6)$$

Here F_1 and F_2 denote the fluxes in the bulk phases (1) and (2) at the interface, i.e. $F_{1/2} = D_{1/2}(\partial \bar{C}_{1/2}/\partial x)|_{x=\delta \mp o}$, with $D_i = d_i^2/\tau_i$ for $i = 1, 2$. The coefficients κ_1 and κ_2 are fitting parameters subject to a constraint ensuring the conservation of the total dopant dose in the vicinity of the interface, for details see ref.[1]. Eqs.(3-5) are solved for the initial distribution C_1^0, C_2^0, C_3^0 at $t = 0$ and eqs.(6) are solved also for some initial distributions $\bar{C}_1^0(x)$, $\bar{C}_2^0(x)$ with the Dirichlet boundary conditions at the interface δ, i.e. $\bar{C}_1(x,t)|_{x=\delta-o} = C_1(t)$ and $\bar{C}_2(x,t)|_{x=\delta+o} = C_2(t)$, where $C_1(t)$ and $C_2(t)$ must be determined from eqs.(3-5). In Figs.(3-5) some applications of the above model to segregation and outdiffusion phenomena are shown. In a stationary version of this model one assumes that the segregation dynamics is much faster than the diffusion dynamics in the bulk phases on the time scale set by the larger of the two diffusion coefficients D_1 and D_2. This means that in a sufficiently small time interval $[t_k, t_{k+1}]$ the quantities $\kappa_i F_i \equiv B_i$ for $i = 1, 2$ in eqs.(3,5) can be regarded to be constant being set to $B_i = \kappa_i F_i(t_k)$ for $t \in [t_k, t_{k+1}]$. In this case eqs.(3,5) can be solved analytically with the stationary solutions $C_i^\infty(t_k)$ for $i = 1, 2, 3$:

$$C_i^\infty(t_k) = f_i(C_{tot}^0, e_{31}/a_{13}^0, e_{32}/a_{23}^0, B_1(t_k), B_2(t_k)) \qquad (7)$$

With the solutions of the stationary model one has to solve only the diffusion eqs.(6) with Dirichlet boundary conditions given by eqs.(7) which can be immediately implemented in such programs like SUPREM III [5].
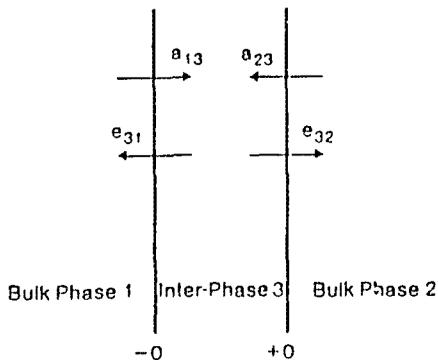
Fig.1 Conceptual diagram of the three-phase model. The emission and absorption rates are indicated.
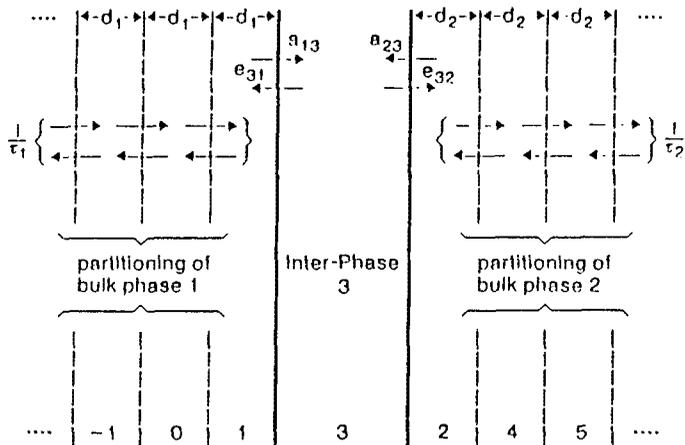
Fig.2 Generalization of the schematic diagram of the three-phase model given in Fig.1. The bulk phases 1 and 2 are now partitioned in stripes of the length d_1 and d_2, respectively. In the bulk phases the model (eqs.(1)) reduces to ordinary diffusion eqs.(6).
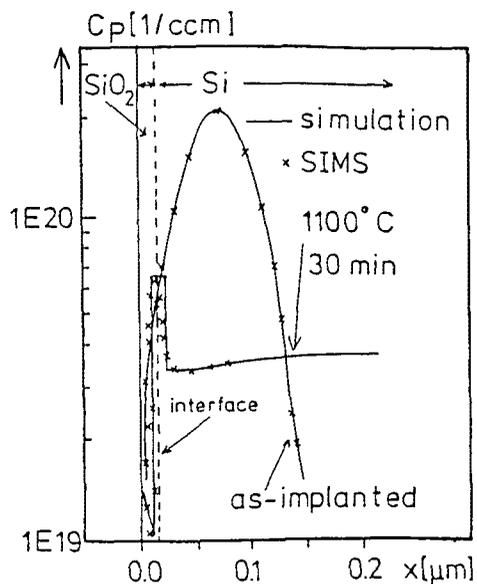
Fig.3 Phosphorus segregation at $Si-SiO_2$ interface after inert anneal at 1100° C for 30 min. The phosphorus has been implanted with $2.5E15\ cm^{-2}$ with 80 keV through an oxide of 25 nm. Note that the dip in the phosphorus profile on the silicon side is also correctly reproduced.
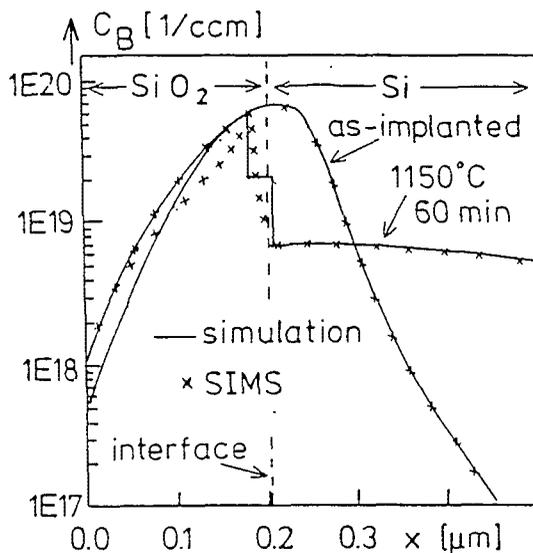
Fig.4 Boron segregation at $Si-SiO_2$ interface after an anneal at 1150° C for 60 min in 1% O_2. The boron has been implanted with $1E15\ cm^{-2}$ with 50 keV through a 215 nm oxide. The as-implanted profile is also indicated. The oxide growth is almost null. Data are taken from ref. [6].
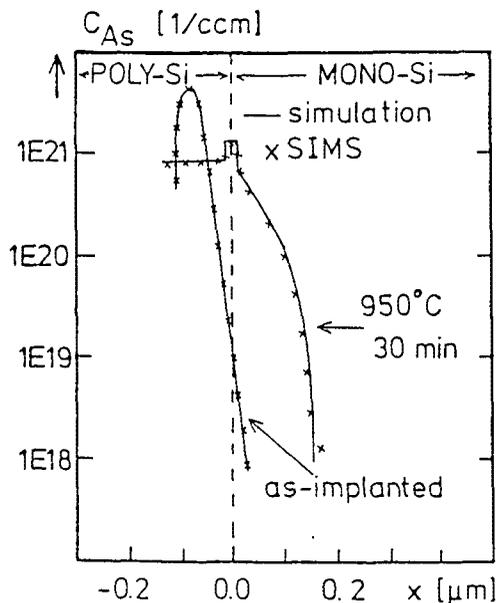
Fig.5 Arsenic outdiffusion from poly silicon into crystalline silicon at 950° C for 30 min. The poly silicon 200 nm thick has been initially implanted with arsenic with $2E16\ cm^{-2}$ at 100 keV; the implantation profile is also indicated. Data are taken from ref. [7].

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