Thin Film Solution of the Cahn Hilliard Equations

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ABSTRACT
The Cahn-Hilliard equation describes phase separation and coarsening in binary MGA's. Perturbation solutions of the one-dimensional Cahn-Hilliard equation for small distances and times are examined. Using a small perturbation a the first-order perturbation expansion, series and Fourier transforms solve the linearized form of the Cahn-Hilliard equation to obtain a general solution. The dispersion relation reveals the growth rates of the perturbation modes, providing insight into the early-time dynamics of phase separation. This analytical approach lays the groundwork for revealing the evolution of small disturbances and their impact on phase separation in binary systems. This work has potential applications in materials science, particularly in the microstructural development of alloys, MGA's and polymer blends.

Keywords: alloy development, Cahn-Hilliard, diffusion, MGA, spinodal, thin films

1.INTRODUCTION

The Cahn-Hilliard equation describes phase separation without the use of classical nucleation theory. This extends for large times to coarsening phenomena. This paper derives the perturbation solutions of the 1D Cahn-Hilliard equation, focusing on small spatial and temporal variables. The first-order perturbation expansions are derived. By employing series, linearized forms of the Cahn-Hilliard equation are solved, yielding the general solution. The dispersion relation obtained from this analysis elucidates the growth rates of perturbation modes, thereby shedding light on the early-time dynamics of phase separation. This analytical framework provides a deeper understanding of the evolution of small perturbations and their significance in the phase separation process within binary systems. The findings have promising implications for materials science, especially in elucidating the microstructural development of alloys and polymer blends.

MGA's (Miscibility gap alloys) , are suitable for spinodal transformations where nucleation can occur spontaneously, depending on inflections in the free energy curves. Hence, the classical nucleation concepts are not applicable. Such alloys retain the spinodal structure even after deformation and so can be reused easily, with less heat treatment. The impact on the environment can be substantially reduced.

2.MATERIALS AND METHODS

The Cahn Hilliard equations are a 4^{th} order set of nonlinear equations, proposed by Cahn & Hilliard [1]. Recently general forms of solutions based on Solitons have been analysed [2]. The exact solutions in closed form have not been published [3-9]. A similarity variable is applied, the resulting equations are then solved using perturbations, revealing the progression of the transformation with time and distance. Physically insightful results are then evaluated for small *x,* and *t.* Boundary Conditions are applied to evaluate constants further. With this , it is hoped to give physical meaning to the theoretical solution especially for thin films where *x* is small. The equations are solved for general Dirichlet conditions,(constant at the boundaries).

3. RESULTS AND DISCUSSION

For the one-dimensional Cahn-Hilliard equation with constant mobility M, we start with the original CH equation: $\partial\phi/\partial t = M\partial^2/\partial x^2(-\partial^2\phi/\partial x^2 + \phi^3 - \phi)$, M=Mobility, ϕ= concentration (1)

Simplifying, we get: $\partial\phi/\partial t = -M\partial^4\phi/\partial x^4 + M\partial^2/\partial x^2(\phi^3 - \phi)$ (2)

We introduce the similarity transformation:

$$\phi(x,t) = \exp(-\lambda t)\psi(\xi), \text{ where } \xi = x/[2M\lambda\tau]^{1/2} \quad (3)$$

The time derivative of ϕ transforms as follows:

$$\partial\phi/\partial t = -\lambda e^{-\lambda t}\psi(\xi) + e^{-\lambda t}[\partial\psi/\partial\xi][\partial\xi/\partial t] \quad (4)$$

Since we have from (3), $\xi = x/[2M\lambda\tau]^{1/2}$, $\partial\xi/\partial t = -\xi/2t$ after simplification (5)

Thus: $\partial\phi/\partial t = -e^{-\lambda t}[\lambda\psi(\xi) + (\xi/2t)\partial\psi/\partial\xi]$ (6)

After simplification, the spatial derivatives transform as follows:

$$\partial^2\phi/\partial x^2 = e^{-\lambda t}\partial^2\psi/\partial\xi^2/[2M\lambda t] \quad (7)$$

$$\partial^4\phi/\partial x^4 = e^{-\lambda t},\ \partial^4\psi/\partial\xi^4/[2M\lambda t]^2 \quad (8)$$

Substituting these into the Cahn-Hilliard equation (1),

Simplifying by cancelling ($e^{-\lambda t}$) and multiplying through by $2M\lambda t$ (9)

Henceforth the function $\psi(\xi)$ is replaced with ψ (10)

$$-2M\lambda^2 t\psi - M\lambda\xi\partial\psi/\partial\xi = -[1/(2M\lambda t)]\,\partial^4\psi/\partial\xi^4 + M\partial^2/\partial\xi^2[\psi^3 - \psi] \quad (11)$$

For large t, the 4th order derivative term $\rightarrow 0$, also $\xi \rightarrow 0$, and the dominant balance gives us:

$$-2M\lambda^2 t\psi - M\lambda\xi\partial\psi/\partial\xi = +M\partial^2/\partial\xi^2[\psi^3 - \psi] \quad (12)$$

The similarity-transformed steady-state equation for $\psi(\xi)$ is then:

$$-2M\lambda^2 t\psi \approx M\partial^2/\partial\xi^2\ (\psi 3 - \psi) \quad (13)$$

Therefore, for small x or **for large t**, $\xi \rightarrow 0$, the equation reduces to the leading order:

$$-2\lambda^2 t\psi \approx \partial^2/\partial\xi^2\ (\psi^3 - \psi) \quad (14)$$

A) For small t, the equation reduces to $\boldsymbol{\partial^4\psi/\partial\xi^4 \rightarrow 0}$ (15)

B) For small x or large t, $\xi \rightarrow 0$, $-2\lambda^2 t\psi = \partial^2(\psi^3 - \psi)/\partial\xi^2$ (16)

To solve the similarity-transformed Cahn-Hilliard equation, we need to start with the transformed equation: $\partial^2/\partial\xi^2\ (\psi 3 - \psi) \approx -2\lambda^2 t\psi$ **(for large t)** (17)

Where $\psi(\xi)$ is the transform form of $\phi(x,t)$, given in eqn(3)

As a first approximation

set $\partial^2/\partial\xi^2\ (\psi 3 - \psi) \approx 0$, which can be integrated approximately to give:

$a\,\psi_0^3 - \psi_0 = A_0\,\xi + B_0$, which shows heuristically that the zeroth order solution goes as the (1/3) root of ξ

Assume a series expansion for ξ around 0, where t is large (from the definition of ξ)

$$\psi(\xi) = \psi_0 + \psi_1\xi^1 + \psi_2\xi^2 + \text{- -} \quad (18)$$

Calculate the first and second derivatives with respect to ξ

$$\partial\psi/\partial\xi = \psi_1 + 2\psi_2\xi + \text{---}$$

$$\partial^2\psi/\partial\xi^2 = 2\psi_2 + 6\psi_3\xi + \text{---} \quad (19)$$

Second Derivative of the Nonlinear Term:

$\partial^2/\partial\xi^2(\psi^3 - \psi) = \partial^2/\partial\xi^2[(\psi_0^3 - \psi_0) + (3\psi_0^2\psi_1 - \psi_1)\xi + (3\psi_0^2\psi_2 + 3\psi_0\psi_1^2 - \psi_2)\xi^2 + \ldots]$

For $\xi \rightarrow 0$, $\psi = \psi_0$ (from (18)),then neglecting 2nd order terms, $3\psi_0^2\psi_1 - \psi_1 = 0$ from the second factor $\rightarrow \boldsymbol{\psi_0^2 = 1/3}$

Proceeding to use this on the RHS of eqn (17) , solve iteratively and get from the 3rd term $2(\psi_2 + \sqrt{3}\psi_1^2 - \psi_2) = -2\lambda^2[1/\sqrt{3}]$, $\boldsymbol{\psi_2}$ cancels out

and $\boldsymbol{\psi_1^2} = -\lambda^2/3$, (20)

which implies that ψ_1 is imaginary. Hence we need to use higher order terms to find this constant. Alternatively, we can put $\psi_1 = 0$ in the above and re derive terms for ψ_2. We see the LHS consistent as zero with the choice of ψ_0, and ψ_1. Since ψ_2 cancels out in (20), we can solve for it further from the Boundary Conditions.
Hence to second order, the prototype solution obtained is

$$\psi(\xi) = \psi_0 + \psi_1\xi^1 + \psi_2\xi^2 = 1/\sqrt{3} + \psi_2\xi^2 \quad (21)$$

Perturbation in ξ approach, taking constants as unknown coefficients.

Assume $\psi = (a + b\xi + c\xi^2 + .. + .. +)$, and proceed only to 2nd order.
We attempt to solve and obtain the constants a,b,c etc:
where $\psi = a + b\xi + c\,\xi^2$
Use the Boundary Condition $\psi(0) = a_0$ where it is small , $a = a_0$; and from the earlier expression, after substituting $\psi = a + b\xi + c\,\xi^2$ in eqn(19-21), from

$$\partial^2/\partial\xi^2\,(\psi^3 - \psi) = \partial^2/\partial\xi^2\,[(\psi_0^3 - \psi_0) + (3\psi_0^2\psi_1 - \psi_1)\xi + (3\psi_0^2\psi_2 + 3\psi_0\psi_1^2 - \psi_2)\xi^2 + \ldots\,] \quad (22)$$

Where from the 3rd factor above $(3a^2c + 3ab^2 - c) = (3\psi_0^2\psi_2 + 3\psi_0\psi_1^2 - \psi_2) \rightarrow 0$ (23)

From(23), if $a = a_0$ (NON ZERO, BUT SMALL), neglecting a_0^2, then $3b^2 = c/a_0$, However directly from $\psi = a + b\xi + c\,\xi^2$, where $\xi = L$, and $\psi(L) = 0$ (given),
If $\psi(L) = 0$, then b is found by solving a quadratic of the form $3b^2a_0 + bL + a_0 = 0$. (24)
Solving : $b = \{-L/2 \pm \sqrt{[L^2/4 - 3a^2_0]}\}/3a_0$
It is seen that as $a_0 \to 0$, b=0 or infinity, is a solution, as was assumed before (imaginary from the previous approximations)
Hence for small x, ξ—>0,

$$\psi(\xi) = 1/\sqrt{3} + \psi_2\xi^2 \quad \text{(from (21),}$$

Hence a solution upto 2nd order is the parabolic function (25)
Comparing with $\psi(L) = 0$, $\psi_2 = -1/\sqrt{3}(L^2)$

<u>Zeroth Order Solution.</u> For the zeroth order, we have:

$$6\psi_2 + 12\psi_1 = -2\lambda^2\,\psi_0$$

Since $\psi_1 = 0$ for reals, $\psi_2 = -\lambda^2/3\psi_0 = -\lambda^2/3\sqrt{3}$ (26)

From $\psi(\xi) = \psi_0 + \psi_2\xi^2$
<u>Final Form</u> for $\psi(\xi)$: $\psi(\xi) = 1/\sqrt{3} - \lambda^2/[3\sqrt{3}]\,\xi^2$ (27)
For large **t** a solution upto 2nd order is the parabolic function

$$\psi(\xi) = 1/\sqrt{/}3[1 - \lambda^2\xi^2/3]$$

Also from the eqn (12) $d^4\psi/d\xi^4 = 0$, $\psi = A + B\xi + C\xi^2 + D\xi^3$ (for small t) (28)
If $\psi(0) = 0$, A=0, then $\psi(L) = 0 \Longrightarrow B + CL + DL^2 = 0$
For solution upto second order, neglect D, $C = -B/L$, $\psi = B\xi - B/L\xi^2 = \mathbf{B(1 - \xi^2/L)}$
Dispersion Relation: Assume a Fourier transform solution for u_1: where we perturb the CH eqn with small parameter ε:
Examine the first perturbed term: $u_1(x,t) = \sum_k \mathbf{u}_1(k)e^{ikx}e^{-\omega(k)t}$ (29)
Where $\mathbf{u}(k)$ is the transformed variable. After simplifications
$\omega(k) = -Mk^2(\epsilon k^2 - 3u_0^2 \quad +1)$
Hence for long time, $\omega(k) = 0 \rightarrow \varepsilon k^2 = \sqrt{[3u_0^2 - 1]}$ (30)

(Derivation in Appendix)

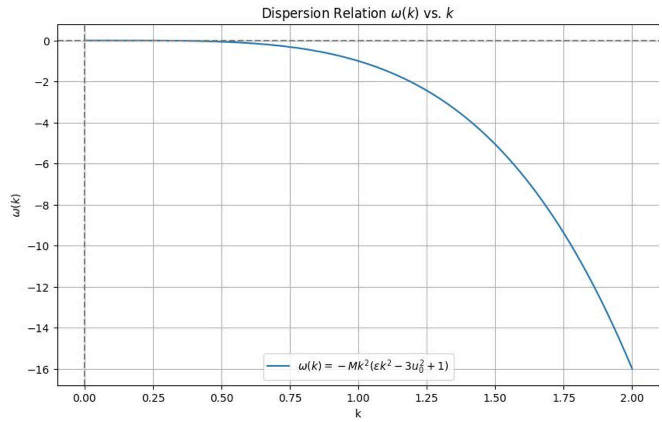

Figure.1 Plot of ω(k) vs k , k on abscissa, ω(k) on ordinate

4. CONCLUSION

Using perturbation theory, the complex nonlinear 4^{th} order partial differential equation can be analysed for various limiting trends as the variables approach small or large values. The simulations for small *x,t* and large *t* show that the approximate solution, including the dispersion relation, goes as a parabolic or quadratic profile. Various tools and approximations were used, and all show a profile which is varying as the square of the spatial variable.

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6.Appendix 1:Program to solve and plot the FT dispersion relation

```
import numpy as np
import matplotlib.pyplot as plt

# Parameters
M = 1  # Mobility
epsilon = 1  # Given epsilon = kappa
u0_squared = 1/3

# Dispersion relation function
def omega(k, M, epsilon, u0_squared):
   return -M * k**2 * (epsilon * k**2 - 3 * u0_squared + 1)

# Generate k values
k_values = np.linspace(0, 2, 400)
omega_values = omega(k_values, M, epsilon, u0_squared)

# Plot the dispersion relation
plt.figure(figsize=(10, 6))
plt.plot(k_values, omega_values, label=r'$\omega(k) = -M k^2 (\epsilon k^2 - 3 u_0^2 + 1)$')
plt.xlabel('k')
plt.ylabel(r'$\omega(k)$')
plt.title('Dispersion Relation $\omega(k)$ vs. $k$')
plt.axhline(0, color='gray', linestyle='--')
plt.axvline(0, color='gray', linestyle='--')
plt.legend()
plt.grid(True)
plt.show()
```

Appendix 2:

Fourier Transform of the CH Equation

(A review of the literature yielded very few results on this aspect, especially regarding perturbation solutions. Some are given in [10,11])

Apply the Fourier transform to the CH equation:

$$\partial \mathbf{u}(k,t)\partial t=-M[-k^2(\mathbf{u}^3(k,t)-\mathbf{u}(k,t)+\epsilon^2k^2\mathbf{u}(k,t))] \qquad (31)$$

The nonlinearity $\mathbf{u}^3$ is complicated to handle directly in Fourier space, but for the purpose of linear stability analysis, we can linearize around a homogeneous state. Assume small perturbations around a constant solution u_0:

$$u(x,t)=u_0+\psi(x,t) \text{ with } (x,t)\ll 1, \qquad (32)$$

Substitute this into the CH equation and linearize by ignoring higher-order terms in ψ:

Since $(u_0^3 - u_0)$ is constant, it drops out upon differentiation:

$$\partial\psi/\partial t = -M\partial^2\partial x^2((3u_0^2 - 1)\psi - \epsilon^2\partial^2/\partial x^2\psi) \quad (33)$$

Applying the FT on this equation: $\partial\psi\hat{}(k,t)/\partial t = Mk^2((1-3u_0^2)\psi\hat{}(k,t) - \epsilon^2k^2\psi\hat{}(k,t))$ (34)

This is a linear ordinary differential equation in $\psi\hat{}(k,t)$, where ^ denotes the Fourier Transformed variable. The solution has the form:

$$\psi\hat{}(k,t) = \psi\hat{}(k,0)e^{\omega(k)t}$$

where $\omega(k)$ is the growth rate: $\omega(k) = Mk^2((1-3u_0^2) - \epsilon^2k^2)$ (35)

Dispersion Relation

The dispersion relation is given by $\omega(k)$

Behavior at Small k

Consider the behavior of the dispersion relation at small wave numbers k: For k small (long-wavelength perturbations): $\omega(k) \approx Mk^2(1-3u_0^2)$

If $1-3u_0^2>0$, (i.e., $u_0^2<1/3$), the growth rate $\omega(k)$ is positive for small k. This implies that long-wavelength perturbations will grow, leading to phase separation or pattern formation.
If $1-3u_0^2<0$ (i.e., $u_0^2>1/3$, the growth rate $\omega(k)$ is negative for small k. This implies that long-wavelength perturbations will decay, and the system is stable against such perturbations. For k large (short-wavelength perturbations): $\omega(k) \approx -M\epsilon^2k^4$. The growth rate $\omega(k)$ is negative, indicating that short-wavelength perturbations will decay due to the stabilizing effect of the term $-^{\epsilon 2k4}$.

Summary

The dispersion relation $\omega(k) = Mk^2((1-3u_0^2) - \epsilon^2k^2)$, describes the growth rate of perturbations in the CH equation.

For small k:

- If $u_0^2<1/3$, long-wavelength perturbations grow, leading to phase separation.
- If $u_0^2>1/3$, long-wavelength perturbations decay, leading to stability.

For large k, perturbations decay due to the stabilizing term $-\epsilon^2k^4$