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On the Determination of Boron Diffusivities and Boron Interstitial Pair Binding Energies in Silicon

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To describe the coupled diffusion of impurities and point defects in silicon, a large number of parameters have to be known and for most of them general agreement about their values has not been reached yet. As far as boron related parameters such as diffusivities of boron interstitial pairs and pair binding energies are concerned, their values have been extracted from experiments of boron diffusion from gaseous sources and doped surface layers [1,2]. However, these values have been extracted assuming isothermal diffusion conditions for the simulations and they are inconsistent with the well verified effective equilibrium diffusivity of the standard type diffusion model [3]. It will be shown here that this inconsistency does not occur, when the temperature ramping conditions of the experiments used for parameter extraction are rigorously taken into account.

The model for the coupled diffusion of boron and point defects in silicon used in this study is based on the model published by Dunham [4]. If pairing reactions and point defect recombination are assumed to be in local equilibrium, an effective diffusivity can be extracted from such kind of models, which can be compared to the effective diffusivity of the standard type diffusion model. Assuming that boron diffuses via negatively and uncharged boron interstitial pairs (BI^-, BI^0), the effective boron diffusivity can be written as [1]:

$$D_{eff} = \frac{4}{n_{Si}} C_I^{eq} \left[\exp\left\{ \frac{E_{BI^-}}{k_B T} \right\} D_{BI^-} + \gamma^+ \cdot \exp\left\{ \frac{E_{BI^0}}{k_B T} \right\} D_{BI^0} \frac{p}{n_i} \right] \tag{1}$$

where $\gamma^+ = \exp\{(E_{I+} - E_F^i)/k_B T\}$. E_{I+} is the energy level of positively charged interstitials and E_F^i the intrinsic Fermi level. n_{Si} is the concentration of Si lattice sites, C_I^{eq} the equilibrium interstitial concentration, E_{BI} are the pair binding energies and D_{BI} the microscopic pair diffusivities. All other symbols have their usual meanings.

On the other side, the effective boron diffusivity of the standard type diffusion model, where pairing reactions and point defect recombination are always assumed to be in equilibrium, is given by [5]

$$D_B^{eff} = D_{B-X^0}^i + D_{B-X^+}^i \frac{p}{n_i} = (0.037 + 0.72 \frac{p}{n_i}) \cdot \exp\{\frac{3.46\text{eV}}{k_B T}\} \,\text{cm}^2/\text{s} \tag{2}$$

The superscript i indicates intrinsic conditions, and X^0, X^+ neutral and positively charged point defects, respectively. The values given in Eq. 2 have been taken from Ref. [3].

The effective diffusivity of the pair diffusion model and of the standard model are equal, when the microscopic pair diffusivities are chosen as follows:

$$D_{BI^-} = \frac{D_{B-X^0}^i}{\frac{4}{n_{Si}} C_I^{eq} \cdot \exp\left\{ \frac{E_{BI^-}}{k_B T} \right\}}, \qquad D_{BI^0} = \frac{D_{B-X^+}^i}{\frac{4}{n_{Si}} C_I^{eq} \gamma^+ \cdot \exp\left\{ \frac{E_{BI^0}}{k_B T} \right\}} \tag{3}$$

These microscopic pair diffusivities not only ensure that the effective equilibrium diffusivity of the pair diffusion model is equal to that of the standard model, but also that the binding energies E_{BI^-} and E_{BI^0} can be changed without changing the effective equilibrium diffusivity. In contrast to the determination of binding energies in Ref. [1], our own simulations of diffusion experiments from gaseous sources and doped surface layers show that the binding energies have negligible influence on the simulation results, as long as the effective equilibrium diffusivity is kept constant. Therefore, the pair binding energies can **not** be extracted from such kind of experiments and rather arbitrarily the values extracted in Ref. [1] have been chosen here. The other significant model parameters and their values are summarized in Table I. The point defect related parameters, namely the diffusivities and equilibrium concentrations of interstitials and vacancies as well as the barrier energy for point defect recombination have been determined by metal diffusion experiments. Good agreement with a broad range of experimental data has been shown recently using these values [6].

The diffusion equation system was solved by ZOMBIE [7] and simulation results of boron diffusion from gaseous sources and doped surface layers as published by Orr Arienzo *et al.* [8] are shown in Fig. 1. Solid lines show the simulation results, when the approximation of isothermal annealing conditions made in Ref. [1] and [2] is dropped, and the temperature ramping conditions shown in Table II are taken into account. For comparison, dashed lines show the simulation results, when the ramping steps are omitted. Obviously, the long temperature ramping times of experiments b) and c) can not be neglected in the simulations. During temperature ramping, the boron surface concentration has been kept constant. This assumption is not justified a priori, but since no parameter fitting was

necessary in order to match the experimental results of Orr Arienzo *et al.* [8] very well and all parameters are based on independent experiments, the surface conditions seem to be sufficiently approximated.

In conclusion, a parameter set for the coupled diffusion of boron and point defects in silicon has been proposed, which is consistent with the macroscopic boron diffusivity of the standard type diffusion model [3]. Using this parameter set, which is entirely based on independent experiments, boron diffusion from gaseous sources and doped surface layers [8] can be simulated accurately, when temperature ramping is taken into account. No fitting was necessary in order to match the experimental results. The binding energies of boron interstitial pairs can not be determined by diffusion experiments from gaseous sources and doped surface layers, since the simulation results are influenced only marginally by these parameters.

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TABLE I. Model parameters for point defects; energy levels of charged defects are given for 0K.

Parameter	Value	Ref.	Parameter	Value	Ref.
C_I^{eq}	$2.9 \times 10^{24} \exp\{-3.18\text{eV}/k_BT\}\ \text{cm}^{-3}$	[9]	D_I	$51 \exp\{-1.77\text{eV}/k_BT\}\ \text{cm}^2\text{s}^{-1}$	[9]
C_V^{eq}	$1.4 \times 10^{23} \exp\{-2.0\text{eV}/k_BT\}\ \text{cm}^{-3}$	[9]	D_V	$3.0 \times 10^{-2} \exp\{-1.8\text{eV}/k_BT\}\ \text{cm}^2\text{s}^{-1}$	[9]
$E_C - E_{I-}$	0.139 eV	[10]	$E_{I+} - E_V$	0.525 eV	[10]
$E_C - E_{V-}$	0.57 eV	[5]	$E_{V+} - E_V$	0.05 eV	[5]
$E_C - E_{V=}$	0.11 eV	[5]	$E_{V++} - E_V$	0.13 eV	[5]
ΔE_{IV}	0.3 eV	[11]			

TABLE II. Annealing conditions of experiments shown in Fig. 1 according to Orr Arienzo *et al.* [8]

exp.	ramp up	isothermal	ramp down
a)	700°C → 850°C: 15min	850°C: 4h	850°C → 700°C: 20min
b)	700°C → 950°C: 30min	950°C: 1h	950°C → 700°C: 50min
c)	700°C → 1050°C: 50min	1050°C: 30min[a]	1050°C → 700°C: 80min

[a] 1h is given in the figure caption and 30min in the text of Ref. [8].

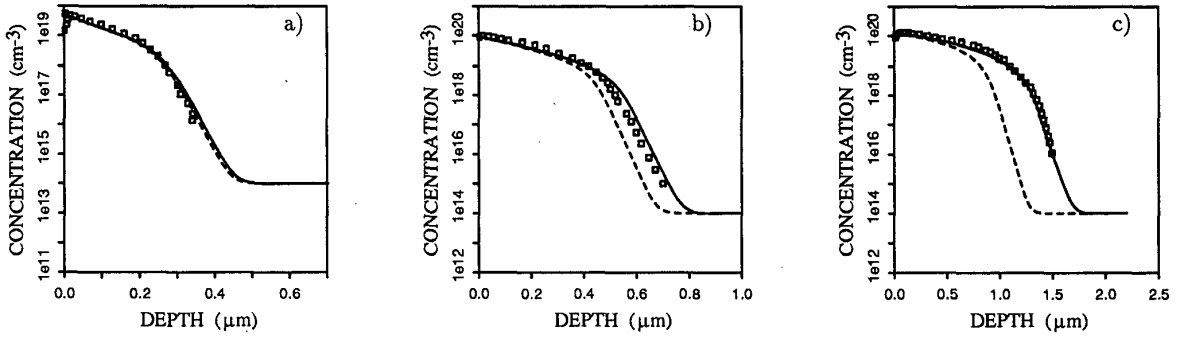

FIG. 1. Comparison between simulation and experimental results of boron diffusion from gaseous sources and doped surface layers. **Symbols:** Experimental results according to Orr Arienzo *et al.* [8]. **Solid lines:** Simulation results, when temperature ramping as given in Table II is taken into account. **Dashed lines:** Simulation results, when ramping up and ramping down steps are omitted.