Dynamic-clustering and Grain-growth Kinetics Effects on Dopant Diffusion in Polysilicon

M. Hane and S. Hasegawa
Microelectronics Research Laboratories, NEC Corporation
1120 Shimokuzawa, Sagamihara 229, Japan

A simulation model for dopant diffusion in polysilicon has been developed considering dynamic clustering and grain growth kinetics tightly coupled with dopant diffusion and segregation. The simulation results show that these effects are significant for high dose implantation case.

More precise models are becoming important for simulating modern polysilicon-related processes used for devices such as poly-Si-emitter BJTs and poly-Si-(p-,n-)gate MOSFETs, which are following the trend toward reduced thermal budget process. For such processes which utilize high-dose implantation and low-temperature annealing, a model for dynamic clustering and de-clustering is necessary to predict accurate dopant profile and its activation in the poly-Si, as well as being encountered in bulk-Si[1]. The situation becomes more complicated in the poly-Si case since clustering tends to compete with segregation and grain growth phenomena during diffusion process. Any advanced model must incorporate these phenomena in a tight coupling manner.

One-dimensional coupled equations for the dopant diffusion in the grain (C_g) and in the grain boundary (C_{gb}) are listed in Table.1. C_{gb} diffusion and segregation kinetics are followed after Refs. [2][3]. As shown in Figure.1, if the poly-Si layer consists of column-like grains with average size L_g surrounded by thin grain boundaries, one-dimensional description is permissible since the dopant diffusion is primarily vertical in a columnar structure through fast path along grain boundary, while lateral diffusion within a grain was taken approximately by the parameter λ [2] in Eqs. 1-2. Segregation coefficient (m_{seg}) was taken from [4]. Tsai's dynamic clustering model for mono-Si[5], was introduced with the modification regarding solid solubility limit, for clustered arsenic (C_{cl} in Eq. 2-3) in the poly-Si grain, which was not taken into account in the previous models[2][6][8]. For grain growth, an empirical model[6] based on Wada et al's experiment[7] was used preliminarily. In the works previously reported[2][8], the grain size was uniformly defined within a poly-Si layer through averaged or parameterized dopant concentration in their calculations. On the other hand, according to [7][9], grain growth depends on carrier concentration (n/n_i). Consequently L_g becomes non-uniform along a depth direction. In the present model, Eq. 4 was introduced to the couple of Eqs.1-3, to enable calculating the local n/n_i -dependent grain growth. The equations were solved by the program "ZOMBIE"[10].

Figure 2 shows the calculation results for implanted arsenic(As) diffusion in a thick poly-Si film for an annealing at 800°C for 6 hours. Here, the grain growth was calculated uniformly within the poly-Si film by using the conventional model[6] instead of using Eq. 4. Accurate reproduction of an experimental data[11](Fig.3) was reflected that the appropriate C_{gb} diffusivity and segregation model parameters. However, the grain growth kinetics effect is not clear in this case, since the grain size was uniformly defined within the poly-Si film and the low temperature grain growth was relatively slow. It becomes clear for much higher dose and temperature conditions.
Fig.4(a) and 4(b) show the results for a high-dose implanted As case, using uniform L_g growth[6][8] and Tsai's clustering parameters[5]. Fig.4(c) shows the result without clustering, for comparison, in which the immobile profile peak could not be reproduced. Experimental data[12] shown in Fig.5, could be reproduced for the 800°C case (Fig.4(a)) while the 900°C case (Fig.4(b)) could not be, where the experimental total As profile for the 900°C case was almost flat within the poly-Si layer. Fig.4(b) shows lower total concentration level than the experimental one (above $10^{21} cm^{-3}$) near the interface region, and also shows insufficient clustered As profile peak collapsing. They are due to both overestimating the grain growth and inadequacies in the clustering model. The grain growth model was modified to include local (n/n_i) dependence by using Eq.4. The clustering model was modified to allow the solubility limit for As in a poly-Si to become higher than that in a mono-Si, according to an experimental data[13]. Fig.6 shows the calculation result adopting the above two additional features. Fig.7 shows the corresponding grain size distribution in which the grain growth was enhanced mainly in the implanted region. In Fig.6, the resulting total As concentration around the flattened profile region agreed with the experimental data (exceeded $10^{21} cm^{-3}$), while the clustered As profile peak still remained near the surface region.

Dopant diffusion in poly-Si was simulated, taking into account the dynamic clustering and local grain growth. Low temperature high dose arsenic diffusion in poly-Si was successfully reproduced. It was found that detailed consideration of the initial condition for the electrical active concentration and more sophisticated de-clustering kinetics are necessary for the higher temperature case.

References

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$$\frac{\partial C_{gb}}{\partial t} = \frac{\partial}{\partial x}\left[D_{gb}\frac{\partial C_{gb}}{\partial x} + D_{gb}\frac{C_{gb}}{L_g}\frac{\partial L_g}{\partial x}\right] + 2\frac{v + D_g/\lambda}{L_g}(C_g - C_{gb}/m_{seg})$$
$$(\lambda = (1/(L_g/4) + 1/(2\sqrt{D_g t}))^{-1}) \quad (1)$$

$$\frac{\partial C_g}{\partial t} = \frac{\partial}{\partial x}\left[D_g\frac{\partial C_g}{\partial x} \pm \frac{q}{kT}D_g C_g\frac{\partial \phi}{\partial x}\right] - 2\frac{v + D_g/\lambda}{L_g}(C_g - C_{gb}/m_{seg})$$
$$-mK_C\,[C_g]^m\,n^k + mK_D C_{cl} \quad (2)$$

$$\frac{\partial C_{cl}}{\partial t} = K_C\,[C_g]^m\,n^k - K_D C_{cl} \quad (3)$$

$$\frac{\partial L_g}{\partial t} = \gamma\left(\frac{n}{n_i}\right)/L_g \quad (4)$$

Table.1 A set of the coupled equations used in the model. K_C and K_D are clustering and de-clustering coefficients[5], respectively, representing dynamic clustering kinetics newly added in the present model. $\gamma(n/n_i)$ implies grain-growth kinetics[7][9].

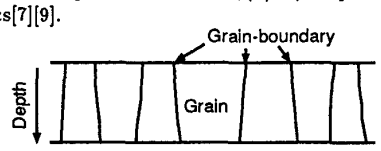


Figure.1 Assumed poly-Si film structure. One-dimensional description is permissible since the dopant diffusion is primarily vertical through fast path along the grain boundaries.

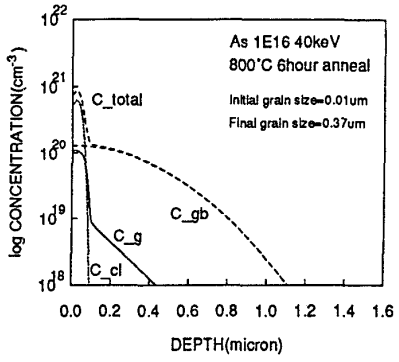


Figure.2 Calculation results for As diffusion in thick poly-Si.

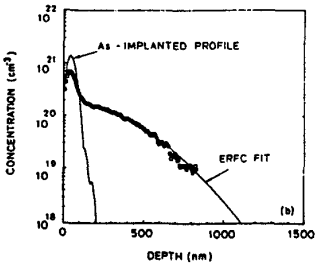


Figure.3 Experimental data corresponding to Fig.2.[11]. (Final grain size was $0.36\mu m$.)

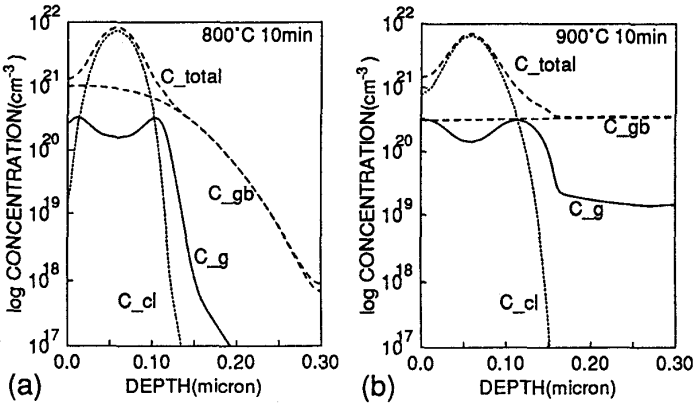


Figure.4 Calculation results for high dose ($5 \times 10^{16} cm^{-2}$) As diffusion in $0.3\mu m$ poly-Si, assuming uniform grain growth. (a) 800°C 10min, $L_g = 0.06\mu m$. (b) 900°C $L_g = 0.56\mu m$. (c) 800°C without clustering.

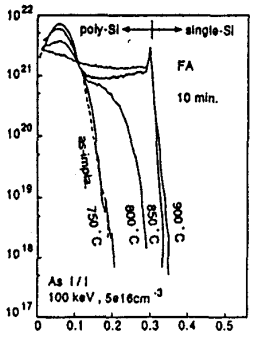
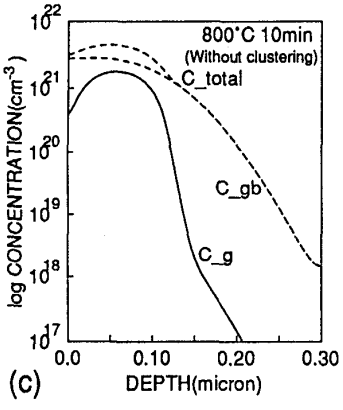


Figure.5 Experimental data for high dose As diffusion in $0.3\mu m$ poly-Si [12].



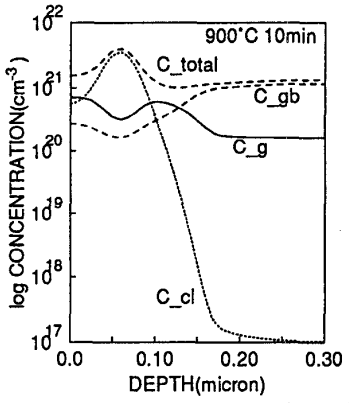


Figure.6 Calculation results for high dose ($5 \times 10^{16} cm^{-2}$) As diffusion for 900°C 10min, in $0.3\mu m$ poly-Si, assuming high solubility value[13] and local (n/ni)-dependent grain growth.

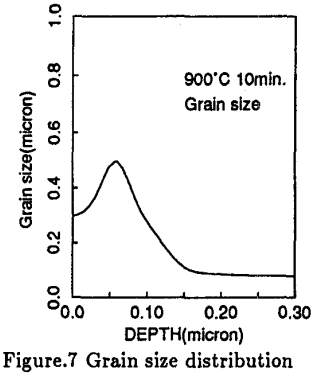


Figure.7 Grain size distribution for Fig.6 case.