

# Theory of dopant diffusion assuming nondilute concentrations of dopant-defect pairs

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(Received 6 June 1991; accepted for publication 30 September 1991)

Current dopant diffusion theory is based on dopant-point-defect interaction, and assumes that the number of dopant-defect pairs is much smaller than the unpaired dopant concentration. In cases where a large number of excess defects are created from implantation damage, this may no longer be a valid assumption. A new derivation of the dopant and defect equations is presented which is valid for any concentration of dopant-defect pairs.

The short time transient enhancement of dopant diffusion in silicon following implantation has been the subject of several studies.<sup>1-7</sup> Producing a physical, point-defect based model for these effects is an important objective for modeling and predicting dopant profiles in silicon. Unlike the conditions present during oxidation enhanced diffusion, the defect excess can be several orders of magnitude greater than the equilibrium defect concentration. Under these conditions, it can no longer be assumed that the concentration of dopant-defect pairs is dilute compared to the dopant concentration. Additionally, Borucki<sup>8</sup> has recently suggested that large numbers of arsenic-defect pairs might be responsible for the underactivation of arsenic. For these cases, the dopant flux equations<sup>9-12</sup> must be rederived.

Mathiot and Pfister<sup>9</sup> derived the equations for defects and impurities by assuming that impurities diffuse only through interaction with point defects. The equations derived are for a single donor impurity, however the acceptors can be treated in much the same way. Assuming that the donor diffuses only when paired with a defect and that the defect-dopant pairs are in equilibrium:

$$\frac{\partial C_A}{\partial t} = -\nabla(J_{AI} + J_{AV}), \quad (1)$$

$$\frac{\partial}{\partial t}(C_V + C_{AV}) = -\nabla(J_V + J_{AV}) - K_{\text{bulk}}, \quad (2)$$

$$\frac{\partial}{\partial t}(C_I + C_{AI}) = -\nabla(J_I + J_{AI}) - K_{\text{bulk}}. \quad (3)$$

$C$  refers to the concentration of the subscripted species,  $J$  is the flux. The subscripts  $A$ ,  $I$ ,  $V$ ,  $AI$ ,  $AV$  refer to the donors, unpaired interstitials, unpaired vacancies, interstitial-donor pairs, and vacancy-donor pairs.  $K_{\text{bulk}}$  represents all of the possible recombination terms, including interstitial-vacancy recombination, dopant mediated recombination, and bulk defect sinks.

The fluxes in Eqs. (1)–(3) have been treated previously<sup>11</sup> when the donor-defect pair concentration is dilute. That derivation led to this expression for the dopant-interstitial flux:

$$-J_{AI} = \sum_c D_{AI^c} C_{AI^c} \nabla \log C_{AI^0}, \quad (4)$$

where the superscript on the  $AI$  pair is the charge state of the pair, and the summation is over all charge states. It is

at this point in the derivation that allowing a nondilute concentration of donor-defect pairs is important. The number of neutral donor-interstitial pairs can be expressed as follows, assuming that electronic processes are faster than any other:<sup>11</sup>

$$C_{AI^0} = K_{AI^0} C_I^- C_A^+ \frac{C_{In}}{C_I^* n_i}, \quad (5)$$

where  $K_{AI^0}$  is a function only of temperature,  $C_A^+$  is the concentration of unpaired, substitutional dopant,  $C_I^-$  is the concentration of negatively charged interstitials in equilibrium during intrinsic doping conditions,  $C_I^*$  is the equilibrium concentration of interstitials, and  $n/n_i$  is the electron concentration divided by the intrinsic carrier concentration. In general  $C_I^*$  is dependent on the charge states of the defects and the local doping level. This allows substitution into Eq. (4) to simplify the flux of the pairs:

$$-J_{AI} = \left( \sum_c D_{AI^c} K_{AI^c} G_{I^c} C_{I^c-1} \right) C_A^+ \frac{C_I}{C_I^*} \nabla \log \left( C_A^+ \frac{C_I n}{C_I^* n_i} \right) \quad (6)$$

where  $G_{I^c}$  is the charge state term, which is equal to  $(n/n_i)^{1-c}$ , where  $c$  is the charge power of the pair and is equal to 0 for neutral pairs,  $-1$  for negative pairs, and  $+1$  for positive pairs, assuming donor diffusion and  $C_{I^c-1}$  is the concentration of interstitials in a charge state one electron more negative than the pair state under inert, intrinsically doped conditions. The quantity in summation is normally associated with the normal concentration dependent diffusivity since all but  $G_{I^c}$  depend solely on temperature. The major difference between Eq. (6) and that found in Law and Pfister<sup>11</sup> is that the total substitutional dopant concentration  $C_A$  has been replaced by the unpaired substitutional dopant concentration,  $C_A^+$ . The two quantities are related through the expressions for the pair concentrations:

$$C_A = C_A^+ + \sum_c K_{AI^c} G_{I^c} C_{I^c-1} C_A^+ \frac{C_I}{C_I^*} + \sum_c K_{AV^c} G_{V^c} C_{V^c-1} C_A^+ \frac{C_V}{C_V^*}. \quad (7)$$

Equations (6) and (7) will generally require numerical solution, however, there are some simplified cases that

can be examined. If the number of pairs is very small compared to the donor concentration, then Eq. (6) can be simplified:

$$-J_{AI} = \left( \sum_c D_{AIc} K_{AIc} G_{Ic} C_{Ic-1} \right) C_A \frac{C_I}{C_I^*} \nabla \log \left( C_A \frac{C_I}{C_I^*} \frac{n}{n_i} \right), \quad (8)$$

which is the expression found in Law and Pfeister.<sup>11</sup> The quantity in parenthesis is the concentration dependent diffusivity, and the expression shows the normal linear dependence of the diffusivity on the scaled interstitial concentration. This equation is similar to those used for diffusion modeling previously.<sup>9-12</sup>

Under large interstitial supersaturation, however, the equation has a different limit. In this case, the donors will be entirely paired, and further increase in the interstitial concentration will not change the donor flux:

$$-J_{AI} = \frac{(\sum_c D_{AIc} K_{AIc} G_{Ic} C_{Ic-1})}{(\sum_c K_{AIc} G_{Ic} C_{Ic-1})} C_A \nabla \log \left( C_A \frac{n}{n_i} \right). \quad (9)$$

The prefactor in the equation is the weighted average of the diffusivity by charge state population, and the second term is the standard drift diffusion expression for the defect flux. The diffusivity no longer depends on the interstitial supersaturation. This approach has been used successfully by Packan<sup>13</sup> in modeling ion-implantation damage effects on boron transient diffusion. Packan limited the maximum diffusivity enhancement by altering Eq. (8) such that any  $C_I$  increase above a parameter  $C_{I\max}$  causes no further increase in the diffusivity. The  $C_{I\max}$  value Packan extracted by comparison to 800 °C boron diffusion corresponds to a boron-interstitial binding energy of 1.7 eV.

The region in between the two limits will look something like that drawn in Fig. 1, which shows a plot of  $D/D^*$  with several values for  $K$ , assuming a single dominant pair state. If  $K$  is very small, then the diffusivity enhancement is proportional to the interstitial supersaturation and remains so even for very large interstitial supersaturation. As  $K$  is increased, the donor atoms become completely paired at a smaller supersaturation and the diffusivity maximum that is reached is also smaller. For comparison, Packan's approximate model is also shown.

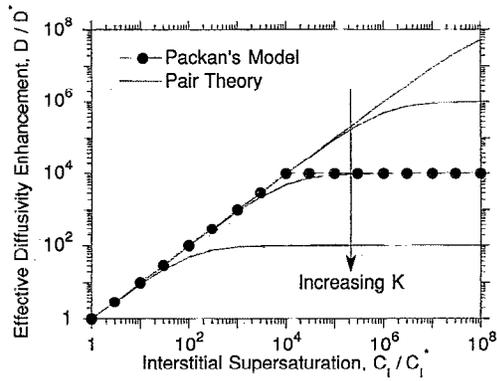


FIG. 1. The effective of dopant-defect pairing on the diffusivity enhancement as a function of excess interstitial concentration. The diffusivity enhancement becomes sublinear for a finite pair reaction coefficient. Packan's model is shown for comparison.

A new theory of defect-dopant interaction has been described which can account for some of the anomalous behavior seen in dopant diffusion in silicon. This theory adds new terms to the dopant flux equation which account for a finite number of defect-dopant pairs. This is most important for developing physical models for implantation damage enhanced transient diffusion, and Packan<sup>13</sup> has successfully used an approximate version of the full equations.

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