# A Two-Dimensional Dopant Diffusion Model for Polysilicon

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We present a two-dimensional simulation model for dopant diffusion in polysilicon, 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 subsequent thermal 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]. Owing 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.

The system in which a dopant diffuses in polysilicon via grain boundaries and grain interiors can be described by a set of coupled PDEs, while the grain growth kinetics can be simulated with an additional PDE. 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. 1-3, where $s$ denotes the charge state of the dopant and $r$ is the effective grain size which can be seen as the reciprocal grain boundary area per unit volume. We calculate different grain sizes for the both coordinates due to different grain growth rates in lateral and vertical direction. The tensor $\gamma$ denotes a weighting factor for the diffusion flux taking into account these different grain sizes to incorporate the specific diffusion behavior of polysilicon; $\gamma_{11}$ is given by the quotient of the lateral and vertical grain size for the lateral diffusion flux, where in vertical direction the whole diffusion flux is taken ($\gamma_{22} = 1$). The electrostatic potential $\psi$ is calculated by assuming Boltzmann statistics for the electron and hole concentration and local charge neutrality. Diffusion and segregation kinetics is followed after [2, 3]. Eq. 3 describes the generation/recombination term of the exchange of dopants between grain interiors and grain boundaries by use of trapping factor $t$ and emission factor $e$, where $T_b^{max}$ denotes the maximum number of free states in the grain boundary. If the grain boundary is not filled with dopants, active dopants from the grain interior sites are delivered if they are not clustered, whereas dopants diffuse into the grain interiors if the maximum number of free states in the grain boundary has been exceeded.

$$\frac{\partial C_{ga}}{\partial t} = \text{div}\left(D_{ga}\cdot\left(\text{grad}\,C_{ga} + s\cdot\frac{C_{ga}}{U_T}\cdot\text{grad}\,\psi\right)\right) - G_{seg} \tag{1}$$

$$\frac{\partial C_{gb}}{\partial t} = \text{div}\left(\gamma\cdot D_{gb}\cdot\left(\text{grad}\,C_{gb} + \frac{C_{gb}}{r}\cdot\text{grad}\,r\right)\right) + G_{seg} \tag{2}$$

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

$C_g^{sol}$ is the solubility limit for the dopant species; it 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 after [4]. Using the static clustering approach implies the assumption that dopants can be delivered fast enough from the grain interior regions into the grain boundary so that no temporary leak of dopants occurs in the grain boundaries. Otherwise a dynamic clustering model has to be implemented. At the moment our results do not give any reason to account for dynamic clustering in the polysilicon material. However, in the crystal silicon dynamic clustering should be included to give a more detailed description of the outdiffusion in mono silicon.

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 [5],[6] and depends on polylayer-thickness $\lambda$, grain boundary energy $\Delta\mu$, diffusion of dopants across the grain boundary $D_{ga}$ and temperature $T$

$$\frac{\partial r}{\partial t} = \frac{D_{ga}}{\lambda} \cdot \left[ 1 - e^{-\frac{\Delta\mu}{K \cdot T}} \right]. \tag{4}$$

Via the diffusion coefficient $D_{ga}$ the grain growth depends on the local net dopant concentration $C_{net}$. Due to the varying local dopant concentration the average grain size becomes non-uniform along the vertical and lateral direction, which agrees with morphological investigations from [7]. On the other hand this non-uniform grain size distribution causes an oriented diffusion flux for the grain boundaries. The above given grain growth model seems to be valid for low thermal budget processing, but by high-thermal processing an additional grain growth starts from the poly-Si/mono-Si interface, due to the large amount of generated impurities (vacancies and interstitials) [8]. To model this phenomenon the interface impurity concentration has to be incorporated into the calculation of the diffusion coefficient.

Figure 1 shows the simulation result for an outdiffusion process of arsenic from a 0.6x0.1$\mu$m poly-layer in mono-Si substrate. By using such a thin poly-layer a characteristic dopant pile-up at the mono-Si/poly interface takes place and fixed the final concentration in the substrate. In our simulations the interface is treated as an extraordinary grain boundary with a smaller number of free states and a higher trapping rate, due to the thin interfacial oxide layer.
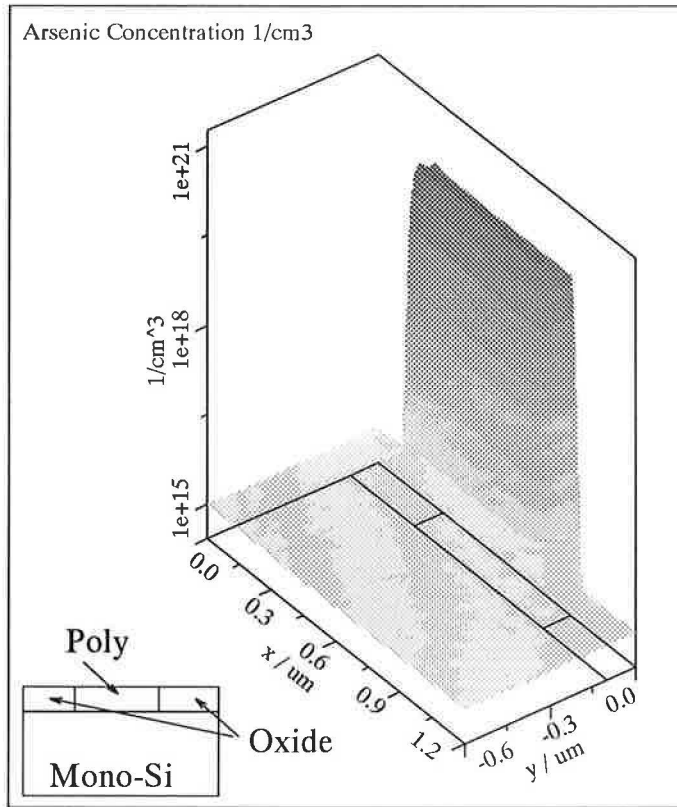


Figure 1: Outdiffusion of Arsenic from 0.6x0.1$\mu$m poly emitter

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