Diffusion in Materials Science: Computational Analysis

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Abstract

This report presents computational analysis of diffusion phenomena in materials science. We examine Fick's first and second laws, analytical solutions including error function profiles, numerical simulation of concentration evolution, and the Kirkendall effect in binary diffusion couples. Python-based computations provide quantitative analysis with dynamic visualization.

Contents

1 Introduction to Diffusion

Diffusion is the net movement of atoms or molecules from regions of high concentration to regions of low concentration. This fundamental transport phenomenon governs numerous materials processes including:

- Heat treatment and phase transformations
- Oxidation and corrosion mechanisms
- Semiconductor doping and device fabrication
- Sintering and powder metallurgy

2 Fick's Laws of Diffusion

2.1 Fick's First Law

Fick's first law describes steady-state diffusion where the flux is proportional to the concentration gradient:

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

where J is the diffusion flux ($\mathrm{mol\,m^{-2}\,s^{-1}}$), D is the diffusion coefficient ($\mathrm{m^2\,s^{-1}}$), and C is concentration.

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Figure 1: Fick's first law: (a) steady-state concentration profile, (b) constant flux through membrane.

The calculated steady-state flux is $J = 9.000e - 07$ $\mathrm{mol\,m^{-2}\,s^{-1}}$.

2.2 Fick's Second Law

For non-steady-state diffusion, Fick's second law describes the time evolution of concentration:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2}$$

3 Analytical Solutions

3.1 Error Function Solutions

For semi-infinite solid with constant surface concentration:

$$\frac{C(x,t) - C_0}{C_s - C_0} = 1 - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{3}$$

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Figure 2: Error function solution showing concentration profiles at different times and penetration depth evolution.

3.2 Thin-Film (Gaussian) Solution

For an instantaneous planar source at $x = 0$:

$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \tag{4}$$

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Figure 3: Gaussian diffusion profile evolution from an instantaneous thin-film source.

4 Temperature Dependence of Diffusion

The diffusion coefficient follows the Arrhenius relationship:

$$D = D_0 \exp\left(-\frac{Q}{RT}\right) \tag{5}$$

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Figure 4: Temperature dependence of diffusion: Arrhenius behavior for various material systems.

Table 1: Diffusion Parameters for Various Systems

System	D_0 ($\mathrm{m^2\,s^{-1}}$)	Q ($\mathrm{kJ\,mol^{-1}}$)	D at 1000 K
C in Fe-alpha	6.20e-07	80	4.11e-11
C in Fe-gamma	2.30e-05	148	4.27e-13
Fe in Fe-alpha	2.00e-04	251	1.55e-17
Cu in Cu	7.80e-05	211	7.42e-16
Al in Al	1.70e-04	142	6.50e-12

5 Numerical Simulation of Diffusion

5.1 Finite Difference Method

We solve Fick's second law numerically using explicit finite differences:

$$C_i^{n+1} = C_i^n + \frac{D\Delta t}{(\Delta x)^2}\left(C_{i+1}^n - 2C_i^n + C_{i-1}^n\right) \tag{6}$$

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Figure 5: Finite difference solution of Fick's second law with mass conservation verification.

The Fourier number (stability criterion) is $Fo = 0.500$, which satisfies $Fo \leq 0.5$ for stability.

6 Kirkendall Effect

The Kirkendall effect demonstrates unequal diffusion rates in binary diffusion couples, resulting in marker movement and void formation.

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Figure 6: Kirkendall effect in a binary diffusion couple showing marker movement due to unequal diffusivities.

The marker shifted by -15.220 mm toward the faster-diffusing side, demonstrating the Kirkendall effect.

7 Interdiffusion Coefficient

The interdiffusion (chemical) coefficient can be determined using the Matano-Boltzmann analysis:

$$\tilde{D} = -\frac{1}{2t}\left(\frac{dx}{dC}\right)_{C^*}\int_0^{C^*} x\, dC \tag{7}$$

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Figure 7: Matano-Boltzmann analysis for determining concentration-dependent interdiffusion coefficient.

8 3D Diffusion Visualization

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Figure 8: Three-dimensional visualization of concentration evolution during diffusion.

9 Conclusions

This analysis demonstrates key aspects of diffusion in materials science:

1. Fick's laws provide the mathematical framework for both steady-state and transient diffusion
2. Error function solutions enable analytical calculation of penetration profiles
3. Temperature dependence follows Arrhenius behavior with characteristic activation energies
4. Numerical methods allow simulation of complex boundary conditions
5. The Kirkendall effect demonstrates the physical consequences of unequal diffusivities
6. Matano-Boltzmann analysis enables experimental determination of diffusion coefficients