

Mass diffusion into two-layer media

S. A. Masoud, A. M. Hassan, M. A. Al-Nimr

Abstract Using Green's function method, an analytical, closed form solution for the problem of transient mass diffusion into a two-layer medium is found. Two problems are considered; composite slab and composite cylinder. Carbon diffusion into slab composed of Ferrite steel and Austenite steel in perfect contact is investigated. From the results, the time required for carbon concentration to reach a certain level is estimated.

List of symbols

a	First layer thickness in the slab, or inner region radius in the cylinder
\bar{A}_1, \bar{A}_2	Initial carbon mass concentration in the first and the second layers respectively
b	Slab thickness, or cylinder total radius
$D_{c1} D_{c2}$	Diffusion coefficients of the first and the second layers, respectively
\bar{E}_1	Maximum carbon concentration at the outer surface of the outer layer
$\bar{m}_{c1}, \bar{m}_{c2}$	Carbon mass concentration in the first and the second layers respectively
r	Radial coordinate
t	Time
x	Transverse coordinate
ρ_1, ρ_2	Mass densities for the first and the second layers respectively

Subscripts

1	First layer
2	Second layer
c	Carbon component

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Introduction

Atoms at finite temperature are not static, but vibrate in three dimensions around the normal atomic position, usually the lattice sites. If an atom moves from one lattice site to another, it must have sufficient energy to break the bonds with its neighbor atoms. This phenomenon of material transport by atomic motion is called diffusion. At

a certain temperature, a small portion of atoms can diffuse within the material. These atoms have enough vibration energies to accomplish such movements. The number of these atoms will increase with the rise in temperature.

The diffusion of atoms within a material is called self-diffusion, while the diffusion of atoms of one material into another material is called inter-diffusion or impurity diffusion [1, 2]. Diffusion can be achieved through several mechanisms. At any instant of time two neighboring atoms are vibrating in directions, so that enough space may exist around the two atoms allowing them to exchange positions simultaneously. Also, it may happen that four neighboring atoms, at some instant, vibrate so that they move cooperatively in a ring, allowing each of them to exchange place simultaneously to a new neighboring position within the ring.

Another suggested mechanism for diffusion is the movement of atom from a position adjacent to vacancy into that vacant lattice site. Conversely, it could be considered that the vacancy had moved to a direction opposite to the direction of atom movement. If a vacancy exists in a lattice, then the movement of the adjacent atom to the vacant site requires less vibration energy than in the other mentioned diffusion mechanisms. It is postulated that dislocation climb can be achieved through the exchange of places between atoms and vacancies, which is rather significant in connection with creep [3].

Diffusion can also be achieved by the migration of small sized atoms from interstitial sites to a neighboring site, which is empty. This diffusion is termed interstitial diffusion. The discontinuous transition from elastic to plastic range in mild steel can be explained by this mechanism [3]. Also, the carbonizing or nitriding of steel is based on this diffusion mechanism. The atoms of carbon or nitrogen penetrate into the surface of steel in order to increase the surface hardness. Many investigators were and still involved, and huge amounts of publications about these surface-hardening processes are available at present [4].

In certain application, a very thin layer of material can be attached to the surface of another material by different surface protection processes such as coating, plating, cladding, etc. In the present work, an attempt has being made to examine the possible diffusion of a specific material through another two materials placed in surface contact with each other, if it may be needed, at certain circumstances, to be done for the products of some of the above mentioned processes. A theoretical analysis has been made and the result, using carbon as the diffused material and two layers of iron as host materials, are

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shown. The mass diffusion equations that describe the transient penetration of carbon into a two-layer media are solved analytically using Green's function method. It is assumed that the two layers are in perfect contact. Two geometry of the two-layer composite medium is considered, which are two-layer slab and cylinder. It is worth mentioning in this respect, that the field of composite materials seems also to be a promising area for the application of this new approach.

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Mathematical analysis

1. Carbon diffusion into a two-layer slab

Two different materials are used to fabricate a two-layer slab as shown in Fig. 1a. The two layers have perfect contact at their interface. Initially, the carbon mass concentration in the first and the second layers are \bar{A}_1 and \bar{A}_2 , respectively. For any time greater than zero, the outer surface of the first layer is maintained at carbon mass concentration of \bar{E}_1 and the outer surface of the second layer is insulated. The governing equations of the problem under consideration are [5]:

$$\frac{\partial^2 \bar{m}_{c1}}{\partial X^2} = \frac{1}{D_{c1}} \frac{\partial \bar{m}_{c1}}{\partial t}, \quad 0 \leq X \leq a \quad (1)$$

$$\frac{\partial^2 \bar{m}_{c2}}{\partial X^2} = \frac{1}{D_{c2}} \frac{\partial \bar{m}_{c2}}{\partial t}, \quad a \leq X \leq b \quad (2)$$

The initial and boundary conditions for Eqs. (1) and (2) are:

$$\begin{aligned} \bar{m}_{c1}(0, x) &= \bar{A}_1, \quad \bar{m}_{c2}(0, x) = \bar{A}_2 \\ \bar{m}_{c1}(t, 0) &= \bar{E}_1, \quad \bar{m}_{c1}(t, a) = \bar{m}_{c2}(t, a) \\ \rho_1 D_{c1} \frac{\partial \bar{m}_{c1}}{\partial X}(t, a) &= \rho_2 D_{c2} \frac{\partial \bar{m}_{c2}}{\partial X}(t, a), \quad \frac{\partial \bar{m}_{c2}}{\partial X}(t, b) = 0 \end{aligned} \quad (3)$$

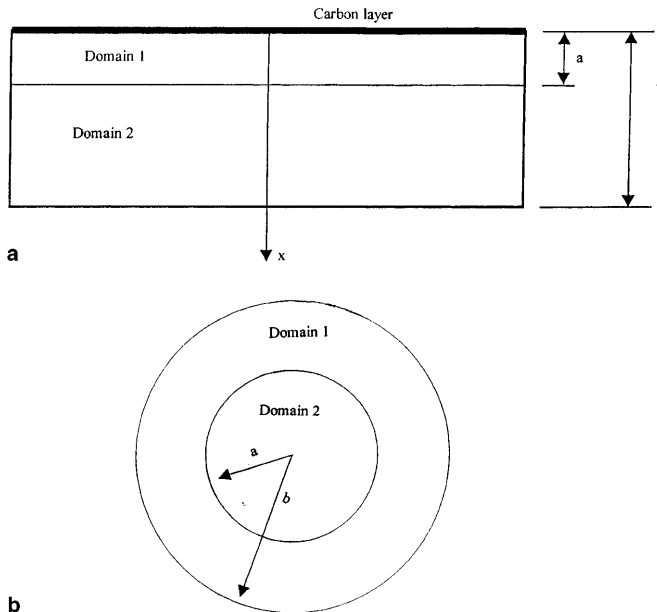


Fig. 1. a Schematic diagram for two-layer Slab, b Schematic diagram for two-layer Cylinder

For homogeneous boundary conditions, the following transformations are used:

$$m_{c1} = \bar{m}_{c1} - \bar{E}_1, \quad m_{c2} = \bar{m}_{c2} - \bar{E}_1$$

Substitute the above transformation into Eqs. (1)–(3) to get:

$$\frac{\partial^2 m_{c1}}{\partial X^2} = \frac{1}{D_{c1}} \frac{\partial m_{c1}}{\partial t} \quad (4)$$

$$\frac{\partial^2 m_{c2}}{\partial X^2} = \frac{1}{D_{c2}} \frac{\partial m_{c2}}{\partial t} \quad (5)$$

with

$$m_{c1}(0, X) = \bar{A}_1 - \bar{E}_1 = A_1,$$

$$m_{c2}(0, X) = \bar{A}_2 - \bar{E}_1 = A_2$$

$$m_{c1}(t, 0) = 0, \quad m_{c1}(t, a) = m_{c2}(t, a)$$

$$\rho_1 D_{c1} \frac{\partial m_{c1}}{\partial X}(t, a) = \rho_2 D_{c2} \frac{\partial m_{c2}}{\partial X}(t, a), \quad \frac{\partial m_{c2}}{\partial X}(t, b) = 0 \quad (6)$$

Using Green's function method [6, 7], the following solution is assumed for Eqs. (4)–(6):

$$\begin{aligned} m_{c1}(t, X) = \sum_{n=1}^{\infty} \frac{e^{-\beta_n^2 t}}{N_n} \psi_{i,n}(X) \left\{ \frac{\rho_1 A_1 \sqrt{D_{c1}}}{\beta_n} [\cos(\alpha_n X)]_0^a \right. \\ \left. - \frac{\rho_2 A_2 \sqrt{D_{c2}}}{\beta_n} [-B_{2n} \cos(\alpha_n X) \right. \\ \left. + C_{2n} \sin(\alpha_n X)]_a^b \right\} \quad i = 1, 2 \end{aligned} \quad (7)$$

where

$$\psi_{1n}(X) = \sin\left(\frac{\beta_n X}{\sqrt{D_{c1}}}\right)$$

$$\psi_{2n}(X) = B_{2n} \sin\left(\frac{\beta_n X}{\sqrt{D_{c2}}}\right) + C_{2n} \cos\left(\frac{\beta_n X}{\sqrt{D_{c2}}}\right)$$

$$\begin{aligned} N_n = \rho_1 \left[\frac{X}{2} - \frac{\sin(2\alpha_n X)}{4\alpha_n} \right]_0^a + \rho_2 B_{2n}^2 \left[\frac{X}{2} - \frac{\sin(2\alpha_n X)}{4\alpha_n} \right]_a^b \\ + \rho_2 C_{2n}^2 \left[\frac{X}{2} + \frac{\sin(2\alpha_n X)}{4\alpha_n} \right]_a^b \\ + 2\rho_2 B_{2n} C_{2n} \left[\frac{\sin^2(\gamma_n X)}{2\gamma_n} \right]_a^b \end{aligned}$$

$$\alpha_n = \frac{\beta_n}{\sqrt{D_{c1}}}, \quad \gamma_n = \frac{\beta_n}{\sqrt{D_{c2}}}$$

B_{2n} and C_{2n} are:

$$B_{2n} = [\sin(\delta_n) \sin(a/b\eta_n) + K \cos(\delta_n) \cos(a/b\eta_n)]$$

$$C_{2n} = [\sin(\delta_n) \cos(a/b\eta_n) - K \cos(\delta_n) \sin(a/b\eta_n)]$$

with

$$\delta_n = \frac{a\beta_n}{\sqrt{D_{c1}}}, \quad \eta_n = \frac{b\beta_n}{\sqrt{D_{c2}}}, \quad K = \frac{\rho_1 D_{c1}}{\rho_2 D_{c2}} \sqrt{\frac{D_{c2}}{D_{c1}}}$$

Also, β_n 's are found by setting the determinant of the following system of algebraic equations to zero:

$$\begin{vmatrix} \sin \delta_n & -\sin(a/b\eta_n) & -\cos(a/b\eta_n) \\ K \cos \delta_n & -\cos(a/b\eta_n) & \sin(a/b\eta_n) \\ 0 & \cos \eta_n & -\sin \eta_n \end{vmatrix} = 0$$

and

$$[f(x)]_a^b = f(b) - f(a)$$

2. Carbon diffusion into a two-layer cylinder

Consider a two-layer composite solid cylinder, as shown in Fig. 1b, where perfect contact is assumed between the cylinder layers. The initial carbon concentration in the first and the second layers are \bar{A}_1 and \bar{A}_2 , respectively. For any time t greater than zero, the outer surface of the cylinder is maintained at carbon mass concentration of \bar{E}_1 . The governing equations for the carbon diffusion in both domains are given as [5]:

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial m_{c1}}{\partial r} \right) = \frac{1}{D_{c1}} \frac{\partial m_{c1}}{\partial t}, \quad 0 \leq r \leq a \quad (8)$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial m_{c2}}{\partial r} \right) = \frac{1}{D_{c2}} \frac{\partial m_{c2}}{\partial t}, \quad a \leq r \leq b \quad (9)$$

where

$$m_{c1} = \bar{m}_{c1} - \bar{E}_1, \quad m_{c2} = \bar{m}_{c2} - \bar{E}_1$$

The initial and boundary conditions for Eqs. (8) and (9) are:

$$m_{c1}(0, r) = \bar{A}_1 - \bar{E}_1 = A_1, \quad m_{c2}(0, r) = \bar{A}_2 - \bar{E}_1 = A_2$$

$$\frac{\partial m_{c1}}{\partial r}(t, 0) = 0, \quad m_{c1}(t, a) = m_{c2}(t, a)$$

$$\rho_1 D_{c1} \frac{\partial m_{c1}}{\partial r}(t, a) = \rho_2 D_{c2} \frac{\partial m_{c2}}{\partial r}(t, a), \quad m_{c2}(t, b) = 0 \quad (10)$$

Using Green's function method, the solutions of Eqs. (8)–(10) are:

$$m_{c1}(t, X) = \sum_{n=1}^{\infty} \frac{e^{-\beta_n^2 t}}{N_n} \psi_{i,n}(r) \left\{ \frac{\rho_1 A_1 \sqrt{D_{c1}}}{\beta_n} \left(a J_1 \left(\frac{\beta_n a}{\sqrt{D_{c1}}} \right) \right) + \frac{\rho_2 A_2 \sqrt{D_{c2}}}{\beta_n} \left[B_{2n} \left[r J_1 \left(\frac{\beta_n r}{\sqrt{D_{c2}}} \right) \right]_a^b + C_{2n} \left[r Y_1 \left(\frac{\beta_n r}{\sqrt{D_{c2}}} \right) \right]_a^b \right] \right\} \quad i = 1, 2 \quad (11)$$

where

$$\psi_{1n}(r) = J_0 \left(\frac{\beta_n r}{\sqrt{D_{c1}}} \right)$$

$$\psi_{2n}(r) = B_{2n} J_0 \left(\frac{\beta_n r}{\sqrt{D_{c2}}} \right) + C_{2n} Y_0 \left(\frac{\beta_n r}{\sqrt{D_{c2}}} \right)$$

$$N_n = \rho_1 \left[\frac{r^2}{2} \left\{ J_0^2 \left(\frac{\beta_n r}{\sqrt{D_{c1}}} \right) - J_{-1} \left(\frac{\beta_n r}{\sqrt{D_{c1}}} \right) J_1 \left(\frac{\beta_n r}{\sqrt{D_{c1}}} \right) \right\} \right]_0^a$$

$$+ \rho_2 \left[\frac{r^2}{2} \left(\frac{B_{2n} \beta_n}{\sqrt{D_{c2}}} J_1 \left(\frac{\beta_n r}{\sqrt{D_{c2}}} \right) + \frac{C_{2n} \beta_n}{\sqrt{D_{c2}}} Y_1 \left(\frac{\beta_n r}{\sqrt{D_{c2}}} \right) \right)^2 + \frac{r^2}{2} \left(B_{2n} J_0 \left(\frac{\beta_n r}{\sqrt{D_{c2}}} \right) + C_{2n} Y_0 \left(\frac{\beta_n r}{\sqrt{D_{c2}}} \right) \right)^2 \right]_a^b$$

$$B_{2n} = \frac{1}{\Delta} \left[J_0(\gamma) Y_1 \left(\frac{a}{b} \eta \right) - K J_1(\gamma) Y_0 \left(\frac{a}{b} \eta \right) \right]$$

$$C_{2n} = \frac{1}{\Delta} \left[K J_1(\gamma) J_0 \left(\frac{a}{b} \eta \right) - J_0(\gamma) J_1 \left(\frac{a}{b} \eta \right) \right]$$

$$\Delta = J_0 \left(\frac{a}{b} \eta \right) Y_1 \left(\frac{a}{b} \eta \right) - J_1 \left(\frac{a}{b} \eta \right) Y_0 \left(\frac{a}{b} \eta \right)$$

and β_n 's are the root of the following determinant:

$$\begin{vmatrix} J_0(\gamma) & -J_0 \left(\frac{a}{b} \eta \right) & -Y_0 \left(\frac{a}{b} \eta \right) \\ K J_1(\gamma) & -J_1 \left(\frac{a}{b} \eta \right) & -Y_1 \left(\frac{a}{b} \eta \right) \\ 0 & J_0(\eta) & Y_0(\eta) \end{vmatrix} = 0$$

where

$$\gamma = \frac{\alpha \beta_n}{\sqrt{D_{c1}}}, \quad \eta = \frac{b \beta_n}{\sqrt{D_{c2}}}, \quad K = \frac{\rho_1 D_{c1}}{\rho_2 D_{c2}} \sqrt{\frac{D_{c2}}{D_{c1}}}$$

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Results

Consider the situation in which a thin layer of carbon is attached at the outer surface of the first layer of the composite slab, as shown in Fig. 1. The slab is made of ferrite iron (α -Fe) and austenite iron (γ -Fe). Properties of these two layers of iron and their interaction with diffusion of carbon (1) are:

$$D_{c,\alpha} = 6.2 \times 10^{-7} \text{ (m}^2/\text{s)}, \quad D_{c,\gamma} = 1 \times 10^{-5} \text{ (m}^2/\text{s)},$$

$$\rho_\alpha = \rho_\gamma = 7870 \text{ (kg/m}^3\text{)},$$

$$a = 0.01 \text{ (m)}, \quad b = 0.02 \text{ (m)}.$$

The results are obtained for two arrangements, where in first one, D_{c1} and ρ_1 stand for the diffusion of carbon into γ -Fe and its density respectively. Also, D_{c2} and ρ_2 stand for the diffusion of carbon into α -Fe and its density, respectively. In the second arrangement, D_{c1} and ρ_1 stand for the diffusion of carbon into α -Fe and its density, respectively. Also, D_{c2} and ρ_2 stand for the diffusion of carbon into γ -Fe and its density respectively. Since the carbon mass concentration in Iron is very important in specifying the mechanical and thermal properties of the Iron, the diffusion of γ -Fe, α -Fe into each other is ignored, and only the carbon diffusion into the iron is investigated. Figure 2 shows the results of the first arrangement, where the carbon layer is attached at the outer surface of γ -Fe. The figure presents the transient variation in the carbon mass concentration within the composite slab at different depths of the slab. It is clear from this figure that locations far away from the surface of the slab requires more time to attain steady state carbon mass concentration. Figure 3 shows similar plots for the second arrangement, in which the carbon layer is attached at the surface of α -Fe. The comparison between the results of the two arrangements

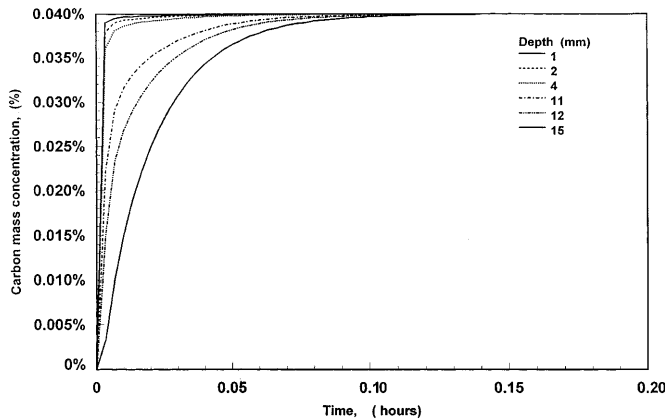


Fig. 2. Carbon mass concentration vs. time for different slab levels in the first arrangement. $D_{c1} = 1.0 \times 10^{-5}$, $D_{c2} = 6.2 \times 10^{-7}$, $a = 10$ mm, $b = 20$ mm

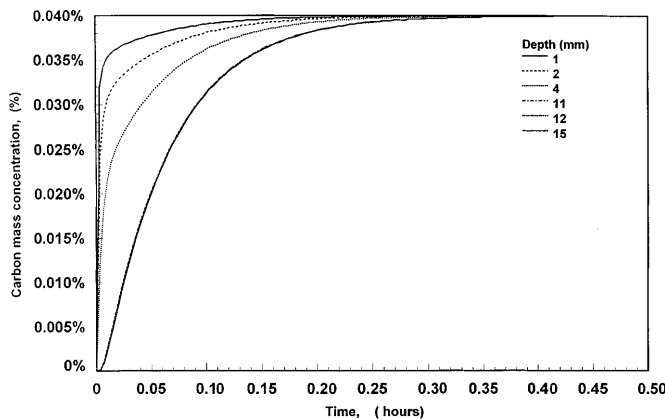


Fig. 3. Carbon mass concentration vs. time for different slab levels in the second arrangement. $D_{c1} = 6.2 \times 10^{-7}$, $D_{c2} = 1.0 \times 10^{-5}$, $a = 10$ mm, $b = 20$ mm

shows that the diffusion process in the second arrangement is much slower than that in the first arrangement. In the second arrangement, carbon has to penetrate through α -Fe, first, which has much lower diffusion coefficient for carbon compared to that for γ -Fe. This implies that the layer of the lower diffusion coefficient is the major controlling agent in the diffusion process.

Ferrite (α -Fe) can not hold usually carbon in solid solution to any great extent, the maximum limits being 0.04 per cent of carbon at eutectoid temperature (723°C), and 0.006 per cent at room temperature. While, austenite (γ -Fe), however, can hold a considerable amount of carbon in solid solution, ranging from 0.87 percent at eutectoid temperature (723°C) to 1.7 percent at eutectic temperature (1130°C). This allotropic changes of iron from α to γ and the change in the amount of dissolved carbon in each of these phases make the use of heat-treating processes for iron possible. These processes

produce a wide range of properties in ferrous alloys. One of these processes is carburizing, which is used on steel to obtain a hard outside layer on a comparatively soft and tough core. These two layers are simulated in the present work as α -Fe layer and γ -Fe layer, especially if there is a perfect contact between these two layers. When carburizing a steel workpiece, it is heated above the allotropic transformation temperature, and then α -phase will change to γ -phase, but if the thickness of the workpiece is large, it is more likely that only the outside layer will be changed to γ , while the core remains unchanged. As carburizing is a surface hardening process, the change of the outer surface to γ -phase is important in order to dissolve more carbon. Figure 2 shows this case where γ -Fe is the first domain and α -Fe is the second domain, which is more common in the heat treatment of steel rather than the arrangement shown in Fig. 3. It is also possible from the above mentioned figures to find out the carbon mass concentration percentage in both α and γ phases at a certain time, which is important in the carburizing process.

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Conclusion

Analytical solution is obtained for the problem of transient mass diffusion into a two-layer composite medium. The solution is obtained for two geometry, which are composite slab and cylinder. Case study is presented in which carbon is diffused into composite slab made of ferrite iron (α -Fe) and austenite iron (γ -Fe) which are in perfect Contact. For this case study two arrangements are considered, where in the first one the carbon layer is attached directly to α -Fe, and in the second one, the carbon layer is attached to γ -Fe. From the obtained results, the time for certain carbon mass concentration is found at any level from slab surface. Also, it is found that the layer of lower diffusion coefficient is the major controlling agent in the diffusion process.

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