An Advanced Model for 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 based on thermodynamic concepts. For high dose implantation cases the trapping/emission mechanism between grain interiors and grain boundaries and the grain growth are the major effects during thermal treatment processes. The polysilicon grains itself are assumed to be tiny squares, growing from initial size. In order to handle nonplanar semiconductor structures, we use a transformation method for the simulation area as well as for the PDE's.**

I. Introduction

COMPUTER modeling of dopant diffusion in various semiconductor materials is a major task in process simulation. Rigorous diffusion models must incorporate a variety of effects such as the dual diffusion mechanism for silicon involving the lattice vacancy, introduced in 1974 by Hu [1], and the silicon self-interstitial for mediating the dopant diffusion. Oxidation enhanced/retarded diffusion [2] and retarded diffusion during thermal nitridation [3] and silicidation [4] are compatible with the dual mechanism. High concentration effects like clustering and precipitation are inherently connected to the processes of activation and deactivation of dopants [5], [6] and are still not quite well understood.

In recent years polysilicon layers are used in modern IC fabrication processes as diffusion sources, for instance for out-diffusion processes by forming an n-polysilicon-gate MOSFET or for emitter- and graft-base formation in high performance bipolar LSI's technology [7]. During annealing the dopant redistribution is strongly affected by the morphological structure of the polysilicon layer. The polysilicon crystal structure consists of mono-crystalline grain interiors and grain boundaries which are used as fast diffusion pathes due to the unusually large amount of lattice defects. If a dopant has diffused away from its lattice site following the grain boundary path, another dopant will be delivered from the surrounding grain interior regions. So four transport mechanisms for dopants can be detected: fast diffusion on grain boundaries, segregation between grain interiors and grain boundaries, dopant transport due to the movement of the grain boundaries related from grain growth, and the grain interior diffusion itself. To predict an accurate dopant profile a polysilicon diffusion model must include the above given transport mechanisms and, in addition, dopant clustering to account for excessively high dopant concentrations.

Previous work to model the diffusion process in polysilicon material has been presented by various authors. O'Neill *et al.* [8] presented a one-stream diffusion model for the grain boundary concentration neglecting the grain interior diffusion and the clustering physics. Jones *et al.* [9] and Lau *et al.* [10] used a two-stream diffusion model for the grain boundaries as well as for the grain interior regions but only a fit formula for the grain growth kinetics. Orlowski *et al.* [11] presented a new concept using a two-stream diffusion model in combination with fractal dimensions to describe the complex irregular structure of polysilicon.

We introduce a new model for the simulation of dopant diffusion in polysilicon using also a two-stream model with a static activation model in the polysilicon but a detailed description of the grain growth kinetics, which is a major task in polysilicon diffusion modeling. In SectionII we describe the basic PDE's for polysilicon diffusion which include the parallel transport mechanism and the dopant clustering. In Section III we give a detailed overview about the polysilicon grain growth kinetics. Finally, in Section IV we present several simulation results and the comparison with experiments.

II. The 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 PDE's, while the grain growth kinetics can be simulated with an additional PDE. To handle dopant clustering we use an algebraic equation to calculate the amount of active dopants which will be described later. The two-dimensional coupled PDE's for the active dopant concentration in the grain interior (C_{ga}) and the grain boundaries (C_{gb}) are given in (1) through (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. Due to different grain growth rates in lateral and vertical direction we calculate different grain sizes for the both coordinates. The tensor γ denotes a weighting factor for the diffusion flux taking into account these different grain sizes to incorporate the specific diffusion behavior of polysilicon; γ_{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 ψ

Manuscript received August 2, 1994; revised March 20, 1995. The review of the work was arranged by Associate Editor A. H. Marshak. This project was supported by the laboratories of SIEMENS Corporation, Munich, Germany, and Digital Equipment Corporation, Hudson, NY, USA.

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IEEE Log Number 9413944.

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is calculated by assuming Boltzmann statistics for the electron and hole concentration and local charge neutrality. Diffusion and segregation kinetics is followed after [10] and [12]. 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.

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

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

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

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 Eq. 4 after [13].

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

Fig. 1 shows the active and total dopant concentration for arsenic and boron using the static clustering model. 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 give no reason to account for dynamic clustering in the polysilicon material, but in the crystal silicon dynamic clustering should be included to give a more detailed description of the outdiffusion in the mono silicon.

III. Dynamic Grain Growth

Grain growth occurs during the thermal treatment. The basic mechanism for polysilicon material growth is the secondary recrystallization. During the growth process the structure of the polysilicon grains are changing. At the beginning we have a large amount of grains with a deposition-dependent average grain size. By applying a temperature gradient the grains are starting to growth via interstates to a small amount of large grains. Now we tried to calculate the migration of the grain boundaries to get a description of the dopant movement during grain growth. In this model the grains of polysilicon are assumed to be squares ($\gamma = 1$) growing from initial grain size r_0. The calculation of the migration of the grain boundaries is based on thermodynamic concepts of surface energy anisotropy and secondary grain growth [14], [15]. Fig. 2 illustrates the process to be modeled during grain growth. We consider growth for a single secondary grain, which has a minimized grain surface energy γ_{min}. To model the growth of secondary grains, we assume a cylindrical grain with predefined radius r_s and thickness h growing into a matrix of normal grains. The change in Helmholtz free energy ΔF for this transformation is given by (5),

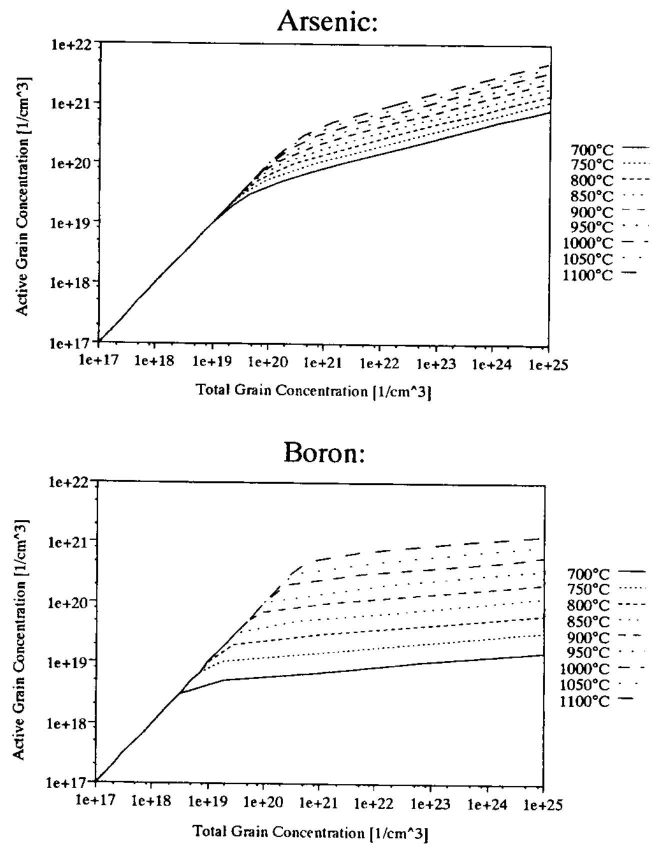

Fig. 1. Active and total dopant concentrations in grain interiors using a static clustering model.

$$\Delta F = -\frac{2 \cdot \Delta\gamma}{h} - N_n \cdot A_{gb} \cdot \gamma_{gb} + \frac{2 \cdot \gamma_{gb}}{r_s} \tag{5}$$

where $\Delta\gamma$ is the surface energy anisotropy, N_n the number of normal grains per unit volume, A_{gb} the grain boundary area and γ_{gb} the average grain boundary energy. Note, that the first two terms in (5) represent energies driving normal grain growth and the third term, due to secondary grain boundary energy, represents a barrier for grain growth. So surface energy and grain boundary energy determine the driving force of grain growth or the energy barrier on the other hand. For instance, grains with a crystallographic orientation near a orientation which minimizes the single surface energy will become secondary grains and this will lead to films composed of large grains with uniform crystallographic texture.

From basic rate theory, the rate of atomic transfer of dopants from lattice sites of one grain to those of a neighbor site is given by a complementary Arrhenius law in (6),

$$\Delta K = K^+ \cdot \left(1 - e^{-\frac{\Delta\mu}{k \cdot T}}\right) \tag{6}$$

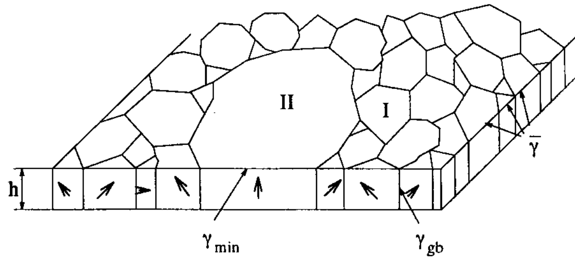

Fig. 2. Polysilicon film with thickness h composed of columnar normal grains **I** and an average surface energy $\overline{\gamma}$ and a single secondary grain **II** with a minimum surface energy γ_{min}.

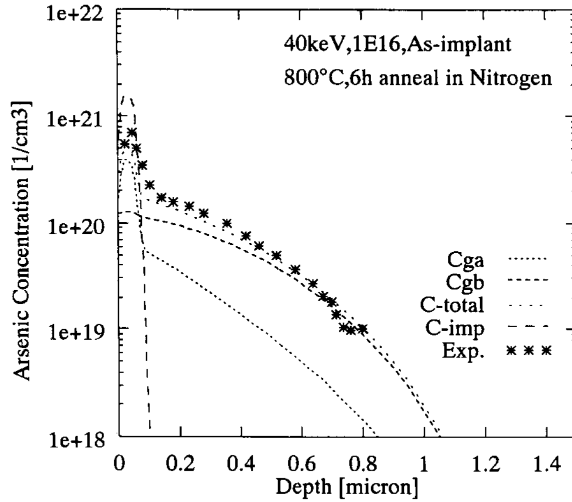

Fig. 3. Arsenic diffusion in 1.5 μm thick polysilicon layer and comparison with experimental results [12].

where K^+ denotes a jump frequency for atoms at the boundary and $\Delta\mu$ is the difference in the electrochemical potential on either side of the boundary and can be seen as an energetic limit for the dopants to diffuse into the neighboring grain. Under constant pressure and volume the electrochemical potential is given by (7). The boundary migration G which can be seen as a growth rate is obtained from (8).

$$\Delta\mu = \frac{\Delta F \cdot \overline{V}}{N}. \quad (7)$$

$$G = \lambda \cdot \Delta K \quad (8)$$

N denotes Avogadro's number, $\overline{V}$ the atomic volume, ΔF the change in Helmholtz free energy is given by (5), and λ the thickness of the boundary. The jump frequency K^+ can be expressed in terms of the temperature dependent diffusivity, thus the growth rate reads

$$\frac{\partial r}{\partial t} = \frac{D_{ga}(C_{net})}{\lambda} \cdot \left[1 - e^{-\frac{\Delta\mu}{k \cdot T}}\right]. \quad (9)$$

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 nonuniform along the vertical and lateral direction, which agrees with morphological investigations from [16]. On the other hand this nonuniform 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) from interface oxidation [17]. To model this phenomenon the interface impurity concentration has to be incorporated into the calculation of the diffusion coefficient.

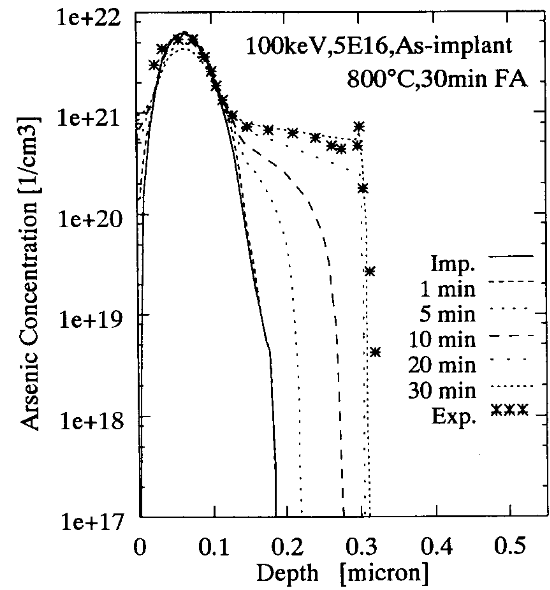

Fig. 4. Arsenic diffusion for 30 min in 0.3 μm polysilicon layer with interface pile-up and comparison with experimental data [16].

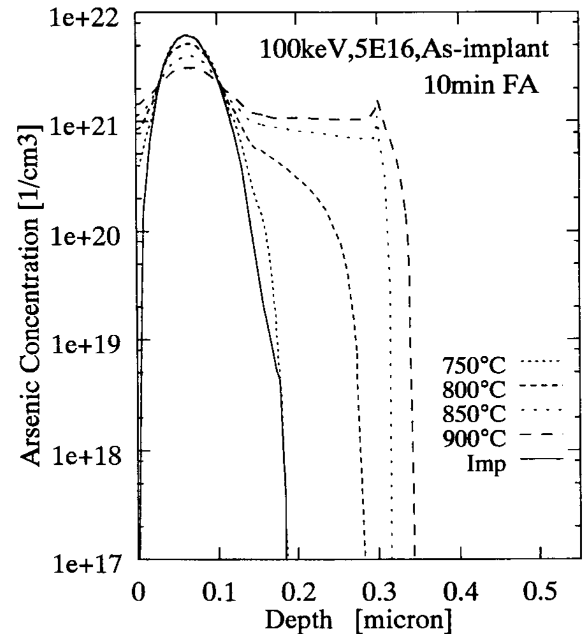

Fig. 5. Arsenic diffusion for 10 min in 0.3 μm polysilicon layer for a temperature range of 750°C–900°C.

IV. Simulation Results

We implemented our model using VISTA's [18] two-dimensional process simulator PROMIS [19]. Fig. 3 shows

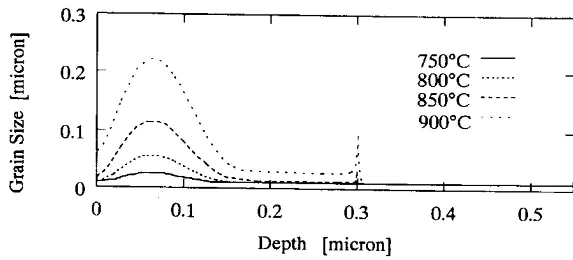

Fig. 6. Temperature- and dopant-dependent grain growth for a temperature range of 750°C–900° C according to concentration profiles of Fig. 5.

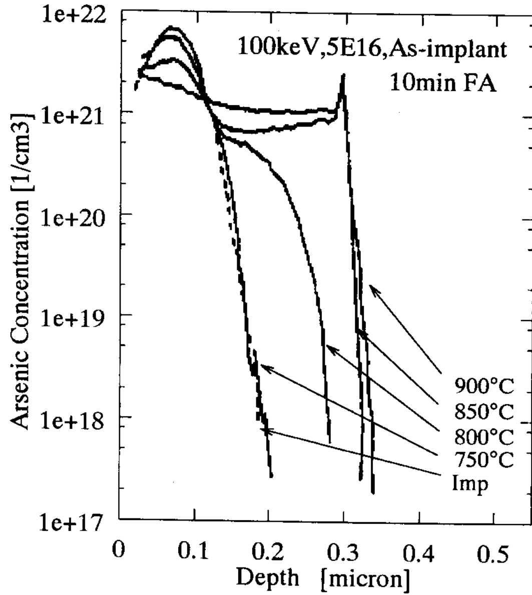

Fig. 7. SIMS profiles for 10-min high dose arsenic furnace annealing received from Kodate *et al.* [17].

the one-dimensional cross section for a 6 h 800°C As-annealing process in nitrogen on a planar 1.5 μm thick poly-layer and the comparison with the experimental RBS profile from Swaminathan *et al.* [15]. The implantation peak near the surface still remains during annealing due to dopant clustering; only dopants below the solubility limit are available for fast diffusion in the grain boundaries, so the concentration tail is determined by the grain boundary diffusivity. In this case the arsenic concentration does 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 the typical pile-up in the arsenic concentration at the interface in Fig. 4. 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. 5 shows the results for high dose As-implantation and 10-min annealing at temperature range from 750°C to 900°C on a 0.3 μm poly-layer. As expected in the 750°C and the 800°C case the dopant diffusion is relatively slow, where in the 850°C and 900°C case the poly-layer is full with dopants, so the dopant exchange between grain interiors and grain boundaries is the dominating dopant transport mechanism.

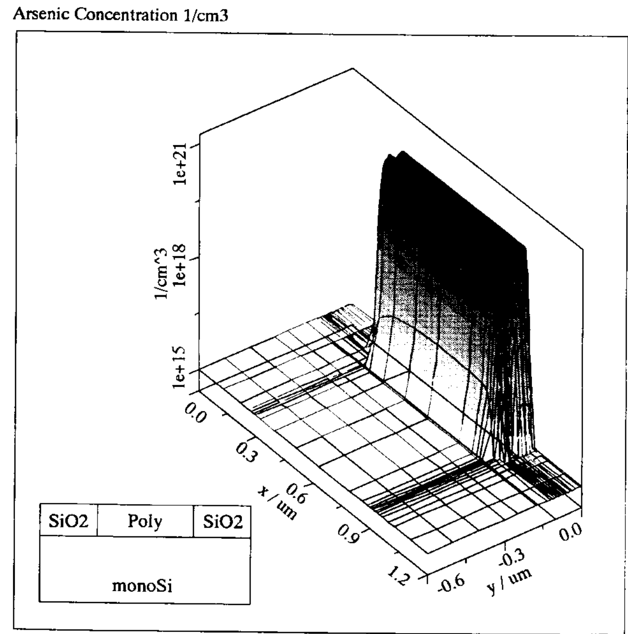

Fig. 8. Simulation of an arsenic outdiffusion from 0.6 × 0.1 μm poly emitter layer at 900°C and 10 min. furnace annealing.

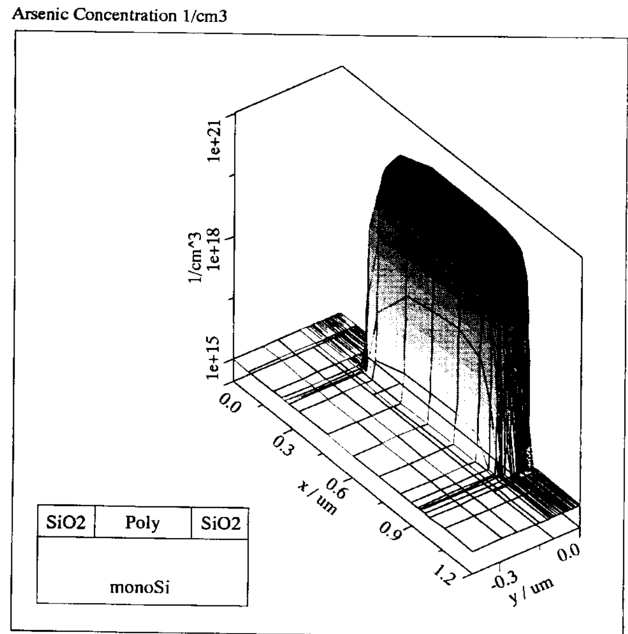

Fig. 9. Simulation of an arsenic outdiffusion from 0.6 × 0.1 μm poly emitter layer at 800°C and 20 min. furnace annealing.

If we look at the vertical grain size in Fig. 6, which is limited by the layer-thickness itself, a strong dopant dependent grain growth has occurred in the high temperature cases. Experimental SIMS results in Fig. 7 from Kodate *et al.* [20] show good agreement with our simulations. We used an initial grain size of 10 nm which corresponds with a previous LPCVD deposition process at 580°C for the grain growth model. Generally, the knowledge of the previous deposition conditions is important for the initialization of the grain growth model.

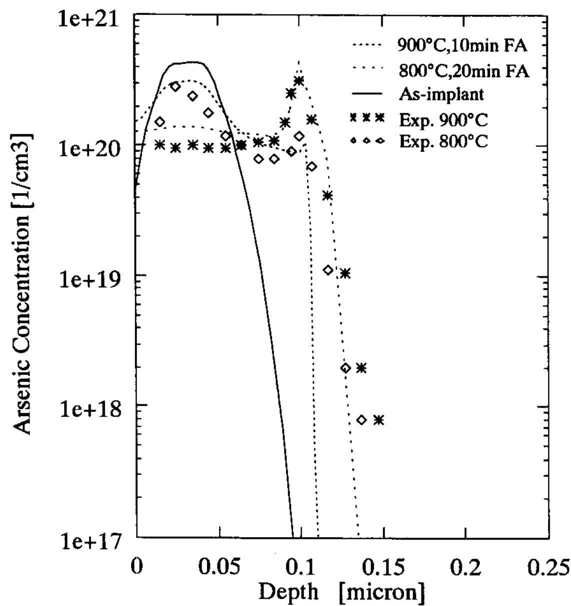

Fig. 10. One-dimensional simulation results in the mid-emitter region and comparison with SIMS profiles [7]. An emitter depth $W_d = 40$ nm for 900°C 10-min furnace annealing can be calculated.

Finally, Fig. 8 shows the result of an outdiffusion simulation from a 0.6×0.1 μm poly-layer in mono-Si substrate for 900°C. The simulation of this example was performed with two different thermal budgets. The first simulation was done at 900°C annealing temperature and 10-min annealing time, where the grain interior cluster concentration in the grain interiors is fully segregated into the poly-Si/mono-Si interface. The same simulation at 800° anneal temperature and 20-min annealing time shows in Fig. 9 a large amount of already clustered dopants near the surface which are not available for dopant segregation at the poly-Si/mono-Si interface due to the low process temperature. In the 900°C case we have a fully established poly-Si/mono-Si interface with a almost constant concentration along the interface, but we get only a weak doping concentration in the polysilicon corners in the 800°C case. Fig. 10 gives the one-dimensional results in the mid-emitter region. For the 900°C case an emitter depth (W_d) of 40 nm is computed, which agrees with SIMS measurements [7] at higher concentrations, where at lower concentrations a significant leak of dopants can be recognized, because vacancy and interstitial diffusion is neglected in our model.

V. Conclusion

A new model for dopant diffusion in polysilicon including dynamic grain growth and dopant clustering was introduced. To model these effects the conventional nonlinear PDE's for dopant diffusion are coupled with a PDE for grain growth and an algebraic equation for dopant activation. The complex morphological structure of polysilicon has demanded models for an effective grain size and grain growth to approximate the real conditions. With low thermal budget processes the major effect is given by fast dopant diffusion in the grain boundaries, whereas with increasing process temperature the grain growth kinetics gain significance.

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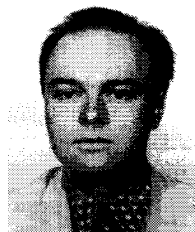

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