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Witold Pogorzelski

Bronisław Bochenek, Janina Wolska-Bochenek

APPLICATION OF INTEGRAL EQUATIONS IN THE THEORY OF DIFFUSION IN THREE-COMPONENT METAL SYSTEMS

I. Introduction

It was a purpose of many authors to find a convenient and concise mathematical framework - as logical extension of the Fick's law - for the description of interdiffusion in multicomponent metallic solid solutions. It is assumed that interstitial components diffuse interstitially and the substitutional components diffuse by a simple exchange mechanism. Thus complications involved in a vacancy mechanism and the associated Kirkendall effect [5] are ignored as well as the general system of one-dimensional diffusion equations for multi-component diffusion in metallic alloys is of the form [1], [3], [4]:

$$\frac{\partial c_\alpha}{\partial t} = \sum_{j=1}^{n-1} \frac{\partial}{\partial x}\left[D_{\alpha j}\frac{\partial c_j}{\partial x}\right] \tag{1}$$

where c_α, $(\alpha=1,2,\ldots,n-1)$ denote concentrations of $(n-1)$ components and $D_{\alpha j}$ coefficients of concentrations.

In the papers [2], [4] there are discussed solutions of the system [1] with the coefficients $D_{\alpha j}$ being constant. In general case the coefficients $D_{\alpha j}$ are variable and moreover they depend on the unknown concentrations c_α.

In the paper [6] an interesting attempt is made to discuss the problem of three-component system in case of variable coefficients depending linearly on two concentrations c_1, c_2 of alloy elements.

In this paper we shall study the following Cauchy problem: Determine functions $c_1(x,t)$, $c_2(x,t)$ satisfying the system

(2) $$\frac{\partial c_\alpha}{\partial t} = \sum_{j=1}^{2} \frac{\partial}{\partial x}\left[D_{\alpha j}(x,t,c_1,c_2)\frac{\partial c_j}{\partial x}\right]$$

($\alpha=1,2$), for every $(x,t) \in (-\infty,+\infty) \times (0,T)$,

and subject to the initial conditions

(3) $$\lim_{t\to 0} c_\alpha = f_\alpha(x), \quad (\alpha=1,2), \quad x\in(-\infty,+\infty),$$

where the functions f_α are given.
We shall try to show the possibility of applying directly to the problem (2), (3) the theory of J.Petrovsky [7], W.Pogorzelski [8], [9], and the results of D.Sadowska [10], and M.Tryjarska [11] concerning parabolic systems of differential equations.

II. Fundamental solution for the system (2) in case of constant coefficients

Let us assume that the coefficients $D_{\alpha j}$, ($j=1,2$) are real constants satisfying the following conditions

(4) $$D_{11} + D_{22} > 0$$

(5) $$\det_{\alpha,j} \| D_{\alpha j} \| > 0$$

Thus the equation, [8 p.154]

$$\det_{\alpha,j} \left\| D_{\alpha j}(-is)^2 - \delta_\alpha^j r \right\| = r^2 + (D_{11}+D_{22})s^2 r +$$

(6) $$+ (D_{11}D_{22} - D_{12}D_{21})s^4 = 0$$

where δ_α^j denotes the Kronecker symbol, has the roots r_j, ($j=1,2$) of the form

(7) $$r_j = -s^2 \varrho_j, \quad (j=1,2),$$

where

(8) $$\varrho_j = \frac{D_{11}+D_{22}+(-1)^j\sqrt{D}}{2}$$

(9) $$D = (D_{11} + D_{22})^2 - 4(D_{11}D_{22}-D_{12}D_{21})$$

The real parts of the roots r_j, $(j=1,2)$ satisfy the inequality

(10) $$\operatorname*{Re}_{j=1,2}(r_j) < -s^2\delta < 0$$

for each value of the real variable s, where $\delta > \mathrm{Re}(\varrho_1)$ is by virtue of (4), (5) a real positive constant. The system (2) with constant coefficients $D_{\alpha j}$, $(\alpha, j = 1,2)$ is then parabolic in the sense of Petrovsky.
According to the general theory given in detail in [7], [8] the elements of the fundamental matrix of solutions of the system (2) have the form of Fourier integrals

(11) $$W_{\alpha\beta}(x,t;\xi,\tau) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} v_\alpha^\beta(t,\tau,s)e^{i(x-\xi)\delta}\,ds$$

$(\alpha, \beta = 1,2)$, where x, ξ denote arbitrary points of the real axis Ox, $\tau < t$ a real value arbitrarily fixed in the interval $[0, T]$.
The functions v_1^β, v_2^β, $(\beta=1,2)$ satisfy the system of ordinary differential equations

(12) $$\frac{dv_\alpha^\beta}{dt} = \sum_{j=1}^{2} D_{\alpha j}(is)^2\, v_j^\beta(t,\tau,s)$$

and initial conditions

(13) $$\lim_{\tau \to t} v_\alpha^\beta(t,\tau, s) = \delta_\alpha^\beta$$

It is easy to show that the solution $\|v_\alpha^\beta\|$ of the problem (12), (13) in case $D \neq 0$ is of the form

(14) $$\|v_\alpha^\beta\| = \begin{Vmatrix} \sum_{j=1}^{2} k_j \exp\left[-s^2 \varrho_j(t-\tau)\right] , & 0 \\ 0, & \sum_{j=1}^{2} k_j \frac{D_{11}-\varrho_j}{D_{12}} \exp\left[-s^2 \varrho_j(t-\tau)\right] \end{Vmatrix}$$

where ϱ_j and D are defined by (8), (9) and

(15) $$k_1 = \frac{D_{11} + D_{12} - \varrho_2}{\varrho_1 - \varrho_2}, \quad k_2 = \frac{\varrho_1 - D_{12} - D_{11}}{\varrho_1 - \varrho_2}$$

In case D=0 the matrix $\|v_\alpha^\beta\|$ is of the form

(16) $$\|v_\alpha^\beta\| = \begin{Vmatrix} \exp\left[-s^2 \frac{D_{11}+D_{22}}{2}(t-\tau)\right], & 0 \\ 0 , & \frac{D_{22}-D_{11}}{2D_{12}} \exp\left[-s^2 \frac{D_{11}+D_{22}}{2}(t-\tau)\right] \end{Vmatrix}.$$

Each element of the matrix (14) or (16) satisfies the inequality

(17) $$\left|v_\alpha^\beta(t,\tau,s)\right| < K \exp\left[-\delta s^2(t-\tau)\right],$$

where K is a positive constant, $K = \max\left(2k_j, 2k_j \frac{D_{11}-\varrho_j}{D_{12}}, 1\right)$, $j=1,2$.

By virtue of the inequality (17) we can assert that the improper integrals (11) are absolutely convergent.

A simple calculus permits us to obtain the matrix of fundamental solutions of the system (2) with constant coefficients, namely in case $D \neq 0$

$$(19)\quad \|W_{\alpha\beta}\| = \left\| \begin{matrix} \sum_{j=1}^{2} \frac{k_j}{2\sqrt{\pi\rho_j(t-\tau)}} \exp\left[-\frac{(x-\xi)^2}{4\rho_j(t-\tau)}\right], & 0 \\ 0, & \sum_{j=1}^{2} \frac{k_j(D_{11}-\rho_j)}{2\sqrt{\pi\rho_j(t-\tau)}D_{12}} \exp\left[-\frac{(x-\xi)^2}{4\rho_j(t-\tau)}\right] \end{matrix} \right\|$$

or in case $D = 0$

$$(20)\quad \|W_{\alpha\beta}\| = \left\| \begin{matrix} \frac{\exp\left[-\frac{(x-\xi)^2}{2(D_{11}+D_{22})(t-\tau)}\right]}{\sqrt{2\pi(D_{11}+D_{22})(t-\tau)}}, & 0 \\ 0, & (D_{22}-D_{11}) \frac{\exp\left[-\frac{(x-\xi)^2}{2(D_{11}+D_{22})(t-\tau)}\right]}{2D_{12}\sqrt{2\pi(D_{11}+D_{22})(t-\tau)}} \end{matrix} \right\|$$

In both cases (19), (20) the elements $W_{\alpha\beta}$ of the fundamental matrix $\|W_{\alpha\beta}\|$ and their derivatives satisfy the inequalities

$$(21)\qquad \left|\frac{\partial^m}{\partial x^m} W_{\alpha\beta}\right| < \frac{\text{const}}{(t-\tau)^{\mu}} \, \frac{\exp\left[-k|x-\xi|\right]}{|x-\xi|^{1+m-2\mu}}$$

where $(m=0,1,2)$ and μ satisfies the inequality

$$(22)\qquad 0 < \mu < \min\left(1, \frac{1+m}{2}\right),$$

k being a positive constant, ([8] p.161).

III. Fundamental solution for the system (2) in case of variable coefficients. The Cauchy problem.

Let us discuss now the system (2) where the coefficients $D_{\alpha j}$, $(\alpha, j=1,2)$ are variable, depend on both concentrations c_1, c_2 and satisfy the following assumptions:

I. The real functions $D_{\alpha j}(x,t,u_1,u_2)$ are defined, continuous and bounded in the domain

$$\Omega : \left\{ (-\infty, +\infty) \times [0,T]; \quad |u_j| < \infty \right\} \tag{23}$$

$$(\alpha, j = 1,2),$$

and satisfy in Ω Hölder conditions

$$\left| D_{\alpha j}(x,t,u_1,u_2) - D_{\alpha j}(x,t',u_1,u_2) \right| < \text{const} \left| t-t' \right|^{h'} \tag{24}$$

where t, t' denote arbitrary values in the interval $[0,T]$ and $h' \in (0,1)$.

Moreover they possess continuous and bounded derivatives[x)] with respect to the variables x, u_1, u_2 uniformly continuous with respect to the variable t and satisfying Hölder conditions

$$\left| \frac{\partial}{\partial x} D_{\alpha j}(x,t,u_1,u_2) - \frac{\partial}{\partial x} D_{\alpha j}(x', t, u_1', u_2') \right| < \text{const} \left[|x-x'|^{h} + \right. \tag{25}$$

$$\left. + t^{\gamma} \sum_{j=1}^{2} |u_j - u_j'|^{h''} \right],$$

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x) In relation with the paper [13] it would be possible to accept some discontinuities concerning the derivatives $\frac{\partial D_{\alpha j}}{\partial x}$, and in relation with the paper [11] (p.154) the inequality

$$\left| \frac{\partial}{\partial u_k} D_{\alpha j} \right| < M t^{-\mu} + M' \sum_{j=1}^{2} |u_j|.$$

$$(26)\qquad \left|\frac{\partial}{\partial u_k}D_{\alpha j}(x,t,u_1,u_2)-\frac{\partial}{\partial u_k}D_{\alpha j}(x',t,u_1',u_2')\right| < \text{const}\left[|x-x'|^{\tilde{h}} + \sum_{j=1}^{2}|u_j-u_j'|^{\tilde{h}''}\right],$$

where x, x' are two arbitrary points of the real axis Ox, h, $\tilde{h},h,\tilde{h}''$, $\gamma\in(0,1)$, $(\alpha,j,k=1,2)$.

II. The system (2) is parabolic in the sense of Petrovsky. Moreover we admit the following assumption concerning the functions of the initial condition (3):

III. The real functions f_α, $(\alpha=1,2)$ are continuous and bounded for every $x\in(-\infty,+\infty)$.

The system (2) can be represented in the form:

$$(27)\qquad \hat{\psi}^{(\alpha)}(c_1,c_2)\equiv\sum_{j=1}^{2}D_{\alpha j}(x,t,c_1,c_2)\frac{\partial^2 c_j}{\partial x^2}+\sum_{j=1}^{2}\frac{\partial D_{\alpha j}}{\partial x}\frac{\partial c_j}{\partial x}-\frac{\partial c_\alpha}{\partial t} = F_\alpha\left(x,t,\frac{\partial c_1}{\partial x},\frac{\partial c_2}{\partial x}\right)\qquad (\alpha=1,2),$$

where we have denoted

$$(28)\qquad F_\alpha\left(x,t,\frac{\partial c_1}{\partial x},\frac{\partial c_2}{\partial x}\right) = -\sum_{k,j=1}^{2}\frac{\partial D_{\alpha j}}{\partial c_k}\frac{\partial c_j}{\partial x}\frac{\partial c_k}{\partial x}$$

The homogeneous system (27) of M-th degree with initial condition (3) in case $\alpha=1,2,\dots,N$, for $x\in E_n$ was studied by D. Sadowska [10]. The unhomogenous system of type (27) with homogeneous initial condition, where the coefficients $D_{\alpha j}$ depend moreover on the derivatives of the unknown functions was studied by M. Tryjarska [11].

We shall look for a solution of the problem (2), (3) (or (27), (3)) in the class of functions $c_\alpha(x,t)$ satisfying following conditions

(29) $$\left| \frac{\partial^m c_\alpha}{\partial x^m} \right| < \infty$$

(30) $$_{t}\gamma\left| \frac{\partial^m c_\alpha}{\partial x^m}(x,t) - \frac{\partial^m c_\alpha}{\partial x^m}(x',t') \right| \leq \varkappa\left[|x-x'|^{\frac{h}{h''}} + |t-t'|^{\frac{h'}{h''}} \right]$$

$(m=0,1)$, $\gamma<\gamma'<\frac{\varkappa}{h''}<1$, and $\varkappa$ denotes a positive constant.

In relation with the papers [8], [9], [10], [11] the elements of the fundamental solution $\Gamma^{(c)}$ of the homogeneous system (27) would be defined by the formula

(31) $$\Gamma^{(c)}_{\alpha\beta}(x,t;\xi,\tau) = W^{\xi,\tau,(c)}_{\alpha\beta}(x,t;\xi,\tau) + \int_{\tau}^{t}\int_{-\infty}^{+\infty}\sum_{\nu=1}^{2} W^{\varrho,\mathfrak{z},(c)}_{\alpha\nu}(x,t;\varrho,\mathfrak{z})\,\phi^{\varrho,\mathfrak{z},(c)}_{\nu\beta}(\varrho,\mathfrak{z};\xi,\tau)\,d\varrho\,d\mathfrak{z}$$

where $W^{\xi,\tau,(c)}_{\alpha\beta}$ denote the elements of the matrix (19),(20) with the coefficients $D^{\xi,\tau,(c)}_{\alpha\beta}$ fixed for $x=\xi$, $t=\tau$ i.e.

(32) $$D^{\xi,\tau,(c)}_{\alpha\beta} = D_{\alpha\beta}\left[\xi,\tau,\ c_1(\xi,\tau),\ c_2(\xi,\tau)\right]$$

The integrals in (31) are the elements of the vector of quasi-potential of linear charge, and the functions $\phi^{\xi,\tau,(c)}_{\alpha\beta}$ form for the fixed β regularly continuous solutions of the system of integral,singular Volterra equations ([10], p.89-91):

(33) $$\phi^{(c)}_{\alpha\beta}(x,t;\xi,\tau) = \hat{\psi}^{(\alpha)}_{(j)(c)}\left[W^{\xi,\tau,(c)}_{j\beta}(x,t;\xi,\tau)\right] + \int_{\tau}^{t}\int_{-\infty}^{+\infty}\sum_{\nu=1}^{2}\hat{\psi}^{(\alpha)}_{(j)(c)}\left[W^{\varrho,\mathfrak{z},(c)}_{j\nu}(x,t;\varrho,\mathfrak{z})\right]\phi^{(c)}_{\nu\beta}(\varrho,\mathfrak{z};\xi,\tau)\,d\varrho\,d\mathfrak{z}$$

Thus the elements of the fundamental solution $\Gamma^{(c)}$ and their first derivatives satisfy the following inequalities:

$$(34)\quad \left|\frac{\partial^m}{\partial x^m}\Gamma^{(c)}_{\alpha\beta}(x,t;\xi,\tau)\right| < \frac{p_m(T,\varkappa)}{(t-\tau)^{\mu_0}}\ \frac{\exp\left[-k|x-\xi|\right]}{|x-\xi|^{2\mu_0-1-m}}$$

(m=0,1) where

$$(35)\qquad \mu_0\in(1-\tfrac{1}{2}\min(h,2h'),\gamma),$$

p_m is a positive constant depending on $T,\varkappa$.

By using the fundamental solution (31) of the homogeneous system (27) one can build generalized potentials relative to this system, namely the Poisson-Weierstrass integral as well the potential of line-charge and seek the solution of the problem (2), (3) (or (27), (3)) in the form

$$c_\alpha(x,t)=\int_0^t\int_{-\infty}^{+\infty}\sum_{\beta=1}^{2}\Gamma^{(c)}_{\alpha\beta}(x,t;\xi,\tau)\,F_\beta(\xi,\tau,\frac{\partial c_1}{\partial\xi},\frac{\partial c_2}{\partial\xi})\,d\xi\,d\tau+$$

$$(36)\qquad +\int_{-\infty}^{+\infty}\sum_{\beta=1}^{2}\Gamma^{(c)}_{\alpha\beta}(x,t;\xi,0)\quad f_\beta(\xi)d\xi$$

$\alpha=1,2$, where F_1,F_2 are defined by (28).

It is obvious that by virtue of the formulae (28), (29), (30) and assumption I we can state that the functions $F_\alpha(x,t,q_1,q_2)$ for every $(x,t)\in(-\infty,+\infty)\times[0,T]$ and $|q_\alpha|<\infty$, $(\alpha=1,2)$, are bounded and satisfy Hölder-Lipschitz conditions

$$(37)\quad \left|F_\alpha(x,t,q_1,q_2)-F_\alpha(x',t,q_1',q_2')\right|<\mathrm{const}\left[|x-x'|^{h^*}+\right.$$

$$\left.+\sum_{j=1}^{2}|q_j-q_j'|\right],$$

where $h^*=\min(h,\tilde{h})$.

On the strength of (29), (30), (34), (37) and supposition III we can examine, instead of the system (36), the following auxiliary system of 4 integral non-linear equations:

$$c_\alpha(x,t) = \int_0^t \int_{-\infty}^{+\infty} \sum_{\beta=1}^{2} \Gamma_{\alpha\beta}^{(c)}(x,t;\xi,\tau)\, F_\beta(\xi,\tau,g_1,g_2)\, d\xi\, d\tau + \tag{38}$$

$$+\int_{-\infty}^{+\infty} \sum_{\beta=1}^{2} \Gamma_{\alpha\beta}^{(c)}(x,t;\xi,0)\, f_\beta(\xi)\, d\xi$$

$$g_\alpha(x,t) = \int_0^t \int_{-\infty}^{+\infty} \sum_{\beta=1}^{2} \frac{\partial}{\partial x} \Gamma_{\alpha\beta}^{(c)}(x,t;\xi,\tau) F_\beta(\xi,\tau,g_1 g_2)\, d\xi\, d\tau +$$

$$+\int_{-\infty}^{+\infty} \sum_{\beta=1}^{2} \frac{\partial}{\partial x} \Gamma_{\alpha\beta}^{(c)}(x,t;\xi,0)\, f_\beta(\xi)\, d\xi$$

$$(\alpha=1,2),$$

with four unknown functions c_1, c_2, g_1, g_2.

The system (38) can be examined by the method of successive approximations, like the system (59) in the paper [11] - and one can prove that a unique solution exists for every $(x,t)\ \varepsilon\ (-\infty,+\infty) \times [0,\varepsilon]$ (where ε is sufficiently small positive constant) that the functions $g_\alpha = \frac{\partial c_\alpha}{\partial x}$, and that $\lim_{t\to 0} c_\alpha = f_\alpha(x)$.

Thus the solution of the system (38) gives also the solution of the system (36) and of the Cauchy problem (2), (3).

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Address of the Author: prof.Bronisław Bochenek, Warszawa, ul.Koszykowa 75 m. 22.

INSTITUTE OF MATHEMATICS, TECHNICAL UNIVERSITY, WARSAW

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