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# A New High-Speed Non-equilibrium Point Defect Model for Annealing Simulation

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## 1. Introduction

As state-of-the-art processes involve fast annealing times at reduced temperatures, it has become increasingly important to incorporate non-equilibrium point defect modeling into the simulation of diffusion [1,2,3]. Non-equilibrium point defect modeling takes into account the actual distribution the defects in the silicon when simulating the annealing of impurities. However, simulation time increases dramatically with the number of equations necessary to simulate multiple types of impurities simulated simultaneously (by a factor of $n^2$, n = no. of equations). Previous physically-based methods used 1D simulation of 1 impurity, since 2D simulation of multiple impurities required excessive CPU time making it difficult to use for practical applications. In this work, for the first time, a high-speed physically-based 2D method of simulating the annealing of multiple impurities is presented which requires only a fraction of the CPU time for simulation of several impurities simultaneously.

## 2. New High-Speed Method for Impurity Annealing Simulation

In this model, impurity diffusion in silicon is modulated through the E-center and kick-out mechanisms by the distribution of point defects. The diffusion of vacancies, interstitials, and impurity-point defect pairs can all be described by equations of the following form,

$$\frac{d x_1}{dt} = f1(x_1) + f2(x_1,...,x_n) \quad , \tag{1}$$

where f f1 is the diffusion term, f2 is the term describing the interaction between diffusion pairs, and $x_i$ represents the concentration of the diffused species i. f1 is described by the following equation,

$$f1(x_1) = \frac{\partial}{\partial \boldsymbol{r}}\left( D_{x_1} \frac{\partial}{\partial \boldsymbol{r}}[x_1] \right) \quad , \tag{2}$$

where $D_{x1}$ is the diffusion constant of the diffused species 1. The actual form of f2 depends upon the diffused element; for vacancies, it is represented by

$$f2 = -k_{bi}\left( [V][I] - [V]^{eq}[I]^{eq} \right) + \sum_D \left( k^r_{DI}[DV] - k^f_{DI}[D^+][V^-] \right) + \sum_A \left( k^r_{AI}[AV] - k^f_{AI}[A^-][V^+] \right) \quad , \tag{3}$$

where V is the vacancy concentration, I is the interstitial concentration, D is the donor concentration, A is the acceptor concentration, DV is the donor-vacancy pair concentration, AV is the acceptor-vacancy pair concentration, and k is the reaction constant.

To simulate the diffusion of four types of impurities taking into account non-equilibrium point defects, it is necessary to solve a system of 10 differential equations of the form of Eq. 1 simultaneously. If n differential equations of the form of Eq. 1 are solved for using the CGS method, the f2 term necessitates the calculation of a n-dimensional tensor, causing the CPU time to increase by a factor of $n^2$ (Fig. 1a). In this work, we have used the explicit method to solve the f2 equations of Eq. 1. Therefore, the calculation of a n-dimensional tensor becomes unnecessary, and CPU time increases only by a factor of n (Fig. 1b). In the case of 10 differential equations, simulation speed is increased by a factor of 10 (Fig. 2).

## 3. Simulation Results

We present results using the new simulation method incorporating non-equilibrium point defects in impurity diffusion. Fig. 3 shows the dose of boron paired with interstitial point defects versus time for diffusion into silicon. BI represents the boron-interstitial pair, and the number in parentheses represents the number of timesteps for the analysis. Because we use the explicit method to solve f2 of Eq. 1, we can see some oscillations of the BI (20) concentrations as time proceeds . Fig. 4 illustrates the impurity profiles of boron (B), interstitials (I), and vacancies (V) for various number of timesteps (again in parentheses). As can be seen from the figure, the number of timesteps has little effect on the impurity profile . As result the impurity profile can be accurately predicted with a minimum number of timesteps using this new method. Fig. 5 shows the impurity profiles of boron, phosphorus and arsenic, which were simulated simultaneously using this new method. The impurity profiles differ due to the different diffusion constants of each species. CPU time for 20 timesteps was 67 seconds on an HP 9000/735 workstation.

## 4. Conclusion

We have made feasible the simultaneous simulation of four different impurities in silicon while incorporating the effects of non-equilibrium point defects by using the explicit method to solve the interaction term between diffusion pairs in the system of differential equations. Using this method, the effect of high time-dependent defect concentration distribution near the initial stages of diffusion can be properly taken into account. This method is thus expected to play an important part to predict device processes utilizing rapid thermal annealing (RTA). Future work includes more detailed verification of simulation results and accurate parameter extraction.

References
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[2] W. B. Richardson and J. Mulvaney, "Noequilibirium behavior of chargedpoint defects during phosphorus diffusion in silicon," J. Appl. Phys., vol.65, pp. 2243-2247, 1989.
[3] W. B. Richardson and J. Mulvaney, "Plateau and kink in P profiles diffused into Si: a result of strong bimolecular recombination?," Appl. Phys. Lett, vol. 53, pp. 1917-1919, 1988.

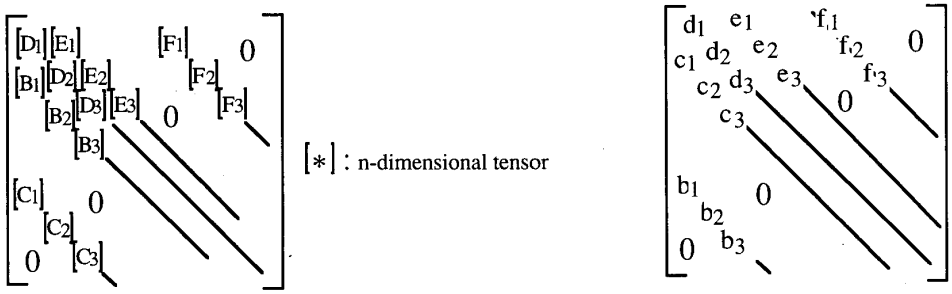


Fig. 1 . The matrix for solving differential equations of the form of Eq.1

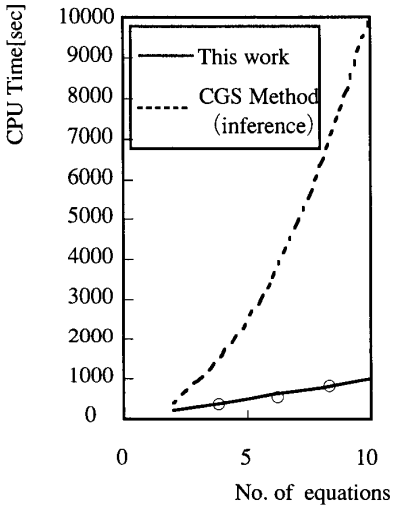


Fig.2 . Comparision of CPU Time for solving the differential equations of Eq. 1.

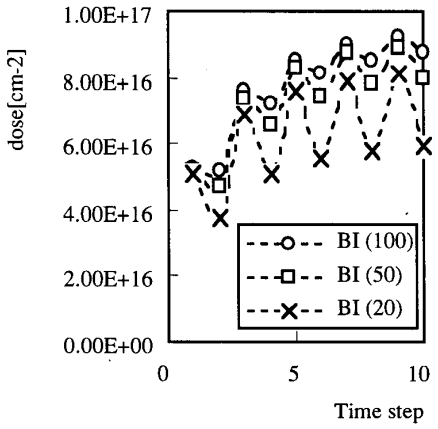


Fig.3. Dose of boron-interstitial pairs at each time step for differnt number of timesteps.

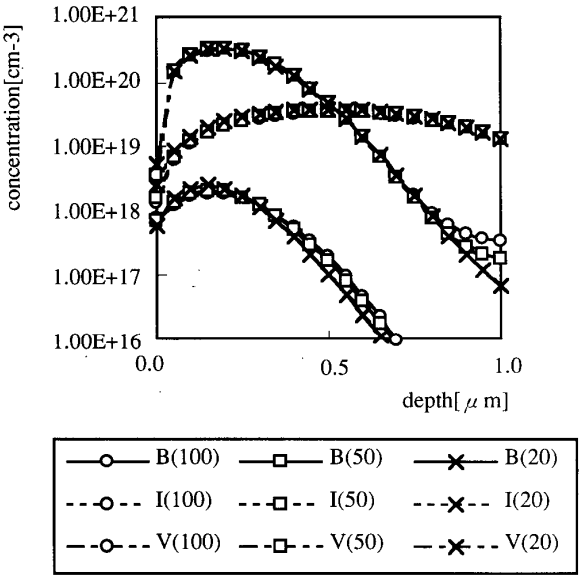


Fig.4. Plots of boron, interstitial, and vacancy concentrations versus depth for different number of timesteps.

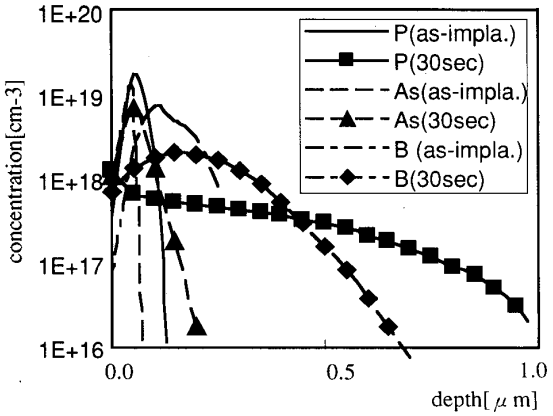


Fig.5. Plots of concentration versus depth of various impurities simulated simultaneously (T=900℃).