Consistent Models for Point Defects in Silicon

P. B. Griffin, P. A. Packan and J. D. Plummer
Stanford University, Stanford, CA 94305.

Introduction

An understanding of the role of point defects in silicon is necessary to rigorously model the evolution of impurity profiles, the growth and shrinkage of stacking faults, the kinetics of gettering and the effects of oxygen precipitation during IC processing. These represent a wide spectrum of physical phenomena, leading different investigators to devise different means to infer the concentrations, diffusivities and recombination velocities of vacancies and interstitials in silicon at processing temperatures. In spite of the fundamental nature of these parameters, there is often poor agreement between different experiments. From a scientific and engineering perspective, it is important to have a model which is consistent over a wide range of experimental results. Indeed, a primary measure of the usefulness of a model is that it self-consistently accounts for a wide range of data.

Here , we propose some key points which a useful model must address, and show how consistency can be maintained in the underlying point defect model for phenomena as different as transient enhanced diffusion due to implant damage, lateral extent of two-dimensional oxidation enhanced diffusion (2D OED), transit times for defects in thin silicon membranes and gettering experiments.

Key Relationships between parameters

$D_iC_i^*$ and $D_vC_v^*$

What are the key relationships that model parameters should maintain? First, since intrinsic point defects in silicon are responsible for self-diffusion, then within some correlation factor the relationship

$$D_{self}C_S = D_iC_i^* + D_vC_v^* \tag{1}$$

must hold. The key experiment separating vacancy from interstitial components of silicon self diffusion has yet to be performed: namely oxidizing and nitriding the surface of a silicon wafer containing a buried silicon isotope layer and observing the enhanced or retarded diffusion of the isotopic silicon marker layer. Such an experiment would determine the magnitude of the $D_iC_i^*$ and $D_vC_v^*$ products unambiguously. In the absence of this data, there are some reasonable approximations to these products, obtained mostly from gold diffusion experiments [1], [2]. These experiments suggest that both I and V contribute to self diffusion at processing temperatures. Additional evidence that this is so comes from Ge marker layer experiments [3]. These showed that the fraction of Ge diffusing by an interstitial mechanism was ≈ 0.4 at processing temperatures. Since Ge diffusion is expected to be similar to silicon self diffusion, this strongly suggests that the $D_iC_i^*$ and $D_vC_v^*$ products are of the same order at processing temperatures. Thus, a large value for D_i obtained in an experiment should give rise to a correspondingly low value for C_i^*, with any consequences that might imply. For modeling OED or stacking fault growth, the value of C_i^* may appear unimportant, since only the effect of the supersaturation C_i/C_i^* is observed. However, for modeling gettering kinetics or transient diffusion during implant damage annealing, the value for C_i^* can strongly influence the prediction.

D_i/K_s

The ratio of the diffusivity of interstitials D_i to their surface recombination velocity K_s has been established from transit time experiments through thin membranes and from 2D OED studies. There is good agreement between different experiments and this suggests that the D_i/K_s ratio should be treated as another fundamental parameter. Clearly, the same D_i/K_s ratio will give rise to the same steady state behavior. We suggest that the D_i and K_s values can be directly scaled, keeping the same ratio and this scaling becomes necessary when we try to reconcile the experiments which measure a high apparent value for D_i with those which measure a low value for D_i.

K_B

Frenkel pair generation/recombination is one of the most important but least well modeled phenomena. The kinetics of $I - V$ generation/recombination have profound implications for understanding the defect kinetics. A question as simple as "How long does it take to establish equilibrium defect population levels after a step change in temperature?" is difficult to answer accurately without a knowledge of the bulk generation constant. Early experiments [4] suggested a time constant of about 60 minutes at 1100 °C, which implies an energy barrier of 1.4eV to I-V recombination. This means that interstitial and vacancy populations are essentially independent at lower temperatures, as pointed out by Tan and Gosele [10]. There is recent strong evidence that suggests that I-V recombination is fast, so these first results may be in error for some subtle but unknown reason. Figure 1 shows the results on the short time retarded diffusion of Sb (which diffuses primarily by vacancies) during interstitial injection. In the light of these results we must conclude that I-V recombination happens quickly, with any consequences that might imply.

D_i and D_v

Because the equilibrium concentrations of I and V are difficult to directly observe in silicon (although the positron technique does offer some hope), much of the experimental work has concentrated on establishing values for D_i and D_v. The interstitial diffusivity D_i presents a most confusing picture, as shown in Figure 2. In general, OED type experiments give rise to smaller values of D_i, while gettering and implant damage studies give large apparent values. Data on the lateral extent of enhanced diffusion during both oxidizing (injecting I) and nitriding (injecting V) conditions can be used to compare values for D_i and D_v over temperature (a full account will be published later). Values for D_i and D_v shown in Figure 3 are similar and are similarly activated with the D_i value representing the lower range of values plotted in Figure 2. Data on lateral enhanced diffusion is useful because it also allows values for the surface recombination velocity K_s to be extracted. Consistent with the points outlined above, a high value for D_i, a reduced value for C_i^* and a scaled up value for K_s for interstitials can also model the data. That a high value for D_i is able to model the 2D OED results on the lateral diffusion length of interstitials at 900 °C equally well is illustrated in Figure 4. It can be noted that the transient observed in the lateral diffusion is of the order of tens of hours at 900 °C , which at first sight is incompatible with the short time constant expected from a very high interstitial diffusivity. But the longer transient can occur if the high D_i reduces to a lower "effective" value. The plots in Figure 5 and 6 show how a large value of D_i can give rise to a much lower value D_i^{eff} if I-V recombination is fast, $D_i C_i^* \approx D_v C_v^*$ and $D_v << D_i$. Thus two very different parameter sets can model the same data if the above relationships between key parameters are maintained and the experimental values for $D_v C_v^*$ in Figure 3 are used.

Extension to transient damage annealing kinetics

We can extend this model to self-consistently predict the time evolution of transient enhanced diffusion after implant damage annealing. Figure 7 shows the behavior of boron in the transient diffusion regime when different doses of Si^{29} are used to create controlled amounts of damage. These simulations use large values of D_i, small values of C_i^* and have a D_i/K_s value which is consistent with 2D OED results.

[1] S. Mantovani, F. Nava, C. Nobili, and G. Ottaviani, *Phys. Rev. B*, **33**, 5536, (1986).

[2] F. Morehead, in *Defects in Electronic Materials- Materials Research Society Symposium Proceedings*, Volume 104, p99, edited by M. Stavola, S.J. Pearton, and G. Davies, (Materials Research Society, Pittsburgh, Pennsylvania, 1988).

[3] P. Fahey, Iyer, S.S., Scilla, G.J. *Appl. Phys. Lett.*, **54**, 843 (1989).

[4] D.A.Antoniadis and I. Moskowitz, *Journal of Applied Physics*, **53**,6788, (1982).

[5] E. Guerrero , W. Jüngling , H. Pötzl , U. Gösele , L. Mader , M. Grasserbauer and G. Stingeder, *Journal of the Electrochemical Society*, 2181, (1986).

[6] S. Mizuo and H. Higuchi, *Jpn. J. Appl. Phys*, **20**, 739, (1981).

[7] P.B. Moynagh and P.J. Rosser, in *ESSDERC '89 - 19th European Solid State Device Research Conference, Berlin*, page 291, edited by A. Heuberger, H.Ryssel, P.Lange, (Springer-Verlag, Berlin, 1989).

[8] P. A. Packan, PhD. Thesis, Feb 1991, Stanford University, Stanford, CA.

[9] F. Morehead. *Defects in Electronic Materials- Materials Research Society Symposium Proceedings Volume 104*, page 99, (MRS, Pittsburgh : Pennsylvania, 1988).

[10] T.Y. Tan and U. Gösele, *Appl. Phys. A*, **37**,1, (1985).

[11] G.B. Bronner and J.D. Plummer, *Journal of Applied Physics*, **61**,5286, (1987).

[12] A. Seeger and H. Föll and W. Frank. *Defects and Radiation Effects in Semiconductors 1976*, page 12, (Inst. Phys. Conf. Ser. No. 31: London, 1977).

[13] P.B. Griffin, P.M. Fahey, and J.D. Plummer, *Appl. Phys. Lett.*, **47**,315, (1985).

[14] M. R. Kump and R. W. Dutton, *IEEE Transactions on Computer-Aided Design*, **7**,191, (1988).

[15] P.B. Griffin and J.D. Plummer. *IEDM Technical Digest*, 522, (1986).

[16] K. Taniguchi, D.A. Antoniadis, and Y. Matsushita, *Appl. Phys. Lett.*, **42**, 961, (1983).

[17] K. Wada and N. Inoue and J. Osaka. *Defects in Semiconductors II-Materials Research Society Symposium Proceedings*, page 125, (North Holland : Palo Alto, 1983).

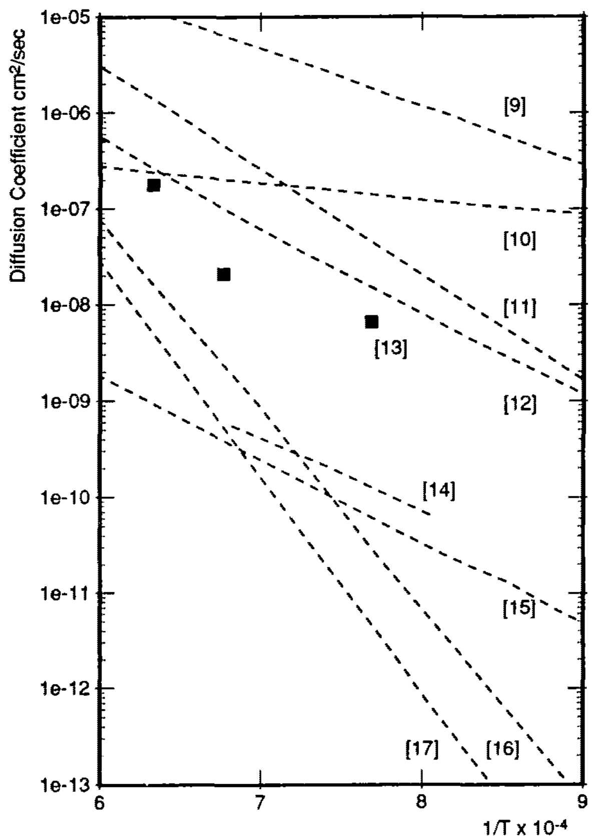

Figure 2: Values of the intersitital diffusion coefficient D_i obtained from studies of transit times across membranes, 2D OED experiments, metal gettering and damage studies.

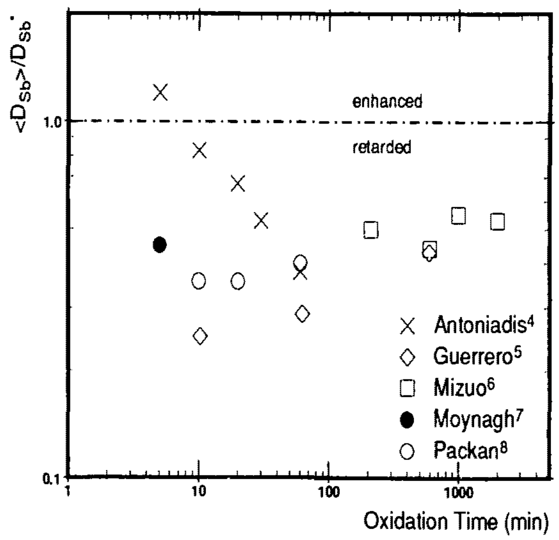

Figure 1: Experimental results on the short time diffusion of Sb at 1100 °C during interstitial injection. With the exception of [4] the results imply that I-V recombination is fast.

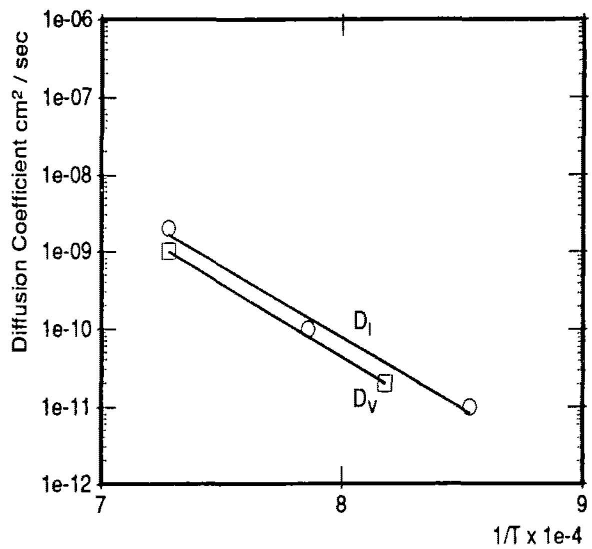

Figure 3: Experimental values for D_i and D_v from observations of the lateral decay of interstitials and vacancies in two-dimensional structures.

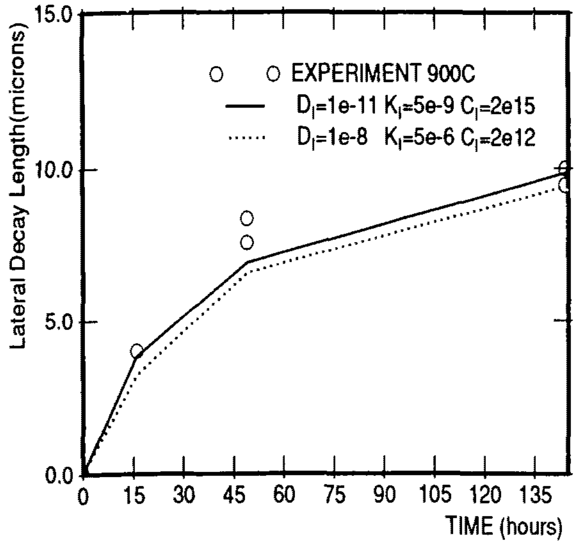

Figure 4: Experimental results and simulations of the lateral interstitial decay length at 900 °C . The lateral decay length exhibits a long transient, and is modeled by a low effective diffusivity of interstitials, or equally well by a high value for D_i with I-V recombintion provided the vacancies have the properties shown in Fig 3.

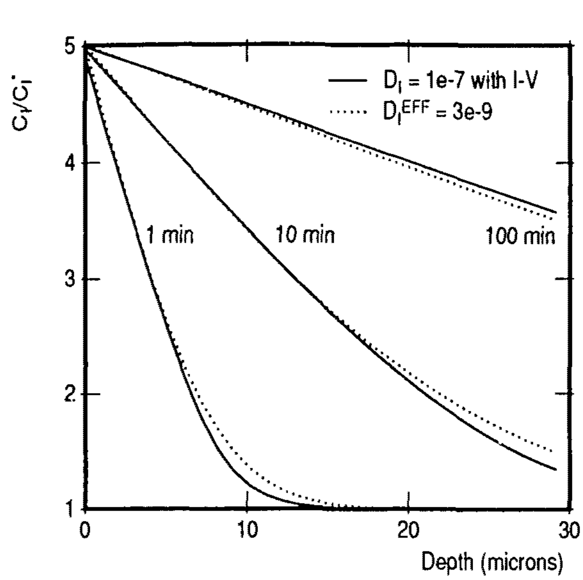

Figure 5: Interstitial supersaturation profiles with a very high interstitial diffusivity ($D_i = 1 \times 10^{-7}\text{cm}^2/\text{sec}$) can give rise to an apparently slower D_i^{eff} if I-V recombination is included with $D_v C_v^*$ from Fig 3.

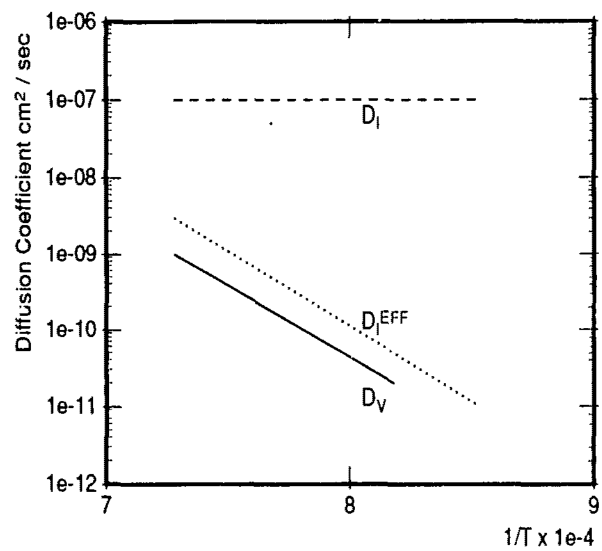

Figure 6: A high value for D_i gives rise to an apparent D_i^{eff} close to and activated similarly to D_v, which seems to be in agreement with the experimental results presented in Figure 3.

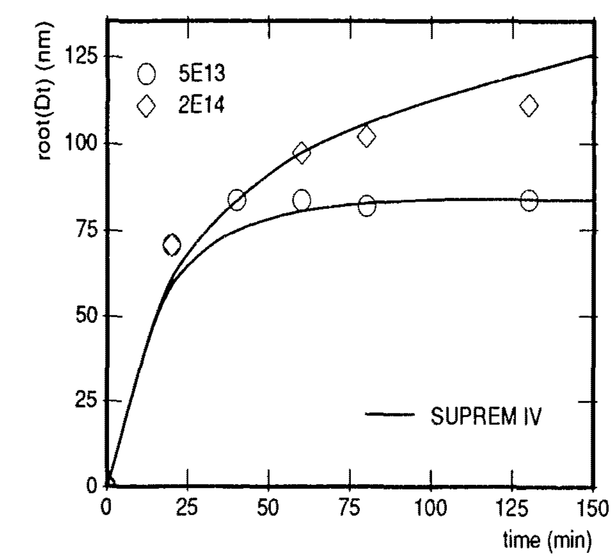

Figure 7: Simulation and experimental results of transient enhanced diffusion of Boron after controlled amounts of damage are introduced by different Si^{29} dose implants. The same parameter set that fits the 2D OED results was used.