

Lawrence Berkeley National Laboratory

Recent Work

Title

A MATHEMATICAL SOLUTION OP THE THREE PHASE-TWO MOVING BOUNDARY PROBLEM

Permalink

<https://escholarship.org/uc/item/45h8p0sz>

Author

Blank, Stuart L.

Publication Date

1969-02-01

c.2

A MATHEMATICAL SOLUTION OF THE THREE
PHASE-TWO MOVING BOUNDARY PROBLEM

Stuart L. Blank

February 1970

RECEIVED
LAWRENCE
RADIATION LABORATORY
MAR 23 1970
LIBRARY AND
DOCUMENTS SECTION

AEC Contract No. W-7405-eng-48

TWO-WEEK LOAN COPY

*This is a Library Circulating Copy
which may be borrowed for two weeks.
For a personal retention copy, call
Tech. Info. Division, Ext. 5545*

LAWRENCE RADIATION LABORATORY
UNIVERSITY of CALIFORNIA BERKELEY

UCRL-19182

25

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Submitted to Scripta Met

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

A MATHEMATICAL SOLUTION OF THE THREE
PHASE-TWO MOVING BOUNDARY PROBLEM

Stuart L. Blank

February 1969

A MATHEMATICAL SOLUTION OF THE THREE PHASE-TWO MOVING BOUNDARY PROBLEM

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 $\text{MgO-Fe}_2\text{O}_3$ system (shown schematically in Fig. 1 with a portion of the phase diagram) (2) in which the phases are MgO , magnesioferrite, and Fe_2O_3 .

Using the notations shown in Fig. 1, C_I , C_{II} , and C_{III} can be obtained by an error function solution:

$$C_I = C_{I,0} + B_I \left[1 - \operatorname{erf} \left(\frac{X}{\sqrt{4D_I t}} \right) \right] \quad \bar{X}_{II,I} < X < \infty \quad (1)$$

$$C_{II} = A + B_{II} \operatorname{erf} \left(\frac{X}{\sqrt{4D_{II} t}} \right) \quad \bar{X}_{III,II} < X < \bar{X}_{II,I} \quad (2)$$

$$C_{III} = C_{III,0} - B_{III} \left[1 + \operatorname{erf} \left(\frac{X}{\sqrt{4D_{III} t}} \right) \right] \quad -\infty < X < \bar{X}_{III,II} \quad (3)$$

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

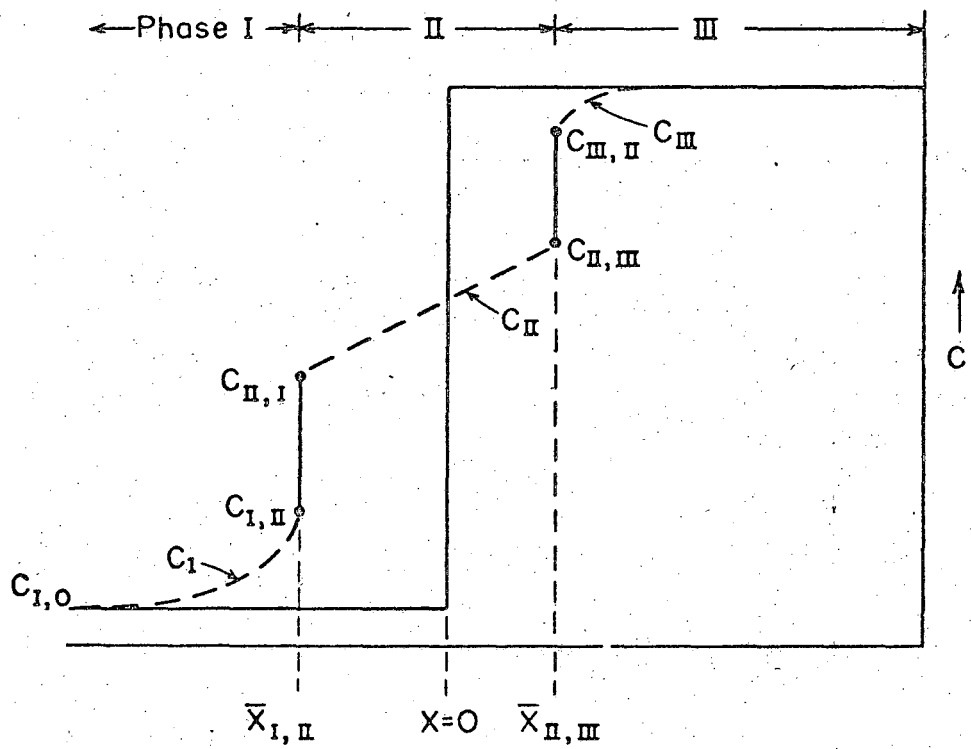
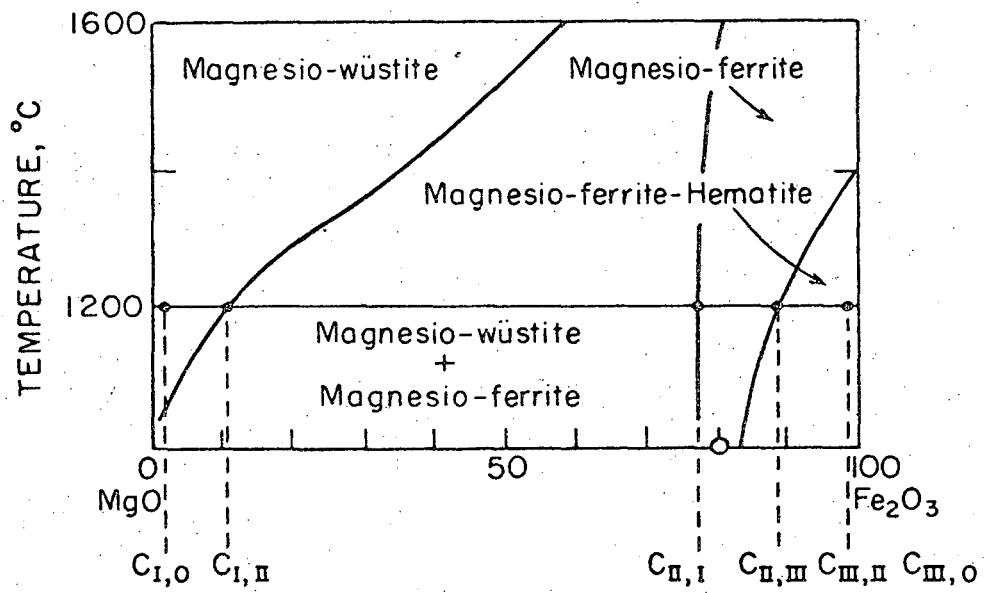
$$\bar{X}_{III,II} = \bar{X}_{II,I} = 0 \text{ when } t = 0,$$

then

$$C_I = C_{I,0} \text{ and } C_{III} = C_{III,0}.$$

The six quantities A , B_I , B_{II} , B_{III} , $\bar{X}_{II,I}$ and $\bar{X}_{III,II}$ must be known in order to obtain an analytical solution. Using Wagner's technique

* Now with Bell Telephone Laboratories, Inc., Murray Hill, N. J. 07974.



XBL 685-750

MgO-FeO phase diagram and schematic diffusion profile for three-phase diffusion problem. (2)

$$\left(\bar{X}_{II,I} = \gamma_I \sqrt{4D_I t} \text{ and } \bar{X}_{III,II} = \gamma_{III} \sqrt{4D_{III} t} \right)$$

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

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

$$C_{II,I} = A + B_{II} \left[\text{erf} \left(\gamma_I \sqrt{\frac{D_I}{D_{II}}} \right) \right] \quad (5)$$

$$C_{II,III} = A + B_{II} \left[\text{erf} \left(\gamma_{III} \sqrt{\frac{D_{III}}{D_{II}}} \right) \right] \quad (6)$$

$$C_{III} = C_{III,0} - \left[\frac{C_{III,0} - C_{III,II}}{1 + \text{erf}(\gamma_{III})} \right] \left[1 + \text{erf} \left(\frac{X}{\sqrt{4D_{III} t}} \right) \right] \quad (7)$$

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

$$C_{II} = C_{II,III} + \frac{(C_{II,III} - C_{II,I}) \left[\text{erf} \left(\frac{X}{\sqrt{4D_{II} t}} \right) - \text{erf} \left(\gamma_{III} \sqrt{\frac{D_{III}}{D_{II}}} \right) \right]}{\left[\text{erf} \left(\gamma_{III} \sqrt{\frac{D_{III}}{D_{II}}} \right) - \text{erf} \left(\gamma_I \sqrt{\frac{D_I}{D_{II}}} \right) \right]} \quad (8)$$

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

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

we obtain

$$\sqrt{\frac{D_{III}}{\pi}} \left[\frac{C_{III,0} - C_{III,II}}{1 + \operatorname{erf}(\gamma_{III})} \right] e^{-\gamma_{III}^2} + \sqrt{\frac{D_{II}}{\pi}} \left[e^{-\left(\gamma_{III}^2 \frac{D_{III}}{D_{II}}\right)} \right] \cdot$$

$$\left[\frac{(C_{II,III} - C_{II,I})}{\left[\operatorname{erf}\left(\gamma_{III} \sqrt{\frac{D_{III}}{D_{II}}}\right) - \operatorname{erf}\left(\gamma_I \sqrt{\frac{D_I}{D_{II}}}\right) \right]} \right] = \gamma_{III} \sqrt{D_{III}} (C_{III,II} - C_{II,III}) \quad (9)$$

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

$$\frac{d\bar{X}_{II,I}}{dt} = \gamma_I \sqrt{D_I} t^{-1/2}$$

$$\sqrt{\frac{D_I}{\pi}} \left(\frac{C_{I,II} - C_{I,0}}{1 - \operatorname{erf}(\gamma_I)} \right) e^{-\gamma_I^2} - \sqrt{\frac{D_{II}}{\pi}} \cdot$$

$$\frac{(C_{II,III} - C_{II,I}) e^{-\left(\gamma_I^2 \frac{D_I}{D_{II}}\right)}}{\left[\operatorname{erf}\left(\gamma_{III} \sqrt{\frac{D_{III}}{D_{II}}}\right) - \operatorname{erf}\left(\gamma_I \sqrt{\frac{D_I}{D_{II}}}\right) \right]} = (C_{II,I} - C_{I,II}) \gamma_I \sqrt{D_I} \quad (10)$$

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

$$\bar{X}_{II,I} - \bar{X}_{III,II} = \left[\gamma_I \sqrt{4D_I} - \gamma_{III} \sqrt{4D_{III}} \right] t^{1/2} \quad (11)$$

which shows that the intermediate phase (magnesian ferrite 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.

ACKNOWLEDGMENT

This work was done under the auspices of the United States Atomic Energy Commission. The approach to this solution was first suggested by Professor J. E. Dorn. I also wish to thank Professor J. A. Pask for fruitful discussions.

REFERENCES

1. J. Crank, Mathematics of Diffusion (Clarendon Press, Oxford, 1956).
2. S. L. Blank and J. A. Pask, Diffusion of Iron and Nickel in Magnesium Oxide Single Crystals, J. Am. Ceram. Soc., V. 52, 669-675, Dec. 1969.

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

- A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or*
- B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.*

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

TECHNICAL INFORMATION DIVISION
LAWRENCE RADIATION LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720