

### Solution 300-3

Problem text repeat:

Consider the diffusivity as denoted in Fairs diffusion model for diffusion of dopant atoms in Si.

- a) Define stringently each symbol.
- b) Explain the equation.

Solution

**a)**

We write the diffusion as a sum of terms, each of which, is considered as a diffusivity associated with one particular charge state of the vacancy.

$$D = D_i^* + D_i^+ \left( \frac{p}{n_i} \right) + D_i^- \left( \frac{n}{n_i} \right) + D_i^{=}\left( \frac{n}{n_i} \right)^2 \quad \text{eq. 1}$$

Just definition of symbols.

$D_i^*$  Diffusivity of dopant (for the intrinsic case) and only due to transport by neutrally charged vacancies.

$D_i^+$  Diffusivity of dopant for the intrinsic case and due only to transport by positively charged vacancies.

$p$ : hole concentration.

$n_i$ : intrinsic carrier concentration.

$D_i^-$  Diffusivity of dopant for the intrinsic case and due only to transport by negatively charged vacancies.

$n$ : electron concentration.

$D_i^{=}$  Diffusivity of dopant for the intrinsic case and due only to transport by doubly negatively charged vacancies.

**b)**

We can understand the additivity from the additivity of fluxes

$$J = J^* + J^+ + J^- + J^{=} \quad \text{eq2}$$

Where each flux term is due to diffusion by the four differently charged vacancies we consider

Each term in eq1 s a diffusivity due to transport by corresponding charge state of vacancy.

Each term in eq1 is written as a product of two terms,  $D$  and the ratio between carrier concentrations:

$$D = \sum_{r=1,0,-1,-2} D^r = \sum_{r=1,0,-1,-2} D_i^r \left( \frac{n}{n_i} \right)^{-r} \quad \text{eq.3}$$

The subscript  $i$  refers the intrinsic case. Intrinsic here means  $n=p$ ; the electron concentration is equal to the hole concentration.

(Alternatively you can take the  $i$  to signal 'impurity' but it is nevertheless for the intrinsic case)

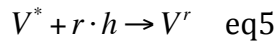
$D_i \cdot r$  are the diffusivities for the intrinsic case as described in a)

The diffusivity due to charged vacancies with charge  $r$  is obviously proportional to the probability that the neighbor site is a vacancy of that charge, which is simply the relative concentration of the vacancy, So we have

$$D^r = D_i^r \frac{[V^r]}{[V^r]_i} \quad \text{eq4}$$

where  $[V^r]$  is the concentration of vacancy in the charge state  $r$ , and  $[V^r]_i$  is that for the intrinsic case.

We can rewrite the vacancy ratio in eq4 to a ratio between carrier concentration by considering a chemical reaction style defect reaction to create a defect. Let's consider a vacancy with a charge  $r$  being created from a neutral vacancy by adding  $r$  holes (negative numbers of holes is here equivalent to electrons)



We write the law of mass action for this reaction

$$\frac{[V^*] p^r}{[V^r]} = K(T) \quad \text{eq6}$$

where  $K(T)$  is the constant of the mass action law and is only a function of temperature  $T$ . So this constant will have the same value also in the special case of intrinsic carrier concentrations so we will have

$$\frac{[V^*]_i p_i^r}{[V^r]_i} = K(T) \quad \text{eq7}$$

We put the left hand of eq6 and eq7 equal to each other and we have

$$\frac{[V^*]_i p_i^r}{[V^r]_i} = \frac{[V^*] p^r}{[V^r]} \quad \text{and since the concentration of neutral vacancies does not}$$

depend on the Fermi level we have  $[V^*]_i = [V^*]$  and thus

$$\frac{[V^r]}{[V^r]_i} = \frac{p^r}{p_i^r} = \left( \frac{n_i^2}{nn_i} \right)^r = \left( \frac{n}{n_i} \right)^{-r} \quad \text{eq9}$$

So we put eq9 into eq4 and the result into 1<sup>st</sup> part of eq3.