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# The Equation of Backward Diffusion and Negative Diffusivity

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**Abstract.** Up to now, all the diffusion theories have shown that the direction of diffusion flux is from high concentration area to lower concentration area (forward diffusion) and diffusivity is positive. In some research on simultaneous diffusion of boron and point defects in Si, the results show that the diffusivity of interstitials can be negative and diffusion process can be backward diffusion. In backward diffusion process, the direction of diffusion flux is from low concentration area to higher concentration area. The phenomenon of backward diffusion and negative diffusivity should be explained. Based on thermodynamic theory, the equation of backward diffusion and negative diffusivity are presented and discussed.

## 1. Introduction

The diffusion is elementary and universal process in natural. The rate law of diffusion had been formulated by A. Fick in which the diffusion flux is proportional to the gradient of the concentration and diffusion flux goes from regions of higher concentration to regions of lower concentration. The some piece of researches of us [1-5] showed that in the simultaneous diffusion of boron and point defect in silicon, the diffusivities of interstitial could be negative and diffusion process of interstitial or vacancy could be backward diffusion in silicon. In this paper, some problems of negative diffusivity, backward diffusion process, backward diffusion equation and solution of backward diffusion equation are presented and discussed.

## 2. Fick's laws of diffusion and forward diffusion process

Fick's first law postulates that the flux goes from regions of high concentration to regions of low concentration (forward diffusion) [6-9]:

$$J = -D \frac{\partial C}{\partial x} \quad (1)$$

in which J is the diffusion flux, D is the diffusivity, C is concentration and x is the position. Fick's second law predicts how diffusion causes the concentration to change with time t [6-9]

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (2)$$



In equation (1) and (2) diffusivity  $D$  is positive and depends on temperature  $T$ , viscosity of fluid or gas and the size of the particles  $r$  according to the Stokes-Einstein relation [6-9]

$$D = \frac{kT}{6\pi\eta r} \quad (3)$$

The diffusivity in solids at different temperatures is found to be well predicted by Arrhenius equation [7]:

$$D = D_o \exp\left(-\frac{E_a}{RT}\right) \quad (4)$$

in which  $D_o$  is the maximum diffusivity and  $E_a$  is the activation energy. Fick's laws have shown that the direction of diffusion fluxes are always the same direction of concentration gradient and the diffusivities are always positive sign.

### 3. The backward diffusion equation and negative diffusivity

Applying the thermodynamics theory on transport process could find the general equation of diffusion and general formula of diffusivity. Assume  $C_1$  is deferent to  $C_2$  and the thermal velocity  $u_1$  and  $u_2$  are not equal [5]

$$u_1 = u \quad (5)$$

$$u_2 = u_1 - nu \quad (6)$$

$$C_1 = C - \frac{\Delta C}{2} \quad (7)$$

$$C_2 = C + \frac{\Delta C}{2} \quad (8)$$

in which  $n$  is natural number and  $\Delta C = C_2 - C_1 > 0$ . The flux of molecules is determined by

$$J = -D \frac{\partial C}{\partial x} + wC \quad (9)$$

in which  $D$  and  $w$  are determined by expressions:

$$D = \frac{(2-n)\sqrt{3}u\lambda}{6} \quad (10)$$

$$w = \frac{\sqrt{3}nu}{3} \quad (11)$$

in which  $\lambda$  is characteristic length. Equation (9) is the general transport equation, equation (10) is the general diffusivity and equation (11) is the advection velocity. We could set up

$$J_{di} = -D \frac{\partial C}{\partial x} \quad (12)$$

$$J_{ad} = wC \quad (13)$$

in which  $J_{di}$  is diffusion flux and  $J_{ad}$  is advection flux. And equation (9) becomes:

$$J = J_{di} + J_{ad} \quad (14)$$

Transport flux  $J$  in equation (14) includes diffusion flux and advection flux.

The general transport equation (9) is also called advection-diffusion equation. This equation showed that the nature of transport process is depends on the difference between the thermal agitation velocity of molecules in high concentration areas and in low concentration areas.

i) If the thermal velocity of molecules in low concentration and in high concentration are equal ( $u_1 = u_2$  or  $n = 0$ ), so diffusivity is positive ( $D > 0$ ) and the advection velocity is vanish ( $w = 0$ ), the transport is only the diffusion process ( the same Fick law - forward diffusion).

ii) If  $u_2 < u_1 < 3u_2$  ( $0 < n < 2$ ), so  $D > 0$  and  $w > 0$ , the transport process includes the forward diffusion and the convection.

iii) If  $u_1 = 3u_2$  ( $n=2$ ), so  $D = 0$  and  $w > 0$ , the transport process is only convection. Although there is difference of concentration in other areas, there is not diffusion process.

iv) If  $u_1 > 3u_2$  ( $n > 2$ ), so  $D < 0$  and  $w > 0$ , the transport process includes the diffusion process with negative diffusivity and the convection.

When diffusivity is negative, the diffusion flux goes from the low concentration areas to high concentration areas. This diffusion process is contrary to Fick's law, so its called backward diffusion process. However, the backward diffusion process is different from forward diffusion process, both of them are described by the similar Fick's equations (1) and (2). If the diffusivity is positive, equation (1) and (2) are forward diffusion equations (FDE) [13-20]. If the diffusivity is negative, equation (1) and (2) are backward diffusion equations (BDE). In other word, process of backward diffusion is described by equation:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} (D < 0) \quad (15)$$

$D$  is negative, so we can set up:

$$D = -D_p \quad (16)$$

in which  $D_p$  is positive. Substituting equation (16) into equation (15) we have:

$$\frac{\partial C}{\partial t} = -D_p \frac{\partial^2 C}{\partial x^2} \quad (17)$$

The theories of partial differential equation showed equation (17) have no solution. But we could find solution for equation (17) with some boundary conditions and initial conditions. We

assume that the diffusion process occur one-dimensional ( $0 < x < L$ ) with boundary conditions and initial conditions are:

$$C(0, t) = C(L, t) = C_0 \quad (18)$$

$$C(x, 0) = f(x) \quad (19)$$

Solution for equation (17) with boundary and initial conditions (18) and (19) is given by:

$$C(x, t) = C_1(x, t) + C_2(x) + C_3(x) \quad (20)$$

Substituting equation (20) into equation (17) we have:

$$\frac{\partial C_1}{\partial t} + D_p \frac{\partial^2 C_1}{\partial x^2} + D_p \frac{\partial^2 C_2}{\partial x^2} + D_p \frac{\partial^2 C_3}{\partial x^2} = 0 \quad (21)$$

The function  $C_2(x)$  is solution of equation:

$$D_p \frac{\partial^2 C_2}{\partial x^2} = 0 \quad (22)$$

with boundary condition:

$$C(0) = C_0 \quad (23)$$

$$C(L) = 0 \quad (24)$$

and function  $C_2(x)$  is found:

$$C_2(x) = C_0 \left(1 - \frac{x}{L}\right) \quad (25)$$

The function  $C_3(x)$  is solution of equation:

$$D_p \frac{\partial^2 C_3}{\partial x^2} = 0 \quad (26)$$

with boundary condition:

$$C(0) = 0 \quad (27)$$

$$C(L) = C_0 \quad (28)$$

and solution  $C_3(x)$  is found:

$$C_3(x) = C_0 \frac{x}{L} \quad (29)$$

The function  $C_1(x)$  is solution of equation:

$$\frac{\partial C_1(x, t)}{\partial t} + D_p \frac{\partial^2 C_1(x, t)}{\partial x^2} = 0 \quad (30)$$

with boundary conditions and initial condition:

$$C_1(0, t) = C_1(L, t) = 0 \quad (31)$$

$$C_1(x, 0) = f(x) - C_2 - C_3(x) = F(x) \quad (32)$$

the solution of equation (34) is:

$$C_1(x, t) = B.e^{(\frac{n\pi}{L})^2 D_p t} . \sin \frac{n\pi}{L} x \quad (33)$$

where ( $n = 0, 1, 2$ ) and factor B is determined by:

$$B = \frac{2}{L} \int_0^L F(\xi) \sin \frac{n\pi}{L} \xi d\xi \quad (34)$$

The particular solution of backward diffusion equation (20) is:

$$C_n(x, t) = C_o + \left( \frac{2}{L} \int_0^L F(\xi) \sin \frac{n\pi}{L} \xi d\xi \right) \exp\left(-\frac{n^2 \pi^2}{L^2} D t\right) \sin \frac{n\pi}{L} x \quad (35)$$

Example, the boundary and initial condition is given by:

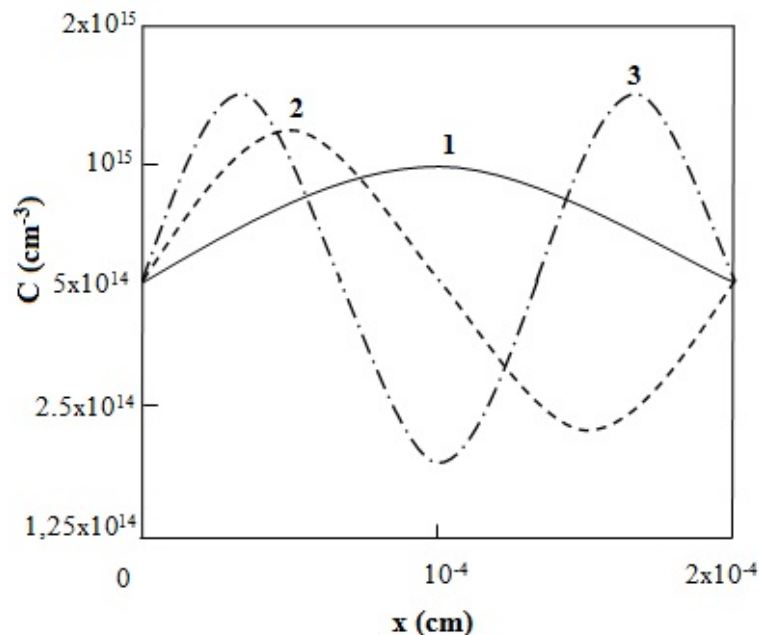
$$C(0, t) = C(L, t) = C_o \quad (36)$$

$$C(x, 0) = f(x) = C_o + C_s . \sin \frac{n\pi}{L} x \quad (37)$$

The particular solution of backward diffusion is:

$$C_n(x, t) = C_o + C_s \exp\left(-\frac{n^2 \pi^2}{L^2} D t\right) \sin \frac{n\pi}{L} x \quad (38)$$

We can plot the graph of function (38) for backward diffusion of self - interstitial defects in silicon. In fig.1 there are graphs of the particular solution of backward diffusion equation with diffusivity of interstitial in silicon  $D = -10^{-12} \text{cm}^2 \text{s}^{-1}$ ,  $C_o = 5.10^{14} \text{cm}^{-3}$ ,  $C_s = 10^{15} \text{cm}^{-3}$  and  $L = 2.10^{-4} \text{cm}$  [1-3]. Line 1 is graphs of the particular solution (38) with  $t = 0$  and  $n = 1$ . Line 2 is graphs of the particular solution (40) with  $t = t_1 = 300 \text{s}$  and  $n = 2$ . Line 3 is graphs of the particular solution (38) with  $t = t_1 = 300 \text{s}$  and  $n = 3$ . However, there is a problem with the general solution of backward diffusion equation (38) that is  $C(x, t)$  becomes extreme when  $n$  is great value.



**Figure 1.** The graph of particular solution of BDE

#### 4. Conclusion

The backward diffusion process and negative diffusivity is contrary to Ficks law, but these are explained by the theory of thermodynamics:

- Cause of backward diffusion and negative diffusivity is the difference between the thermal velocity of molecules in low concentration areas and the thermal velocity of molecules in high concentration areas.
- The backward diffusion process is described by an equation similar to Ficks equation.
- The backward diffusion equation could have particular solutions.
- Some problems of the particular solutions of the backward diffusion equation should be studied more in the future.

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