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GREEN'S FUNCTION METHODS FOR MATHEMATICAL MODELING OF UNIDIRECTIONAL DIFFUSION PROCESS IN ISOTHERMAL METALS BONDING PROCESS

ABSTRACT

Application of Green's Function Methods for mathematical modeling of isothermal diffusion process in metals has been presented in the paper. This article presents the physical model of unidirectional diffusion in isothermal process of metals bonding. For given initial and boundary conditions of diffusion the solution to a mathematical problem which describes the rate of change in concentration of one metal in the other with a constant diffusion coefficient was shown.

Key words: *unidirectional diffusion, mathematical model of diffusion*

INTRODUCTION

Diffusion process in crystalline solids is thermally activated movement of atoms as a results of concentration gradient of defects causing mass (atoms) transport [1,2].
Solutions (atomic diffusion) or intermetallic phase (reactive diffusion) can form in crystalline solids as a consequence of diffusion process [3].
Crosslinking diffusion dominates in case of atomic diffusion processes running above Tammanna temperature. Whereas grain boundary diffusion, interfacial diffusion and diffusion in dislocation prevail in lower temperatures. Unidirectional diffusion process can be describe in the mathematic way by Fick's laws [4].
Fick's First Law (1) describes correlation between mass and concentration gradient of diffusing atoms.

$$J = - D \frac{\partial c}{\partial x} \tag{1}$$

where:

J – flux of the diffusing elementary substance
x – line coordinate
t – time
c = c(x , t) – distribution of elementary substance in time
D – diffusion coefficient

Fick's Second Law describes a correlation between concentration gradient and rate of concentration change in defined point of unidirectional diffusion for constant diffusion coefficient (D).

$$\frac{\partial c}{\partial t}(x,t) = D\frac{\partial^2 c}{\partial x^2}(x,t) \tag{2}$$

The problem can be reduced by solution of differential equation (2) with c(x,t) from the mathematical point of view (for defined physical model). It is possible for defined initial and final conditions of specified physical model.
The method of Fick's Second Law solution for unidirectional diffusion of metal A into metal B and creation of solid solution of metal A in B (α) during isothermal diffusion connection A and B metals showing in Fig. 1 have been presented in the paper.

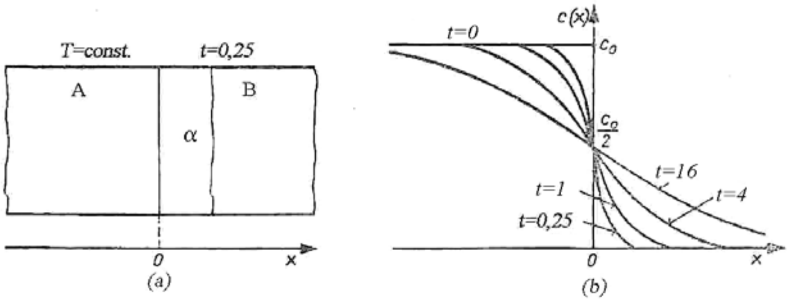

Fig. 1. Physical model of isothermal diffusion connection A and B metal (a) and concentration distribution of metal A into B depending on diffusion duration (b)

MATHEMATICAL DESCRIPTION OF DIFFUSION PROCESS IN ISOTERMAL DIFUSION BONDING OF METALS

Concentration distribution of A metal into B metal for arrangement showing in Fig. 1 enable to specify following initial and final results for t = 0.

$c(x, 0) = c_o = \text{const.}$ for $-\infty \le x \le 0$
$c(x, 0) = 0$ for $0 < x \le \infty$

Gaussian function describes normal distribution probability function of elementary substance diffusion from one point. Gaussian function curve is called „the bell curve".

$$g(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\xi)^2}{2\sigma^2}} = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\xi)^2}{2\sigma^2}\right] \tag{3}$$

where: $\sigma \in [0,+\infty)$ is a standard deviation (diffusion radius). When

$$\sigma \longrightarrow 0 \quad \text{to} \quad g(x) \longrightarrow \delta(\xi)$$

Green's Function method using for evaluation of diffusion models consist in finding of solution in the following form:

$$c(x,t)=\int_{-\infty}^{+\infty}G(x,\xi,t)\varphi(\xi)d\xi \tag{4}$$

where:

$$G(x,\xi,t)=\frac{1}{\sigma(t)\sqrt{2\pi}}\exp\left[-\frac{(x-\xi)^2}{2\sigma^2(t)}\right] \tag{5}$$

and function $\sigma(t)$ is ascending from 0 to $+\infty$.

Function $\sigma(t)$ is a standard deviation (diffusion radius) individual elementary substance for diffusion from one point:

$$c(x,0)=\int_{-\infty}^{+\infty}\delta(\xi)\varphi(\xi)d\xi=\varphi(x) \tag{6}$$

$$c(x,t)=\int_{-\infty}^{+\infty}\frac{1}{\sigma(t)\sqrt{2\pi}}e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}}\varphi(\xi)d\xi \tag{7}$$

$$\frac{\partial^2 c}{\partial x^2}=\frac{1}{\sigma^5(t)\sqrt{2\pi}}\int_{-\infty}^{+\infty}\varphi(\xi)e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}}\left[(x-\xi)^2-\sigma^2(t)\right]d\varsigma \tag{8}$$

$$\frac{\partial c}{\partial t}=\frac{\sigma'(t)}{\sigma^4(t)\sqrt{2\pi}}\int_{-\infty}^{+\infty}\varphi(\xi)e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}}\left[(x-\xi)^2-\sigma^2(t)\right]d\xi \tag{9}$$

As a result of substitution (8) and (9) to (2) we getting:

$$\sigma'(t)\int_{-\infty}^{+\infty}\varphi(\xi)e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}}\left[(x-\xi)^2-\sigma^2(t)\right]d\xi=$$
$$=\frac{D}{\sigma(t)}\int_{-\infty}^{+\infty}\varphi(\xi)e^{-\frac{(x-\xi)^2}{2\sigma^2(t)}}\left[(x-\xi)^2-\sigma^2(t)\right]d\xi$$

hence:

$$\sigma'(t)=\frac{D}{\sigma(t)} \tag{10}$$

and:

$$\sigma(t) = \sqrt{2Dt} \tag{11}$$

$$c(x,t) = \frac{1}{2\sqrt{\pi Dt}} \int_{-\infty}^{+\infty} \varphi(\xi) e^{-\frac{(x-\xi)^2}{4Dt}} d\xi \tag{12}$$

Let for t = 0 be satisfied initial and final conditions:

$$\begin{aligned} c(x,0) &= c_0 = \text{const} \quad \text{for} \quad -\infty \le x \le 0 \\ c(x,0) &= 0 \quad\quad\quad\quad\quad \text{for} \quad 0 < x \le +\infty \end{aligned} \tag{13}$$

Taking into consideration (6) and (13) we getting $\varphi(\xi) = c_0$ for $\xi \le 0$, and for $\xi > 0$, $\varphi(\xi) = 0$. The formula (12) converting to the equation of the form:

$$c(x,t) = \frac{c_0}{2\sqrt{\pi Dt}} \int_{-\infty}^{0} e^{-\frac{(x-\xi)^2}{4Dt}} d\xi \tag{14}$$

Applying substitution:

$$\frac{\xi - x}{2\sqrt{Dt}} = z \ \text{ for } -\infty \le z \le \frac{-x}{2\sqrt{Dt}}$$

and adequate evaluation maps we getting:

$$c(x,t) = \frac{c_0}{\sqrt{\pi}} \left[\int_0^{+\infty} e^{-z^2} dz - \int_0^{\frac{x}{2\sqrt{Dt}}} e^{-z^2} dz \right] \tag{15}$$

Appling Gaussian Error Distribution:

$$\mathrm{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-z^2} dz$$

and taking into consideration following the equality:

$$\int_0^{+\infty} e^{-z^2} dz = \frac{\sqrt{\pi}}{2}$$

we getting the final result for solution of equation No. 2.

$$c(x,t) = \frac{c_0}{2}\left[1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right] \tag{16}$$

CONCLUSIONS

The Fick's Second Law (2), which can be solved on the base of Gaussian function and by usage of Green's Function, can be applied in mathematical modeling of unidirectional diffusion for isothermal bonding of metals. The equation (16) is the final result, which showing that distribution of diffusing metal A to B is a function of initial concentration (c_o) metal A in time t = 0 and isothermal diffusion coefficient (D).

REFERENCES

1. Mrowec S., *Teoria dyfuzji w stanie stałym. Wybrane zagadnienia*, PWN, Warszawa 1989.
2. Crank J., *The mathematics of diffusion,* Oxford at the clarendon press, 1967.
3. Jarzębski Z.M., *Dyfuzja w metalach. Podstawy teoretyczne i metody doświadczalne,* Wyd. „Śląsk", Katowice 1975.
4. Mrowec S., *Defects and diffusion in solids*, Elsevier, Amsterdam 1980.