Defect-Coupled Dopant Diffusion at High Concentrations

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ABSTRACT

This paper investigates the role of defects in the diffusion of dopants in silicon under extrinsic conditions. The form of the diffusivity is rewritten to make the presence of each charged defect explicit, and this form is used to extract coefficients from experimental measurements of diffusivity under extrinsic conditions in inert and oxidizing ambients.

The role of point defects in the diffusion of dopants in silicon has been extensively studied over many years. The traditional formulation for concentration-dependent diffusivity is derived from the variation in vacancy concentrations with fermi level, and the same form applies equally well to an interstitialcy mechanism. More recently this has been modified to include the effect of defects injected during oxidation. So far, explicit modeling of defect diffusion has emphasised the low dopant concentration regime. This paper considers the explicit modeling of diffusion in the presence of high dopant concentrations. The role of defects can be more clearly seen if the dependence of defect concentration on n/n_i is made explicit. For example, in the case of boron in an oxidizing ambient:

$$D = D_{I_0}\frac{C_{I_0}}{C_{I_0}^*} + D_{I_+}\frac{C_{I_+}}{C_{I_+}^*} + D_{V_0}\frac{C_{V_0}}{C_{V_0}^*} + D_{V_+}\frac{C_{V_+}}{C_{V_+}^*} \quad \text{and} \quad \frac{C_{I^+}}{C_{I^+}^*} = \frac{\left(C_I + C_{inj}\right)\gamma\frac{p}{n_i}}{\left(1 + \gamma\frac{p}{n_i} + \beta\frac{n_i}{p}\right)} \quad \text{etc.}$$

where D_{I_0} is the neutral interstitialcy component of diffusion, C_{I_0} is the concentration of neutral vacancies (C^* denotes intrinsic, inert conditions), γ and β are derived from the interstitial energy levels and C_{inj} is the injected interstitial concentration due to oxidation.

Two-dimensional modeling of this diffusion equation has been performed by modification of the Suprem-IV program,[1] including terms for doping-dependent defect lifetime. Figure 1 shows an example calculation for boron diffusing at 1000°C. Excess interstitials are generated near the surface, where the boron concentration is high. The vacancy concentration is slightly depressed because of the positions of the vacancy energy levels (in n^+ layers a large enhancement is seen). The net difference in vacancy and interstitial concentrations is supplied by the free surface. Drift due to the electric field established by the boron profile is much greater in magnitude than the diffusion term for defects. The dominant defect charge state is positive so defects are completely retarded by the field and are not injected into the substrate. Neutral defects could diffuse into the substrate, but no gradient in neutral defects is caused fermi level effects. Diffusion into the substrate will occur if a neutral defect gradient is established by injection at the surface. It is interesting to note that these simple considerations rule out a pair dissociation model for the phosphorus tail based on P^+V^- pairs since these pairs will be held in by the electric field.

Given the above form for diffusivity, values for the physical constants involved can be extracted from diffusivity measurements under extrinsic conditions in oxidizing ambients. Such experiments have been performed by Miyake.[2] An earlier analysis of these results[3] omitted the contribution of the I^- defect in n^+ layers and the dependence of defect concentration on fermi level. Correcting these deficiencies, we can extract the position of the I^+ and I^- energy levels, the relative contributions of charged and neutral defects to boron diffusion and the product $f_I C_{inj}/C_I^*$. Figure 2 shows the fit for the diffusion enhancement due to oxidation as a function of background doping level, $\Delta D = D_{ox} - D_{inert}$.

REFERENCES

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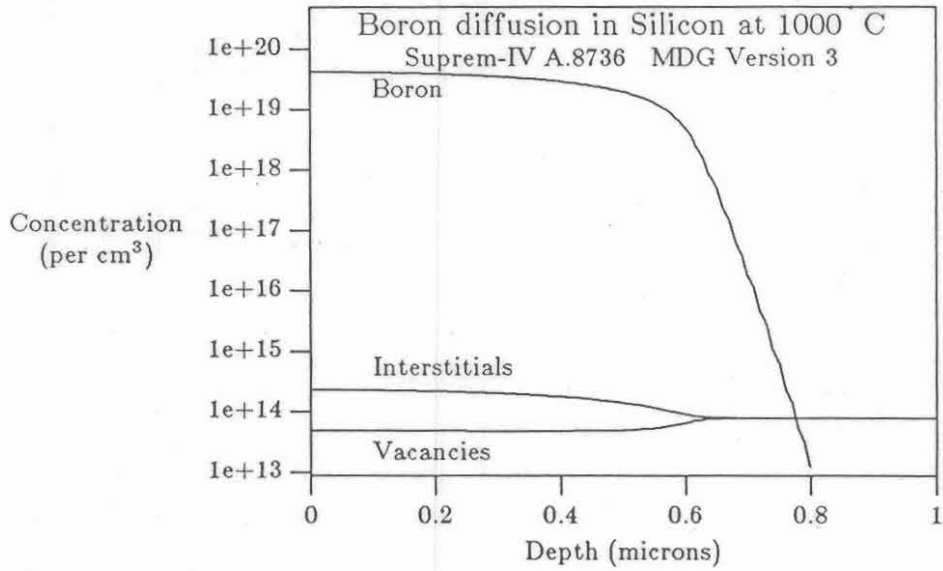
Figure 1. Defect distributions during the diffusion of boron.
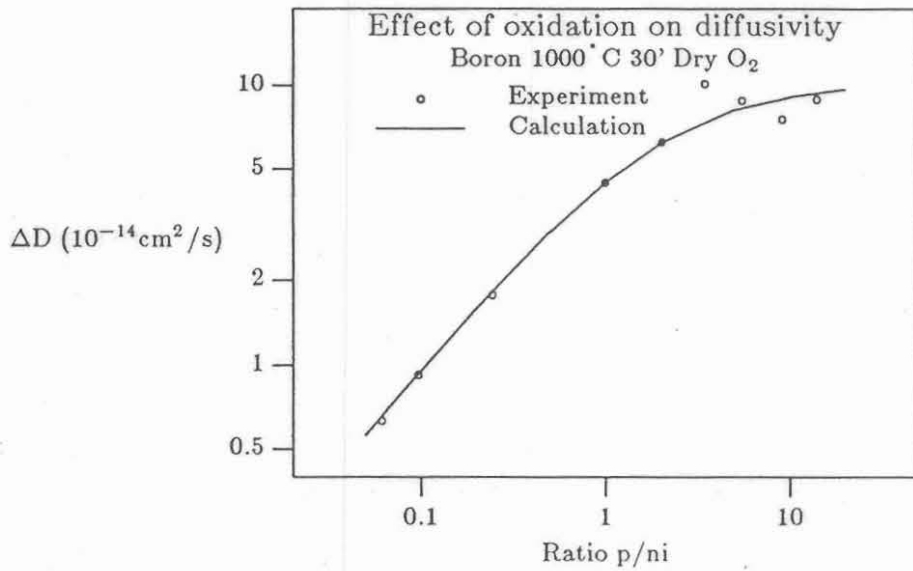

Figure 2. Oxidation enhancement of boron diffusivity in extrinsic conditions.