

> restart;

SOLUTION Suggestion FYS9n4310 300-5

Problem

Assume we have a dopant with a concentration $C(z)$ and a concentration gradient.

> diff(C(z), z) <> 0;

$$\frac{d}{dz} C(z) \neq 0$$

Then, since we assume dopants to be ionized, we have an electrical field increasing the flux of dopants. We are asked to show that the flux of atoms can be written as

$$J = -D \left(1 + \eta \right) \frac{d}{dz} C(z)$$

where η is due to the electrical field.

Solution

Lets assume our dopants are donors.

Since we have an electrical field we have to write the atomic flux with two driving forces:

> eq1:=J=-D*diff(C(z), z)+mu*C(z)*Epsilon(z);

$$eq1 := J = -D \left(\frac{d}{dz} C(z) \right) + \mu C(z) E(z)$$

Here E is the electrical field and μ is the atomic mobility related to the diffusivity by the Einstein relation.

> eq1b:=mu=D*q/k/T;

$$eq1b := \mu = \frac{D q}{k T}$$

We will have a situation where the net electron current can be assumed to be very small (compared to diffusion or drift term) in transport equation for electrons.

(Note the two terms, drift and diffusion are opposite each other for electrons, but have same direction for ions. So J is not small compared to the terms

Then we have (it is similar to eq1, but for electron current)

> eq2:=0 = q*D[n]*(diff(n(z), z))+q*mu[n]*n(z)*Epsilon(z); eq2b:=mu[n]
=D[n]*q/k/T;

$$eq2 := 0 = q D_n \left(\frac{d}{dz} n(z) \right) + q \mu_n n(z) E(z)$$

$$eq2b := \mu_n = \frac{D_n q}{k T}$$

> eq3:=Epsilon(z) =solve(subs(eq2b,eq2),Epsilon(z));

$$eq3 := E(z) = - \frac{\left(\frac{d}{dz} n(z) \right) k T}{q n(z)}$$

We can put this expression for the electrical field into equation 1

> eq4:=subs(eq1b,subs(eq3,eq1));

$$eq4 := J = -D \left(\frac{d}{dz} C(z) \right) - \frac{D C(z) \left(\frac{d}{dz} n(z) \right)}{n(z)}$$

We then write eq4 in the prescribed form, by putting $D*dC/dz$ outside a parenthesis

> eq5:=J=-D*diff(C(z), z)*(1+eta);

$$eq5 := J = -D \left(\frac{d}{dz} C(z) \right) (1 + \eta)$$

That makes eta equal to

> **eq6 := eta = C(z)*(diff(n(z), z))/(n(z)*(diff(C(z), z)));**

$$eqb := \eta = \frac{C(z) \left(\frac{d}{dz} n(z) \right)}{n(z) \left(\frac{d}{dz} C(z) \right)}$$

$$\text{or } \eta = \frac{\frac{d}{dz} \ln(n(z))}{\frac{d}{dz} \ln(C(z))} \quad \text{or even } \eta = \frac{C(z) \left(\frac{d}{dC} n(C) \right)}{n(C)}$$

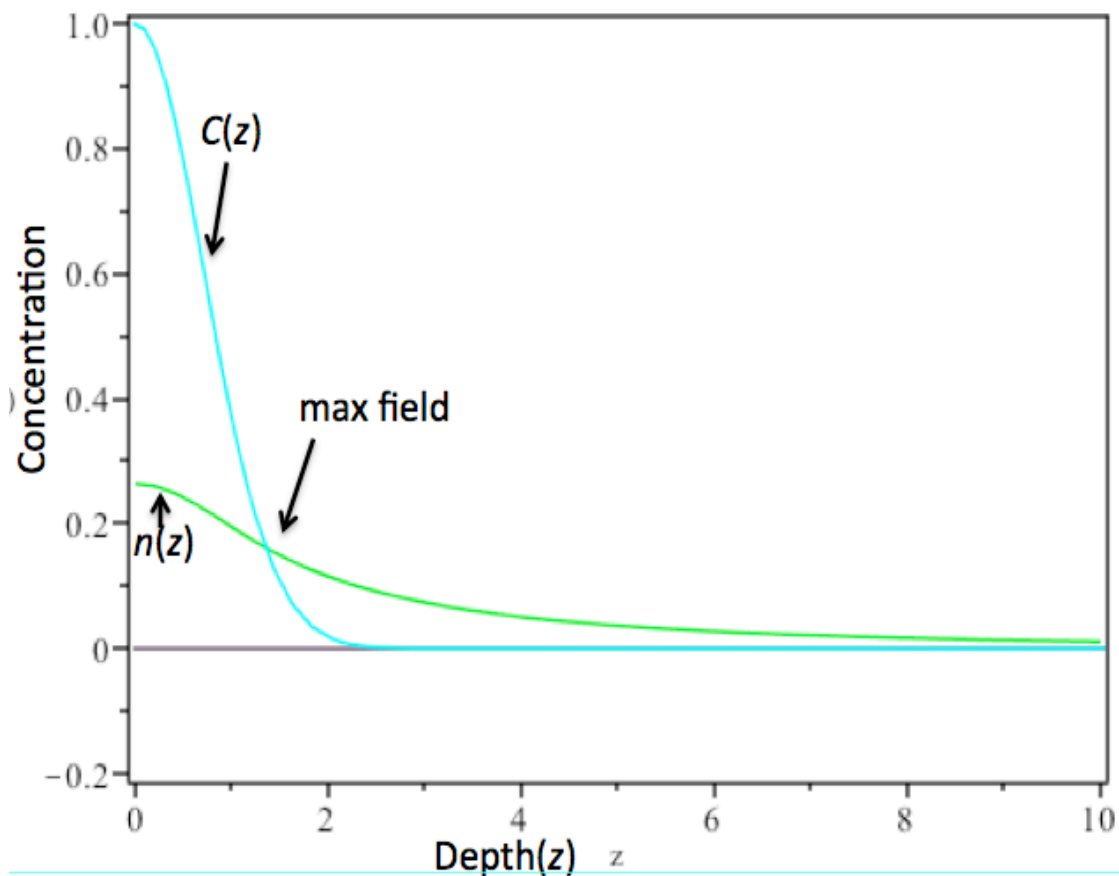
b) show that eta, η , will have a value between 0 and 1

We can argue that eta, η , is between 0 and 1, so the electric field correction is 1..2, for a typical case quite easily

We consider we a uniformly decreasing doping concentration from the surface, assume it is donors

That will tend to give a high concentration of electrons close to the surface and less further in.

We thus will have diffusion of electrons, (this is very fast compared to ions). The flux of electrons will cause buildup of net charge, we have charged donors with net positive charge close to surface, while excess electrons and a negative charge further in. This will set up an electrical field and we have a drift current opposing the diffusion current



The electric field can be obtained from Gauss law (or Poissons equation) by integrating the charge distribution.

Thus if we integrate over z , the electrical field will be maximum when $C(z)$ and $n(z)$ crosses, because the excess charge changes sign for this point, (when integrating)

We may think that the enhancement of the diffusivity is largest when the electrical field is largest.

So we consider that point.

We have that

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> eq7:=n(z)=C(z);#
eq8:=abs((diff(n(z), z)))<=abs((diff(C(z), z)));
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$$eq7 := n(z) = C(z)$$

$$eq8 := \left| \frac{d}{dz} n(z) \right| \leq \left| \frac{d}{dz} C(z) \right|$$

Thus we have that

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> eq9:=eta<=1;
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$$eq9 := \eta \leq 1$$

Further digression. FD and comments on **

The reason we have an electric field is because we have a net charge. Charge and electric field are accompanying each other as described by Gauss law or Poissons equation.

$$\frac{d}{dz} E(z) = \frac{q \left(C(z) + \frac{ni^2}{n(z)} - n(z) \right)}{\epsilon_0 K_s} \quad (\text{FD1})$$

This equation together with a similar equation to eq1 for electrons will give us an expression for the electrical field

$$0 = q D_n \left(\frac{d}{dz} n(z) \right) + q \mu_n n(z) E(z) \quad \text{gives} \quad E(z) = - \frac{\left(\frac{d}{dz} n(z) \right) k T}{q n(z)} \quad (\text{FD2})$$

We see this (FD2) is identical to eq3 above. By combining (FD1) and (FD2) we get a differential equation

$$- \frac{\left(\frac{d^2}{dz^2} n(z) \right) k T}{q n(z)} + \frac{\left(\frac{d}{dz} n(z) \right)^2 k T}{q n(z)^2} - \frac{q \left(C(z) + \frac{ni^2}{n(z)} - n(z) \right)}{\epsilon_0 K_s} = 0 \quad (\text{FD3})$$

which can be solved to find the relationship between $n(z)$ and $C(z)$, when we supply boundary conditions

(this can be accomplished by so-called 'shoot method': we know n and its derivative, but at different points, so we may see if we hit the other point by trial and error in our aiming with our gun.) This is in principal straight forward when we know $C(z)$, but if we really need to find the electrical field to find $C(z)$ we are in a not so unusual 'catch 22'-situation which sometimes can be handled by multiple iteration and consistency checks.

We realize that in a diffusion profile the electron concentration is lower than the donor concentration in the highest concentration parts (in between the surface donor concentration and much higher than the intrinsic carrier concentration) while it is higher than the donor concentration at lower concentrations. See the schematics above showing the situation qualitatively. (The figure is a solution of the differential equation with one particular set of parameters)

c) Discuss very briefly whether the results would be principally different if we consider interstitial diffusion

Let's rephrase the question: Is the above derivation also valid for interstitial diffusion?

Answer : Why not! :-)

Nothing is assumed that explicitly refer to substitutional dopants, however, if we think of cases where we have interstitial atoms that do not alter the carrier concentration then we don't get an electrical field. So while the derivation of equation eq6 here is general and apply for interstitial and vacancy diffusion, the analysis does not necessarily apply,