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Author
Blank, Stuart L.

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Stuart L. Blank
Inorganic Materials Research Division, Lawrence Radiation Laboratory,
and Department of Materials Science and Engineering
College of Engineering, University of California,
Berkeley, California

The solution of the diffusion problem involving two phases with a moving boundary was given by Crank. (1) This solution is extended here to systems with three phases and two moving boundaries. It has been applied to the diffusion profile for the MgO-Fe₂O₃ system (shown schematically in Fig. 1 with a portion of the phase diagram) (2) in which the phases are MgO, magnesioferrite, and Fe₂O₃.

Using the notations shown in Fig. 1, C₁, C₁I, and C₁II can be obtained by an error function solution:

\[ C₁ = C₁,0 + B₁ \left[ 1 - \text{erf}\left( \frac{X}{\sqrt{4D₁t}} \right) \right] \quad X₁ < X < \infty \]  

\[ C₁II = A + B₁II \text{erf}\left( \frac{X}{\sqrt{4D₁IIt}} \right) \quad X₁ < X < \infty \]  

\[ C₁III = C₁III,0 - B₁III \left[ 1 + \text{erf}\left( \frac{X}{\sqrt{4D₁IIIt}} \right) \right] \quad \infty < X < \infty \]  

Equations (1), (2) and (3) satisfy Fick's second law. Equations (1) and (3) also satisfy the initial conditions of

\[ \bar{X}₁₁ = \bar{X}₁₁,1 = 0 \quad \text{when} \quad t = 0, \]

then

\[ C₁ = C₁,0 \quad \text{and} \quad C₁III = C₁III,0. \]

The six quantities A, B₁, B₁I, B₁II, C₁, and \( \bar{X}₁₁,1 \) and \( \bar{X}₁₁,II \) must be known in order to obtain an analytical solution. Using Wagner's technique

MgO-Fe₂O₃ phase diagram and schematic diffusion profile for three-phase diffusion problem. (2)
\[
\left( \bar{X}_{II,I} = \gamma_I \sqrt{4D_{II} t} \quad \text{and} \quad \bar{X}_{III,II} = \gamma_{III} \sqrt{4D_{III} t} \right)
\]

and applying the boundary conditions of \( \bar{X}_{II,I} \) and \( \bar{X}_{III,II} \) one then obtains

\[
C_I = C_{I,0} + \left[ \frac{C_{II,III} - C_{I,0}}{1 - \text{erf}(\gamma_I)} \right] \left[ 1 - \text{erf} \left( \frac{X}{\sqrt{4D_{II} t}} \right) \right]
\]

\[
C_{II,I} = A + B_{II} \left[ \text{erf} \left( \gamma_I \sqrt{\frac{D_{II}}{4D_{III}}} \right) \right]
\]

\[
C_{II,III} = A + B_{II} \left[ \text{erf} \left( \gamma_{III} \sqrt{\frac{D_{III}}{4D_{II}}} \right) \right]
\]

\[
C_{III} = C_{III,0} - \left[ \frac{C_{III,0} - C_{III,II}}{1 + \text{erf}(\gamma_{III})} \right] \left[ 1 + \text{erf} \left( \frac{X}{\sqrt{4D_{III} t}} \right) \right]
\]

Solving for \( B_{II} \) and \( A \) and substituting into Eq. (2) results in

\[
C_{II} = C_{II,III} + \frac{\left( C_{II,III} - C_{II,I} \right) \left[ \text{erf} \left( \frac{X}{\sqrt{4D_{II} t}} \right) - \text{erf} \left( \gamma_{III} \sqrt{\frac{D_{III}}{D_{II}}} \right) \right]}{\left[ \text{erf} \left( \gamma_{III} \sqrt{\frac{D_{III}}{D_{II}}} \right) - \text{erf} \left( \gamma_{II} \sqrt{\frac{D_{II}}{D_{II}}} \right) \right]}
\]

Two additional equations are now needed in order to obtain \( \bar{X}_{III,II} \) and \( \bar{X}_{II,I} \) and to complete the solution. These are obtained by examining the flux at \( \bar{X}_{III,II} \) and at \( \bar{X}_{II,I} \). In each case the flux into the boundary minus flux out of the boundary equals the rate of increase of material in region II. By applying a mass balance at \( \bar{X}_{III,II} \)

\[
\text{Flux in} = -D_{III} \left( \frac{\partial C_{III}}{\partial X} \right) \bar{X}_{III,II}
\]

\[
\text{Flux out} = -D_{II} \left( \frac{\partial C_{II}}{\partial X} \right) \bar{X}_{III,II}
\]

and realizing that

\[
\frac{d\bar{X}_{III,II}}{dt} = \gamma_{III} \sqrt{D_{III}} \quad t^{-1/2}
\]

we obtain
By applying a mass balance at \( \bar{x}_{II,I} \):

\[
\text{Flux in} = - D_{II} \left( \frac{\partial c_{II}}{\partial x} \right) \bar{x}_{II,I}
\]

\[
\text{Flux out} = - D_{I} \left( \frac{\partial c_{I}}{\partial x} \right) \bar{x}_{II,I}
\]

and using the relation that

\[
\frac{d\bar{x}_{II,I}}{dt} = \gamma_{I} \sqrt{D_{I}} \quad t^{-1/2}
\]

\[
\sqrt{\frac{D_{I}}{\pi}} \left( \frac{c_{II,I} - c_{II,0}}{1 - \text{erf} \left( \gamma_{I} \right)} \right) e^{-\gamma_{I}^2} - \sqrt{\frac{D_{II}}{\pi}} = \frac{(c_{II,I} - c_{II,0})}{1 - \text{erf} \left( \gamma_{I} \right)} e^{-\gamma_{I}^2} - \sqrt{\frac{D_{II}}{\pi}} = (c_{II,I} - c_{II,0}) \gamma_{I} \sqrt{D_{I}}
\]

Equations (9) and (10) can now be solved for \( \gamma_{I} \) and \( \gamma_{III} \). One procedure is to assume \( \gamma_{III} \) in Eq. (9) and to calculate \( \gamma_{I} \), and to assume \( \gamma_{I} \) in Eq. (10) and to calculate \( \gamma_{III} \). These can then be plotted and the values for \( \gamma_{III} \) and \( \gamma_{I} \) obtained. It is also evident from this treatment that

\[
\bar{x}_{II,I} - \bar{x}_{III,II} = \left[ \gamma_{I} \sqrt{D_{I}} - \gamma_{III} \sqrt{D_{III}} \right] t^{1/2}
\]

which shows that the intermediate phase (magnesioferrite in this example) grows as \( t^{1/2} \).
Using the above solution a diffusion experiment can be designed to measure all the necessary parameters and therefore obtain an exact analytical solution.

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REFERENCES


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