# Dynamic Grain-Growth and Static Clustering Effects on Dopant Diffusion in Polysilicon

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**Abstract**

**A two-dimensional simulation model for dopant diffusion in polysilicon has been developed, which includes dopant clustering in grain interiors as well as in grain boundaries. The grain growth model is coupled with the diffusion coefficient of the dopants and the process temperature. For all high dose implantation cases the trapping/emission mechanism in polysilicon and the grain growth are the major effects during thermal treatment processes.**

For recent device fabrication techniques polysilicon-related processes have become more important, e.g. emitter out-diffusion by forming a poly-Si-(p-,n-)gate MOSFET or in high performance bipolar LSI's technology [1]. Due to the low thermal budget and high dose implantation polysilicon processes, more accurate physical models are required. To predict precise concentration profiles in polysilicon layers various phenomena such as clustering, segregation at material interfaces, generation/recombination mechanism and grain growth must be incorporated in any advanced polysilicon diffusion model.

## 1 Polysilicon Diffusion Model

The two-dimensional coupled PDEs for the active dopant concentration in the grain interior ($C_{ga}$) and the grain boundaries ($C_{gb}$) are given in Eq.s (1)-(2). $\gamma$ denotes a geometric factor taking into account the different average grain size of polysilicon material in lateral and vertical direction. Diffusion and segregation kinetics is followed after [2].

$$\frac{\partial C_{ga}}{\partial t} = \mathrm{div}\ \left(D_{ga} \cdot \left(\mathrm{grad}\ C_{ga} + s \cdot \frac{C_{ga}}{U_T} \cdot \mathrm{grad}\ \psi\right)\right) - G_s \quad (1)$$

$$\frac{\partial C_{gb}}{\partial t} = \mathrm{div}\ \left(\gamma \cdot D_{gb} \cdot \left(\mathrm{grad}\ C_{gb} + \frac{C_{gb}}{r} \cdot \mathrm{grad}\ r\right)\right) + G_s \quad (2)$$

$$G_s = t \cdot \left(\frac{T_b^{max}}{r} - C_{gb}\right) \cdot C_{ga} - e \cdot \left(C_g^{sol} - C_{ga}\right) \cdot C_{gb} \quad (3)$$

Eq. (3) describes the generation/recombination term of the exchange of dopants between grains interiors and grain boundaries by use of trapping $t$ and emission $e$ factors, where

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$T_b^{max}$ denotes the maximum number of free states in the grain boundary. $C_g^{sol}$ is the solubility limit for the dopant species:

$$\frac{C_g^t}{C_g^{sol}} = \frac{C_{ga}}{C_g^{sol}} + m_g \cdot \left(\frac{C_{ga}}{C_g^{sol}}\right)^{2.m_g} \tag{4}$$

$C_g^{sol}$ is also taken to calculate the active grain interior concentration $C_{ga}$ from the total interior concentration $C_g^t$ in the static clustering model Eq. (4) after [3].

## 2 Dynamic Grain Growth

In our model the grains of polysilicon are assumed to be tiny squares with an initial grain size $r_0$. During the thermal treatment the grain boundaries will migrate, so grain growth occurs. The calculation of the migration is based on thermodynamic concepts [4],[5] and depends on polylayer-thickness $\lambda$ , grain boundary energy $\Delta\mu$ , diffusion of dopants across the grain boundary $D_{ga}$ and temperature $T$

$$\frac{\partial r}{\partial t} = \frac{D_{ga}}{\lambda} \cdot \left[1 - e^{-\frac{\Delta\mu}{K \cdot T}}\right]. \tag{5}$$

Via the diffusion coefficient $D_{ga}$ the grain growth depends on the local dopant concentration. Due to the anisotropic material properties of polysilicon the average grain size becomes non-uniform along the vertical and lateral direction. On the other hand this non-uniform grain size distribution causes an oriented diffusion flux. On the other hand this non-uniform grain size distribution causes an oriented diffusion flux.

## 3 Simulation Results

Fig.1 shows the one-dimensional calculation result for a 6h 800°C As-annealing process in nitrogen on a planar 1,5 $\mu$m thick poly-layer. In this case the arsenic concentration did not reach the interface poly-Si/mono-Si. Therefore the interface conditions can be neglected. By decreasing the poly-layer thickness, interface segregation takes place and forms a pile-up in the arsenic concentration at the interface (Fig.2). Here the interface region is simulated as an interface grain boundary with a smaller number of free states due to the interfacial oxide layer. Fig.3 shows the results for high dose As-implantation and 10 min annealing at temperature range from 750°C - 900°C on a 0.3$\mu$m poly-layer. Experimental data (Fig.4)[7] are reproduced. Fig.5 shows the result of an out-diffusion simulation from a 0.6x0.1$\mu$m poly-layer in substrate, where Fig.6 gives the one-dimensional result in the mid-emitter region. For the 900°C case an emitter depth($W_d$) of 40nm is computed, which agrees with SIMS measurements (Fig.7)[1].

## 4 Conclusion

A new model for dopant diffusion in polysilicon including dynamic grain growth and dopant clustering was introduced. To model this requirements the conventional nonlinear PDEs

are coupled with a PDE for grain growth and an algebraic equation to calculate the active dopant concentration.

## 5 Acknowledgements

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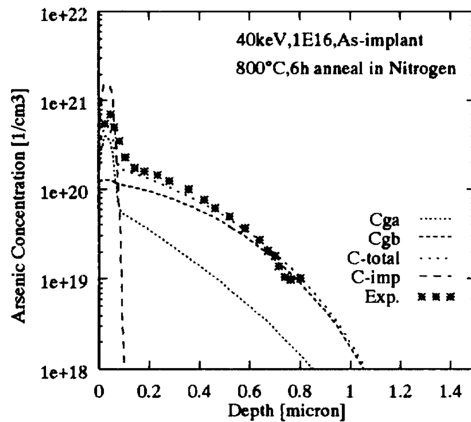


Figure 1: As diffusion in thick poly-layer and comparison with experimental results [6].

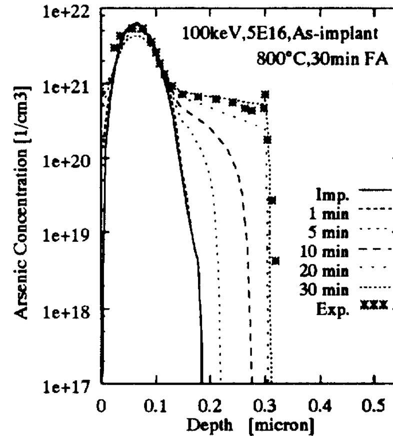


Figure 2: As diffusion in 0.3$\mu$m poly-layer with interface pile-up and comparison with experimental data [7].

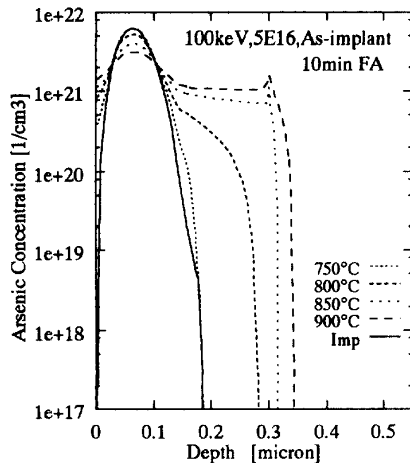


Figure 3: Simulation As-diffusion in 0.3$\mu$m poly-layer from 750°C - 900°C.

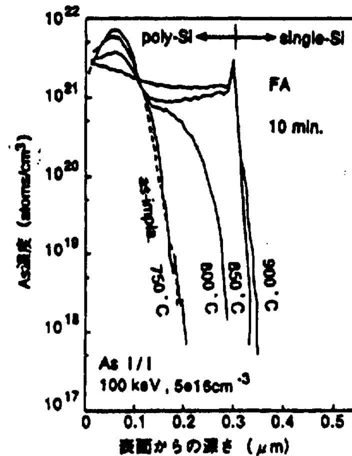


Figure 4: SIMS-profiles for 10 min. high dose As-diffusion

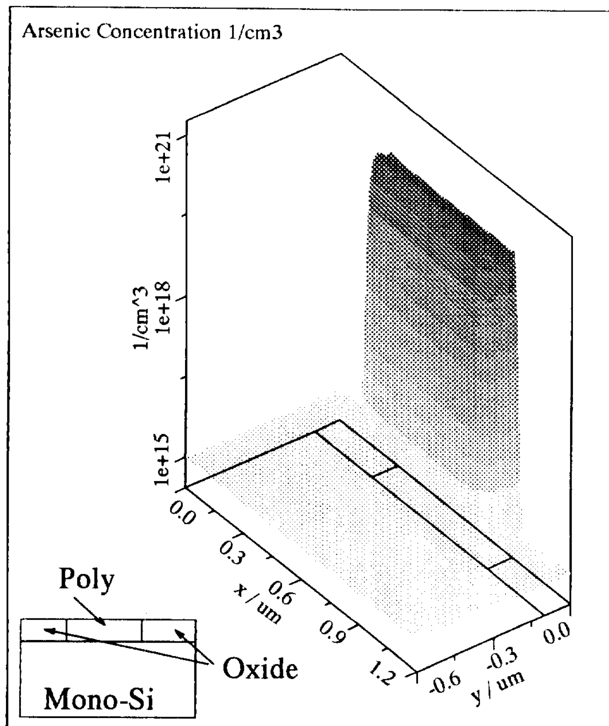


Figure 5: Outdiffusion of Arsenic from 0.6x0.1$\mu$m poly emitter

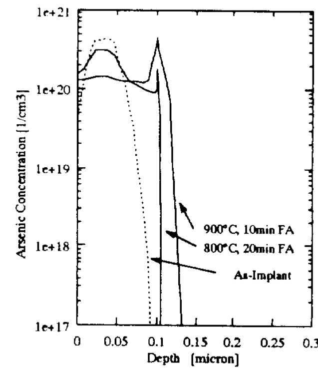


Figure 6: One-dimension Simulation results; emitter depth $W_d$=40nm for 900°C 10min.FA.

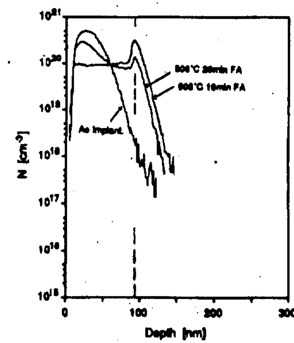


Figure 7: SIMS-measured As profile in a poly-Si emitter

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