NON-EQUILIBRIUM DIFFUSION PROCESS MODELING BASED ON THREE-DIMENSIONAL SIMULATOR AND REGULATED POINT DEFECT INJECTION EXPERIMENTS

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During the last decade, it has been continued to develop process simulation system which can predict impurity redistribution with final device structure, in order to have better understandings in advance of process operation[1-4]. Furthermore, very many improvements have been carried out each individual process simulator, for instance, implementation of point defect diffusion model, renewing of segregation coefficients,etc. Much more attention should be paid, however, to process modeling and process parameter than before, since without properly controlled they could have less margin in definite requirements and/or could alter completely device characteristics. On this view point, a new sophisticated experiment has been conducted for precise estimation of point defect diffusion coefficients and dopant diffusion coefficients in non-equilibrium condition.

Figure 1 shows a general concept of this experiment, in which total amount of point defect injection flux has been well regulated by varying the window area. Monitor region which has been buried underneath in the substrate is studied by SIMS and angle-bevel after oxidation, drive-in, or silicidation process. Various kinds of samples which have different thickness of silicon epitaxial layer and some other dopant layer are prepared. Anomalous dopant diffusion phenomena during a phosphorus drive-in diffusion and during a Ni silicidation process are summarized in Table 1. The results indicate that Si self-interstitial atoms are largely generated during the phosphorus drive-in process and that vacancies are generated during the silicidation process. Typical experimental results are presented in Fig.2 for various kinds of window area ratio. It should be noticed that the junction depths decrease markedly with decreasing the ratio.

Dopant diffusion coefficients are chosen to fit best the profiles by means of the least square method, which are represented in Fig.3, as a function of window area ratio. Dopant independent diffusion characteristic is obviously revealed for the first time. Dopant diffusion coefficient under equilibrium point defect concentration are considered entirely different from each other, however, observed diffusion coefficient under non-equilibrium condition is almost unique regardless of dopant species. Furthermore, dopant diffusion coefficients are found to increase in proportion to point defect injection flux.

Using the series of experimental results, the values of point defect diffusion coefficients(D_I, D_V), recombination rate(k_R), and so-forth have been obtained precisely as a parameter of a temperature ranged down to 750 °C through adjusting of 3-D process simulator. Silicon self-interstitial diffusion coefficient and equilibrium concentration measured in this work are shown in Fig.4. Previously wide scattered silicon self-interstitial diffusion coefficient comes well reliable by the accurate experiment at low temperature. Figure 5 shows a flow chart of newly developed 3-D simulator, in which a direct coupling model is adopted for calculation of dopant concentration profiles. Basic equations which govern diffusion characteristics are also presented. Finite deferential method using the discretized equation shown in Fig.6 is adopted. Figure 7 indicates a typical simulated result of 3-D point defect distribution using the measured values.

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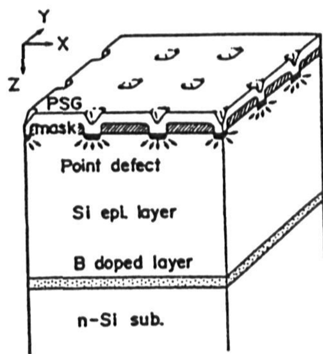


Fig.1 A general concept of sample structure.

Table 1 Summary of non-equilibrium dopant diffusion phenomena during a phosphorus drive-in diffusion and during a nickel silicidation process.

	Phosphorus drive-in diffusion	Ni silicidation
Boron	enhanced	not enhanced
Arsenic	enhanced	enhanced

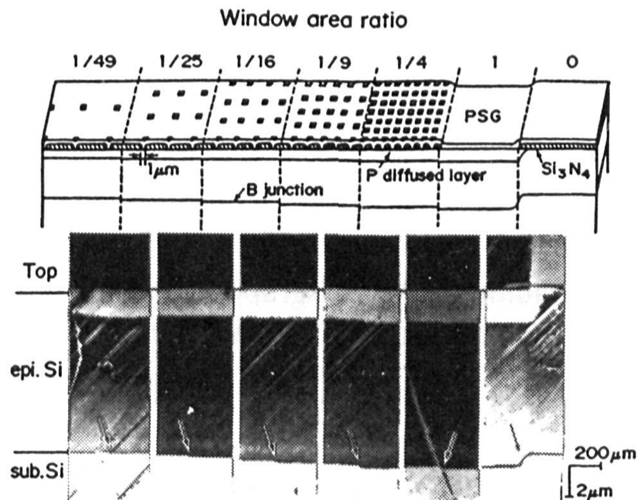


Fig.2 Typical experimental results of angle-lapped surfaces after the annealing of 16 hours at 850 °C. PSG films have been deposited for the point defect injection sources. Angle of bevelled sample was 34'. Arrows indicate junctions of monitor region.

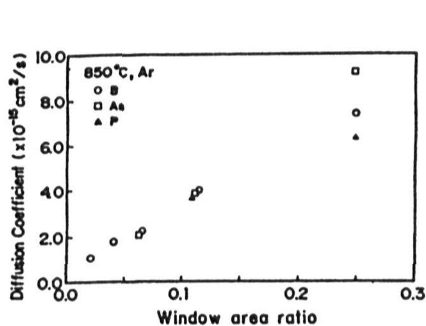
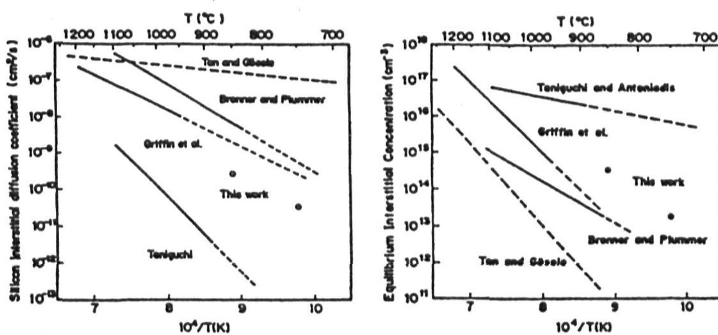


Fig.3 Dopant diffusion coefficients as a function of window area ratio.



(a) Diffusion coefficient. (b) Equiribrium concentration.

Fig.4 Silicon self-interstitial characteristics.

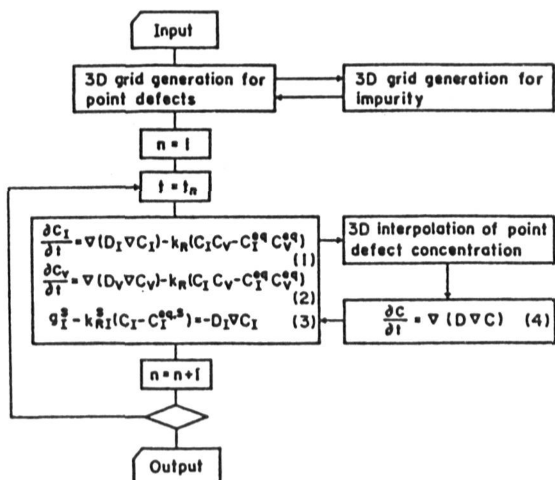


Fig.5 Flow chart of a 3-D simulator. Basic diffusion equations are written down in the figure. In the impurity diffusion equation (4), diffusivity(D) is defined to be $D=D_i(FC_I/C_I^*+(1-F)C_V/C_V^*)$, where C^* is point defect concentration in equilibrium, C_V, vacancy concentration, and C_I, interstitial concentration.

$$\frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial t}\right)\rightarrow\left\{\left(\frac{D_{i+1,j,k}+D_{i,j,k}}{2}\cdot\frac{C^{n+1}_{i+1,j,k}-C^{n+1}_{i,j,k}}{\Delta x_i}\right)-\left(\frac{D_{i,j,k}+D_{i-1,j,k}}{2}\cdot\frac{C^{n+1}_{i,j,k}-C^{n+1}_{i-1,j,k}}{\Delta x_{i-1}}\right)\right\}\Big/\left(\frac{\Delta x_{i-1}+\Delta x_i}{2}\right)$$

ΔZ_{k-1}, ΔY_j, (i,j,k), ΔX_{i-1}, ΔX_i, ΔY_{j-1}, ΔZ_k

Fig.6 Example of discretization method.

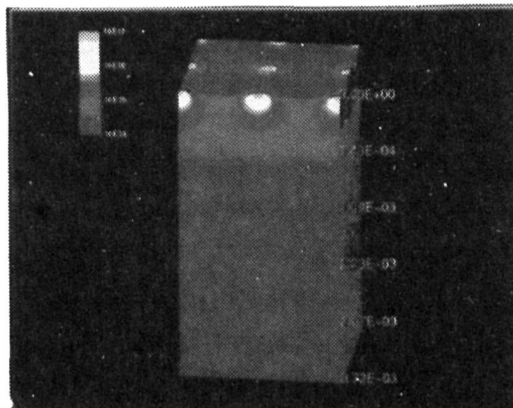


Fig.7 3-D simulation result of point defect distribution.