TWO STREAM MODEL FOR DOPANT DIFFUSION IN POLYSILICON INCORPORATING EFFECTS OF GRAIN GROWTH

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Abstract

We have developed a two stream model for dopant diffusion in polysilicon which also takes into account dopant incorporation into the grain boundary from the grain interiors as a result of grain boundary movement. With this model we are able to match dopant profiles following implants and low thermal budget anneals. Grain growth in polysilicon is accounted for using a model similar to that of Kim and Thompson [1]. We have also carried out further experiments, including investigation of TED in polysilicon.

INTRODUCTION

Doped polysilicon films are widely used in the semiconductor industry as gate electrodes, emitters and diffusion sources for shallow junctions. With dimensions and junction depths tending towards the deep submicron (with corresponding lower thermal budgets), accurate predictions of the doping profile in polysilicon has become necessary for efficient process development.

Dopant redistribution in polysilicon is strongly affected by the morphological structure of the material itself. Thin polysilicon films typically have columnar grains separated by regions of high defect concentrations referred to as grain boundaries. There are at least four important processes involving dopants in polysilicon: grain interior diffusion (both laterally towards the grain boundaries and vertically), dopant transport due to dopants being swept up by grains as they grow, segregation from the grain interiors to the grain boundaries, and fast diffusion along the grain boundaries. Accurate modeling of dopant diffusion in polysilicon requires that all four of these processes be correctly accounted for in the model. Figure 1 illustrates a typical arsenic profile in polysilicon after annealing at 800°C for 6 h [2]. The peak region near the surface is caused by the relatively slow diffusion of arsenic in the grain at this temperature (further reduced since the peak concentrations exceed the solid solubility limit), and the tail is caused by fast diffusion of the dopants which have become incorporated into the grain boundaries. This work aims at developing consistent models for dopant diffusion in polysilicon, grain growth kinetics and grain boundary segregation, as well as the interactions between these processes.

TWO STREAM MODEL

Implementing a full 2D or 3D model incorporating all four processes is difficult due to the moving boundaries associated with grain growth. However, grain growth effects can be incorporated relatively easily into two-stream models. Two stream models divide the dopant concentration into dopants within the grain and dopants in the grain boundary, coupled by dopant transfer from the grains to the grain boundaries and have previously been used by several groups [3, 4, 5].

In one dimension, the model equations are:

$$\frac{\partial C_{\mathrm{A}}^{\mathrm{g}}}{\partial t} = \frac{\partial}{\partial x}\left(D_{\mathrm{A}}^{\mathrm{grain}}\frac{\partial C_{\mathrm{A}}^{\mathrm{g}}}{\partial x}\right) - k_{\mathrm{eff}}\left(C_{\mathrm{A}}^{\mathrm{g}} - \frac{C_{\mathrm{A}}^{\mathrm{gb}}}{s}\right) \tag{1}$$

$$\frac{\partial C_{\mathrm{A}}^{\mathrm{gb}}}{\partial t} = \frac{\partial}{\partial x}\left(\frac{D_{\mathrm{A}}^{\mathrm{gb}}}{L_{\mathrm{g}}}\frac{\partial\left(C_{\mathrm{A}}^{\mathrm{gb}}L_{\mathrm{g}}\right)}{\partial x}\right) + k_{\mathrm{eff}}\left(C_{\mathrm{A}}^{\mathrm{g}} - \frac{C_{\mathrm{A}}^{\mathrm{gb}}}{s}\right) \tag{2}$$

$C_{\mathrm{A}}^{\mathrm{g}}$ is defined as the concentration of dopant A in the grain interior averaged over both the grain and grain boundary volumes,

$$C_{\mathrm{A}}^{\mathrm{g}} = \left(\frac{\text{number of dopants in grain interior}}{\text{unit polysilicon volume}}\right). \tag{3}$$

Similarly, $C_{\mathrm{A}}^{\mathrm{gb}}$ is defined as the concentration of dopant A in the grain boundary averaged over both the grain and grain boundary volumes,

$$C_{\mathrm{A}}^{\mathrm{gb}} = \left(\frac{\text{number of dopants in grain boundary}}{\text{unit polysilicon volume}}\right). \tag{4}$$

The total doping is then just the sum of the grain and the grain boundary components,

$$C_{\mathrm{A}}^{\mathrm{total}} = C_{\mathrm{A}}^{\mathrm{g}} + C_{\mathrm{A}}^{\mathrm{gb}}. \tag{5}$$

For the grain interior diffusvity, we use a model identical to the single crystal model with parameters from isoconcentration experiments. For arsenic, we also incorporate the effect of very high concentrations on diffusivity [6],

$$D_{\mathrm{A}}^{\mathrm{g}} = D_0 + D_{-}\left(\frac{n}{n_{\mathrm{i}}}\right)\left[1 + \left(\frac{n}{C_{\mathrm{ref}}}\right)^3\right]. \tag{6}$$

We also have incorporated solid solubility effects for arsenic in the grain interiors. Hence, $C_{\mathrm{A}}^{\mathrm{g}}$ in equations (1) and (2) actually represents $\min(C_{\mathrm{A}}^{\mathrm{ss}}, C_{\mathrm{A}}^{\mathrm{g}})$. Also when calculating $D_{\mathrm{A}}^{\mathrm{g}}$ we use the solid solubility for arsenic [7] to calculate the active concentration of dopants in the grain interior. The grain boundary diffusivity is given by

$$D_{\mathrm{A}}^{\mathrm{gb}} = D_0^{\mathrm{gb}} \exp\left(-E_{\mathrm{A}}^{\mathrm{gb}}/kT\right), \tag{7}$$

where D_0^{gb} and $E_{\mathrm{A}}^{\mathrm{gb}}$ are calculated from experimental observations [2].

The effective segregation coefficient between grain interiors and grain boundaries is normalized by the relative volumes giving

$$s = 2m_{\mathrm{seg}}W_{\mathrm{gb}}/L_{\mathrm{g}}, \tag{8}$$

where m_{seg} is the grain boundary segregation coefficient, W_{gb} is the average width of a grain boundary and L_{g} is the average grain diameter. Segregation has been characterized from data by Mandurah *et al.* [8] and Swaminathan *et al.* [9] and the dependence on dopant concentration has been included.

Throughout our analysis we have assumed circular cylindrical grains although most of the results are equivalent for square cylindrical grains. For transfer of dopants from the grain interior to the grain boundaries, there are two important mechanisms: lateral diffusion of dopants within the grains towards the grain boundaries and sweeping up of dopants by the grain boundaries as the grains grow. If $\sqrt{D_{\mathrm{A}}^{\mathrm{g}}t}$ is much smaller than the grain diameter, not much dopant can be transferred to the grain boundaries by lateral diffusion of dopants only. Hence, we will grossly underestimate the amount of dopant which segregates to the grain boundary if we do not account for grain growth. We also assume that the segregation at the grain/grain boundary interface is fast. The effective transfer rate k_{eff} is given by

$$k_{\mathrm{eff}} = k_D + k_v. \tag{9}$$

The transfer rate component arising out of lateral dopant diffusion within the grain, k_{D}, is similar to a model by Sadovnikov [4],

$$k_D = \frac{D_{\mathrm{A}}^{\mathrm{g}}}{L_{\mathrm{g}}}\left[\frac{2\beta}{L_{\mathrm{g}}} + \frac{1}{2\sqrt{D_{\mathrm{A}}^{\mathrm{g}}t}}\right]. \tag{10}$$

The factor β is calculated to be 2.9 based on steady state diffusion in a cylindrical grain [10], while Sadovnikov used $\beta = 2$.

The contribution of grain boundary motion to dopant incorporation into the grain boundary, k_v, includes the time rate of change of grain size. We assume that the effective average grain boundary velocity is proportional to the grain growth rate,

$$v_{\mathrm{eff}} = \gamma \frac{dL_{\mathrm{g}}}{dt}, \tag{11}$$

so that

$$k_v = \frac{2v_{\mathrm{eff}}}{L_{\mathrm{g}}} = \frac{2\gamma}{L_{\mathrm{g}}} \frac{dL_g}{dt}. \tag{12}$$

The grain growth model is based on the work of Kim and Thompson [1] which assumes that grain growth is proportional to the square root of time,

$$L_{\mathrm{g}}(t) = \left[L_{\mathrm{g}0}^2 + 2\sigma t\right]^{\frac{1}{2}}, \tag{13}$$

where σ is a parameter which depends on the grain boundary mobility and the grain boundary energy. Grain boundary mobility is dependent on local Fermi level and hence on local dopant concentration. As the dopant concentration varies with depth, grain boundary mobility also varies with depth, and hence we get different amounts of grain growth in different regions of the sample. Figure 2 shows a comparison of grain growth predicted by the model with data from Kim and Thompson [1]. The grain growth parameter σ has been optimised to fit grain growth data over a range of temperatures and doping levels.

EXPERIMENTS

The models were compared to the experimental work of Swaminathan *et al.* [2], which consisted of arsenic implants into thick polysilicon with varying grain sizes and followed by annealing. We also carried out further similar experiments to investigate transient enhanced diffusion effects as well as the impact of initial grain size on post-anneal dopant profiles and grain growth. Polysilicon was deposited by LPCVD at 625°C and a pressure of 0.25 Torr. The as-deposited grain size was found to be 0.2μm. Samples of polysilicon were annealed at 1100°C for 0 to 6.5 h to get different grain sizes. Subsequently, all samples were implanted with an arsenic dose $7 \times 10^{15}\mathrm{cm}^{-2}$ at 40 keV. A cap oxide was deposited to prevent loss of dopants and the samples were annealed. The dopant profiles were measured using secondary ion mass spectroscopy (SIMS). Grain sizes were measured using transmission electron microscopy (TEM) and scanning electron microscopy (SEM). For SEM measurements, grain boundaries were delineated using an etchant comprised of nitric acid, hydrofluoric acid and deionized water [11].

RESULTS AND DISCUSSIONS

We implemented the model described above in PEPPER [12] using the "dial-an-operator" mode. Figures 1 and 3 compare model simulations to Rutherford backscattering (RBS) profiles from Swaminathan *et al.* [2] for a 6 h anneal at 800°C in a 1 μm thick poly layer. The peak remians near the surface due to the low diffusivity at low temperature and solid solubility effects. The reduction in the peak from the as-implanted profile is due to transfer of dopants from the grain interior to the grain boundary, primarily as a consequence of grain growth. The tail region of the profiles is due to rapid diffusion of dopants which have been incorporated into the grain boundary regions.

As seen in Figure 3, the model does a good job of accounting for the effects of initial grain size on the profiles. However, to match the dopant incorporation into the grains in our model with experimental data, it was necessary to use a γ of about 5 at 800°C. Possible explanations for the value of γ being substantially higher than 1 include dopant incorporation into grain boundaries during epitaxial regrowth following ion implantation, transient enhanced diffusion (TED) due to excess defect concentrations following the implant, and grain boundary motion which does not result in grain growth. The first two possibilities would lead to strongly enhanced dopant incorporation into the grain boundaries at short times. Figure 4 shows that the simulated profiles for annealing at 800°C for 25 min matches the data for a 20 min (plus push and pull of wafers into furnace) anneal. Since, the model described above is able to predict profiles for short times without incorporating effects of TED or dopant incorporation during regrowth, we conclude that these two processes have minimal effects for arsenic doped poly.

Figure 6 shows an example of comparison of the model predictions to data from our experiments. The same parameters do a reasonable job of matching the experimental results, but, in contrast to the profiles from Swaminathan *et al.* [2], there seems to be evidence for an effective grain boundary diffusivity which is concentration dependent.

CONCLUSIONS

A two stream model for dopant diffusion in polysilicon incorporating effects of grain growth has been developed and implemented. The model parameters were characterized based on experimental measurements of grain growth kinetics and grain boundary segregation. The model accounts for the dependence of arsenic diffusion profiles on initial grain size, with grain boundary motion providing the dominant mechanism for transfer of dopant to grain boundaries. Investigation of the time-dependence of profile evolution lead to the conclusion that TED effects are neglible for arsenic.

ACKNOWLEDGEMENTS

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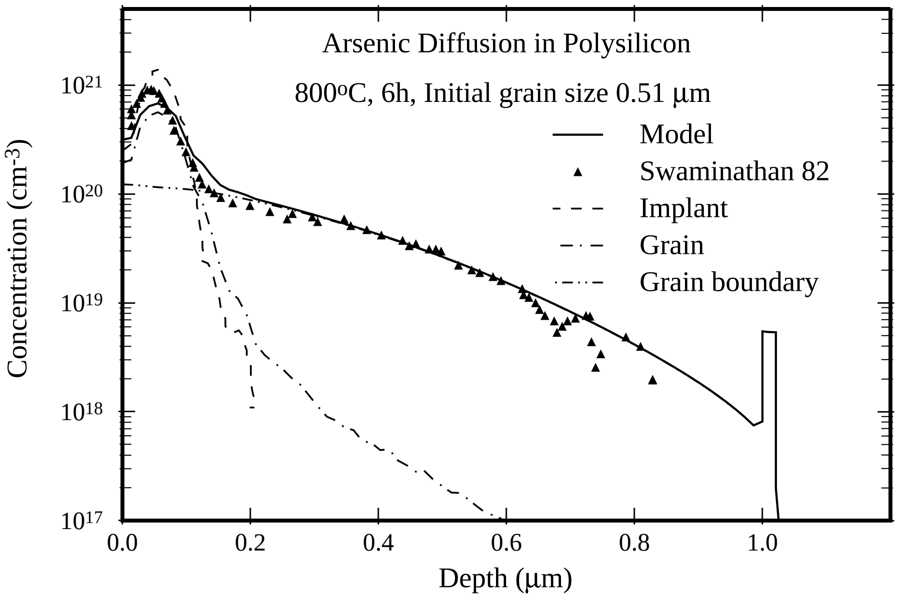

Figure 1: Comparison of RBS data from Swaminathan [2] with simulation of arsenic diffusion in 1μm poly annealed for 6 h at 800°C for a starting grain size of 0.51μm. Note that the width of interface peak is chosen to approximate SIMS broadening.

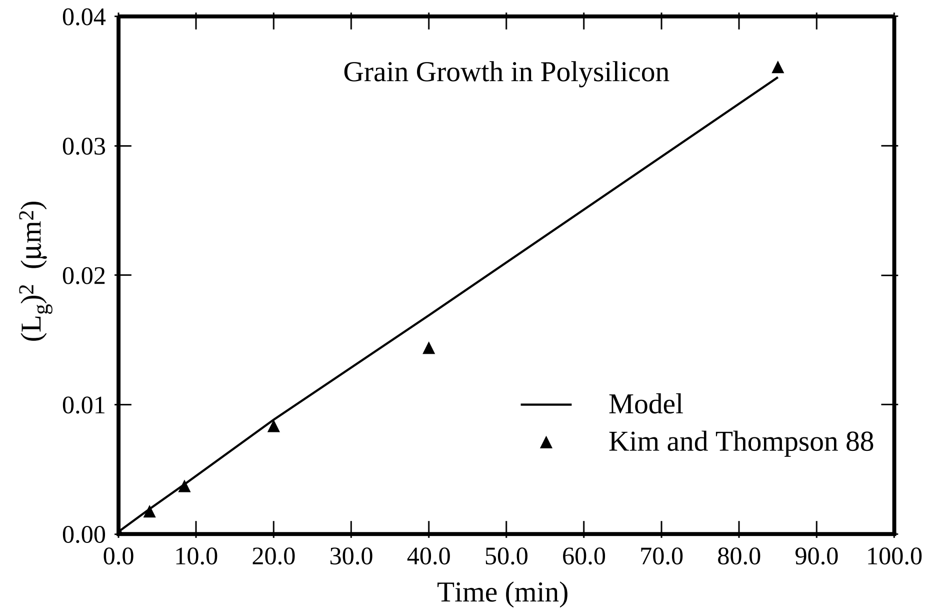

Figure 2: Comparison of predicted values of grain growth to experimental data from Kim and Thompson [1] for polysilicon doped uniformly with $5 \times 10^{20}\mathrm{cm}^{-3}$ of phosphorus and annealed at 950°C.

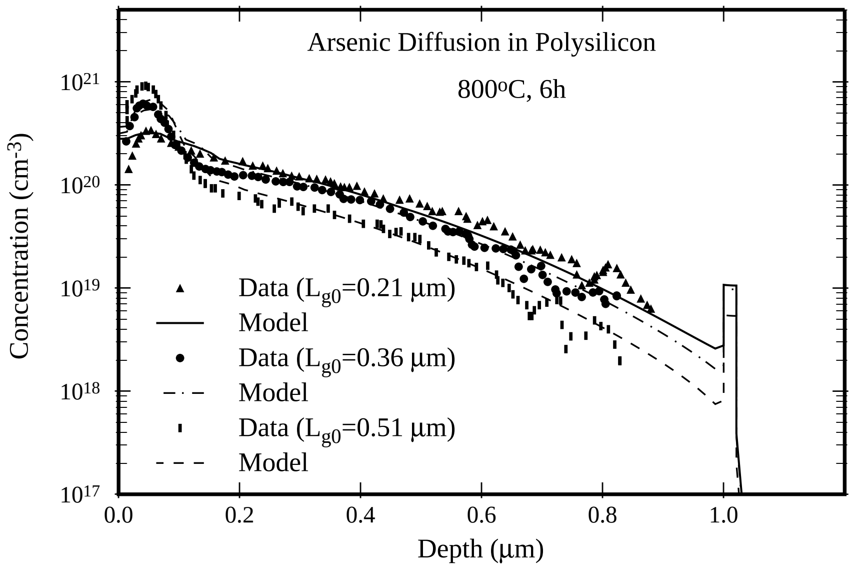

Figure 3: Comparison of RBS data from Swaminathan [2] with simulation of arsenic diffusion in 1μm poly annealed for 6 h at 800°C for different starting grain sizes.

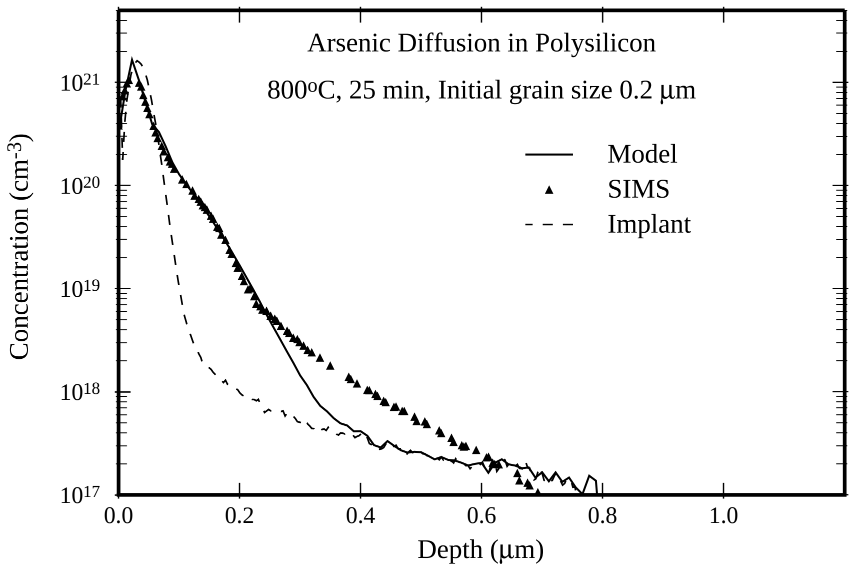

Figure 4: Comparison of arsenic profile from SIMS for implanted 0.8μm thick polysilicon film subjected to 20 min anneal at 800°C plus furnace push/pulls with simulation of 25 min anneal at 800°C. Starting grain size in poly is 0.2μm.

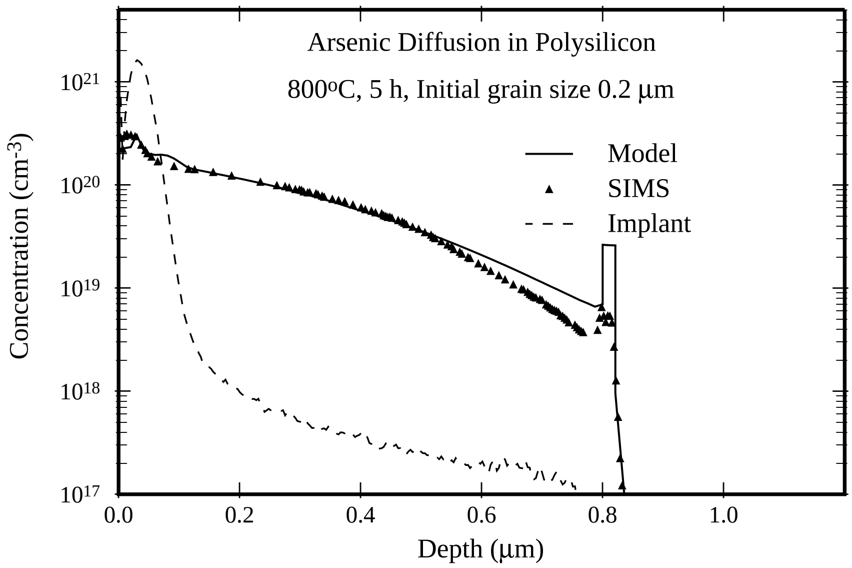

Figure 5: Comparison of SIMS data with simulation of arsenic diffusion in 0.8μm poly annealed for 5 h at 800°C. Starting grain size in poly is 0.2μm.

KEYWORDS

Polysilicon, poly, grain, grain boundary, grain growth, segregation, dopant diffusion, modeling, simulation.