**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)
$D_i^{-r}$ 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

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

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)

$$V^* + r \cdot h \rightarrow V^r \qquad \text{eq5}$$

We write the law of mass action for this reaction

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

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 walue also in the special case of intrinsic carrier concentrations so we will have

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

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

$$\frac{[V^*]_i p_i^r}{[V^r]_i} = \frac{[V^*]p^r}{[V^r]}$$

and since the concentration of neutral vacancies does not depend on the Fermi level we have $[V^*]_i = [V^*]$ and thus

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

So we put eq9 into eq4 and the result into 1st part of eq3.