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The Perturbation Analysis of a Planar Liquid-Solid Interface in Undercooled Pure Melt

Fengying Wang

School of Information, Beijing Wuzi University, Beijing101149, China

Abstract: This paper establishes a non dimensional model, considers the influence of the far field flow and dynamic cooling on the flat surface of the pure melt during the solidification process by using the method of asymptotic analysis. The ground state solution and the asymptotic solution of the solidification system are given, and the dispersion relation of the disturbance frequency and wave number is derived, according to this relationship, the stability of the solidification process of liquid solid flat interface can be determined, which can offer theoretical foundation for theoretical research of crystal growth and experimental work.

Keywords solidification process; planar interface; perturbation; asymptotic analysis

INTRODUCTION

In the solidification process, it is important to study the shape and stability of liquid solid interface of crystal. As early as 1960s,Mullins and Sekerka put forward the theory of linear stability of the crystal plane (M - S theory) [Mullins *et al.*,1964].This theory has become an important basis for the study of the characteristics of liquid solid interface form . Based on the assumption that the perturbation wavelength is much smaller than the thermal diffusion length, the dispersion relation was introduced to determine the stability of the interface[Langer *et al.*, 1978] [huang *et al.*, 1981] [Bahrenberg *et al.*, 2001] [Li *et al.*, 2005]. So it was obtained that in the process of the cold melt, the interface growth rate is much larger than that of the flat interface. Trivedi and Kurz demonstrated that the M - S theory is ineffective in the rapid solidification of the melt. Trivedi and Kurz thought that the interface is absolutely stable if the interface growth velocity is greater than a certain critical velocity[Trivedi *et al.*, 1986]. Xu introduced the interfacial wave to the solid-liquid interface, and gained a second-order approximate solution to the differential equation by perturbation method, and pointed out that anisotropy was not a requisite condition for stable state crystal growth[Xu., 1998]. Boettinge r*et al.* studied the interfacial stability combined with the crystal growth kinetics, but they put the kinetic undercooling as a linear function of the interface growth velocity, so derived an incorrect conclusion that the dynamic coefficient has no effect on the stability of the liquid solid interface[Boettinger *et al.*, 1984] [Galenko *et al.*, 2004]. The effect of crystal growth kinetics on the absolute stability of the interface of the fast solidified pure melt was studied by Li Jinfu.[Li *et al.*, 2000]. In this paper, we will establish a non dimensional model, study the influence of the far field flow and dynamic cooling on the flat surface of the pure melt during the solidification process by using the method of asymptotic analysis. The ground state solution and the asymptotic solution of the solidification system will be given, and the dispersion relation of the disturbance frequency and wave number will be obtained, according to this relationship, the stability of the solidification process of liquid solid flat interface can be determined.

ESTABLISHMENT OF MATHEMATICAL MODEL AND NON-DIMENSIONLIZATION

Mathematical model

We assume that the liquid solid flat interface is at the beginning of the coordinate plane, and the interface temperature is the thermodynamic equilibrium temperature T_M, the far field temperature is T_∞ ($T_\infty < T_M$), the interface is moving with the characteristic velocity along the Z axis direction. In the moving coordinate system, the temperature field satisfies the heat conduction equation:

$$\frac{\partial T_L}{\partial t} = k_L\left(\frac{\partial^2 T_L}{\partial x^2} + \frac{\partial^2 T_L}{\partial z^2}\right)$$

$$\frac{\partial T_S}{\partial t} = k_S\left(\frac{\partial^2 T_S}{\partial x^2} + \frac{\partial^2 T_S}{\partial z^2}\right)$$

Where T_L 、 T_S are the liquid phase and solid phase temperature respectively, k_L 、 k_S are liquid phase and solid phase thermal diffusion coefficients respectively.

The boundary conditions include:

1) The far field condition in the liquid phase domain: as $z \to \infty$, $T_L \to T_\infty$;

2) The side-wall condition in the solid phase domain: as $z = -t$, $T_S = T_I$ (where T_I is the interface temperature);

Corresponding Author: Fengying Wang, School of Information, Beijing Wuzi University, Beijing 101149, China.

3) The solid-liquid interface condition: at the interface $z = h(x,t)$,

The thermo-equilibrium condition:

$$T_L = T_S = T_I$$

The Gibbs-Thomson condition:

$$T_I = T_M(1 + 2K\frac{\gamma}{\Delta H}) - \frac{1}{\mu}V_I$$

The heat balance condition:

$$(\Delta H + 2K\gamma)V_I = (k_S\frac{\partial T_S}{\partial n} - k_L\frac{\partial T_L}{\partial n})$$

where γ is the surface free energy, ΔH is the latent heat of melt, μ is the interface dynamic coefficient, n is the interface unit law direction(from solid phase to liquid phase), $K = \frac{h_{xx}}{2(1+h_x^2)^{3/2}}$ is the interface curvature, $V_I = \frac{1+h_t}{(1+h_x^2)^{1/2}}$ is the velocity along the direction from the solid phase to the liquid phase, h_x and h_t are respectively the first order partial derivatives of x and t of the interface shape function $z = h(x,t)$.

Dimensionless mathematical model

To get the dimensionless forms of the problem, we use the thermal diffusion length $l_T = k_L/V$ as the length scale, the interface pulling velocity V is used as the velocity scale, κ_L/V^2 is used as the time scale and $\Delta H/(c_p\rho_L)$ is used as the temperature scale. Where c_p is specific heat, ρ_L is the density of the melt. So we can define dimensionless quantities as

$$\bar{x} = \frac{x}{l_T},\ \bar{z} = \frac{z}{l_T},\ \bar{h} = \frac{h}{l_T},\ \bar{t} = \frac{t}{l_T/V},$$

$$\bar{T}_L = \frac{T_L - T_M}{\Delta H/(c_p\rho_L)},\ \bar{T}_S = \frac{T_S - T_M}{\Delta H/(c_p\rho_L)}.$$

Where we assume $k_T = k_S/k_L$, get the dimensionless equations and boundary conditions. But for the sake of convenience, in the following discussion, we shall omit the bar "-" over the dimensionless quantities, and still use the original mark. After finishing, the dimensionless equations are the following:

$$\frac{\partial T_L}{\partial t} = \frac{\partial^2 T_L}{\partial x^2} + \frac{\partial^2 T_L}{\partial z^2} \quad (1)$$

$$\frac{\partial T_S}{\partial t} = k_T\left(\frac{\partial^2 T_S}{\partial x^2} + \frac{\partial^2 T_S}{\partial z^2}\right) \quad (2)$$

The dimensionless boundary conditions are:

1) The far field condition in the liquid phase domain: as $z \to \infty$, $T_L \to T_\infty$ (i.e. dimensionless temperature $\frac{T_\infty - T_M}{\Delta H/(c_p\rho_L)}$). (3)

2) The side-wall condition in the solid phase domain: as $z = -t$, $T_S = T_I$ (i.e. dimensionless temperature $\frac{T_I - T_M}{\Delta H/(c_p\rho_L)}$). (4)

3) The solid-liquid interface condition: at the interface $z = h(x,t)$,

The thermo-equilibrium condition:

$$T_L = T_S = T_I \quad (5)$$

The Gibbs-Thomson condition:

$$T_I = 2K\Gamma - C^{-1}MV_I \quad (6)$$

The heat balance condition:

$$(1 + 2KC\Gamma)V_I = k_T\frac{\partial T_S}{\partial n} - \frac{\partial T_L}{\partial n} \quad (7)$$

where $\Gamma = \frac{\gamma c_p\rho_L T_M}{(\Delta H)^2 l_T}$, $C = \frac{\Delta H}{c_p\rho_L T_M}$, $M = \frac{V}{T_M\mu}$.

SOLUTION OF MATHEMATICAL MODEL AND PERTURBATION ANALYSIS

From (1) ~ (7) we can see that temperature field and interface conditions are free boundary value problem of nonlinear partial differential equations coupled together, it is difficult to obtain the analytical solution. But due to the influence of some physical parameters, the liquid-solid interface is very easy to be interfered which leads to tiny fluctuations in the interface. We will study the asymptotic analysis for liquid-solid straight interface stability in small perturbations. When there is no disturbance in the flow field, we let the liquid-solid straight interface $z = h_B(x,t) = 0$ as the interface basic state, and let $\frac{\partial}{\partial x} = \frac{\partial}{\partial t} = 0$. The basic steady state solution of (1)~(7) is easy to be obtained:

$$T_{BL}(x,z) = T_\infty + e^{-z} \quad (8)$$

$$T_{BS}(x,z) = -C^{-1}M \quad (9)$$

At the same time, the characteristic velocity of the interface motion is determined as $V = \frac{\mu\Delta H}{c_p\rho_L}(|T_\infty| - 1)$.

When small perturbation appears in the temperature field and the interface, in order to analyze the linear stability of planar interface, we make a small perturbation to the steady state solution, express the solution as follows:

$$\begin{cases} T_L(x,z,t) = T_{BL}(x,z,t) + \tilde{T}_L(x,z,t) \\ T_S(x,z,t) = T_{BS} + \tilde{T}_S(x,z,t) \\ h(x,t) = h_B + \tilde{h}(x,t) \end{cases} \quad (10)$$

Where the amplitude of the perturbation dynamic $\tilde{q} = \{\tilde{T}_L, \tilde{T}_S, \tilde{h}\}$ is an infinitesimal. By substituting (8)(9)(10) into (1)~(7), neglecting the infinitesimal of higher order, we obtain the linear perturbed equations:

$$\begin{cases} \dfrac{\partial \tilde{T}_L}{\partial t} - \dfrac{\partial \tilde{T}_L}{\partial z} = \dfrac{\partial^2 \tilde{T}_L}{\partial x^2} + \dfrac{\partial^2 \tilde{T}_L}{\partial z^2} \\ \dfrac{\partial \tilde{T}_S}{\partial t} - \dfrac{\partial \tilde{T}_S}{\partial z} = k_T \left(\dfrac{\partial^2 \tilde{T}_S}{\partial x^2} + \dfrac{\partial^2 \tilde{T}_S}{\partial z^2} \right) \end{cases} \quad (11)$$

with the boundary conditions for dynamic disturbance:

In far field: as $z \to \infty$, $\tilde{T}_L \to 0$ (12)

At the side-wall : as $z = -t$, $\tilde{T}_S \to 0$ (13)

At the interface $z = \tilde{h}(x,t)$, since $|\tilde{h}| \ll 1$, we make the Taylor expansion along the z=0, eliminate the various terms of the basic solution and high order infinitesimal, obtain the interface conditions of linearization after finishing, that is, at $z = 0$,

$$\tilde{T}_L - \tilde{T}_S + \left(\frac{\partial T_{BL}}{\partial z} - \frac{\partial T_{BS}}{\partial z} \right) \tilde{h} = 0 \quad (14)$$

$$\tilde{T}_S + \left(\frac{\partial T_{BS}}{\partial z} \right) \tilde{h} = \Gamma \frac{\partial^2 \tilde{h}}{\partial x^2} - C^{-1} M \frac{\partial \tilde{h}}{\partial t} \quad (15)$$

$$C\Gamma \frac{\partial^2 \tilde{h}}{\partial x^2} + \frac{\partial \tilde{h}}{\partial t} = \frac{\partial^2}{\partial z^2}(k_T T_{BS} - T_{BL})\tilde{h} + \frac{\partial}{\partial z}(k_T \tilde{T}_S - \tilde{T}_L) \quad (16)$$

From the form of the basic steady solution we can deduce the temperature gradient and the two order derivative of the basic state solution in the interface $z = 0$:

$$G_{1L} = \left. \frac{\partial T_{BL}}{\partial z} \right|_{z=0} = -1, \quad G_{1S} = \left. \frac{\partial T_{BS}}{\partial z} \right|_{z=0} = 0,$$

$$G_{2L} = \left. \frac{\partial^2 T_{BL}}{\partial z^2} \right|_{z=0} = 1, \quad G_{12S} = \left. \frac{\partial^2 T_{BS}}{\partial z^2} \right|_{z=0} = 0.$$

The perturbed system (11) ~ (16) contains three parameters: $\{\Gamma, M, C\}$, where C^{-1} is dimensionless solidification temperature. The surface tension parameter Γ is a microscopic length, which is a very small parameter (usually $10^{-2} \sim 10^{-5}$) for solidification, so it can be set up $\Gamma = \varepsilon^2$ ($\varepsilon \ll 1$), and ε is called surface tension stability parameter. M is the interface dynamic parameter.

The interface condition (14) shows that, when $\varepsilon \to 0$, all disturbance quantity should be of the same order of magnitude, again by (15), $\tilde{T}_S$ and $\tilde{h}$ to have the same order of magnitude, $\tilde{h}_{xx}$ must be $O(\tilde{h}/\varepsilon^2)$, and this is only possible when $\tilde{h}$ is a combination of variable function of (x/ε). So we introduce the following fast variables:

$$\begin{cases} x_+ = \dfrac{k(\varepsilon)}{\varepsilon} x \\ z_+ = \dfrac{g(\varepsilon)}{\varepsilon} z \\ t_+ = \dfrac{\sigma(\varepsilon)}{\varepsilon} t \end{cases} \quad (17)$$

The original variables (x, z, t) can be called slow variables, the fast and slow variables are regarded as independent variables, such as $\varepsilon \to 0$, the asymptotic expansions of perturbed solution are as follows:

$$\tilde{q}(x,z,x_+,z_+,t,t_+) = \mathrm{e}^{t_+}[\tilde{q}_0(x,z,x_+,z_+,t) + \varepsilon \tilde{q}_1(\bullet) + \cdots]$$

$$\begin{aligned} k(\varepsilon) &= k_0 + \varepsilon k_1 + \cdots \\ g(\varepsilon) &= k_0 + \varepsilon g_1 + \cdots \\ g_S(\varepsilon) &= k_0 + \varepsilon g_{S1} + \cdots \\ \sigma(\varepsilon) &= \sigma_0 + \varepsilon \sigma_1 + \cdots \end{aligned} \quad (18)$$

The solution of the solid phase domain is denoted in the form of $g_S(\varepsilon)$ (different from $g(\varepsilon)$ in the liquid phase domain). In order to obtain the asymptotic solution, the parameter $\sigma(\varepsilon)$ and the wave numbers $k(\varepsilon)$, $g(\varepsilon)$, $g_S(\varepsilon)$ are expanded by ε. Further derivation shows that the first term of the asymptotic expansion of these wave numbers are the same, set to the same value k_0 as shown in (18).

All the partial derivatives above are substituted as follows:

$$\begin{cases} \dfrac{\partial}{\partial x} \Rightarrow \dfrac{\partial}{\partial x} + \dfrac{k}{\varepsilon} \dfrac{\partial}{\partial x_+} \\ \dfrac{\partial}{\partial z} \Rightarrow \dfrac{\partial}{\partial z} + \dfrac{g}{\varepsilon} \dfrac{\partial}{\partial z_+} \\ \dfrac{\partial}{\partial t} \Rightarrow \dfrac{\partial}{\partial t} + \dfrac{\sigma}{\varepsilon} \dfrac{\partial}{\partial t_+} \end{cases} \quad (19)$$

They can change the linear perturbation system (11) ~ (16) to the multiple independent variables of the system. By letting $\varepsilon \to 0$, substituting (17)(18) into the perturbation system, comparing the order of ε of the two sides of the equation, we can get all order approximate equations.

Assuming $k_0 = O(1)$, the zeroth order approximation can be derived that

$$\begin{cases} k_0^2 \left(\dfrac{\partial^2 \tilde{T}_{L0}}{\partial x_+^2} + \dfrac{\partial^2 \tilde{T}_{L0}}{\partial z_+^2} \right) = 0 \\ k_0^2 \left(\dfrac{\partial^2 \tilde{T}_{S0}}{\partial x_+^2} + \dfrac{\partial^2 \tilde{T}_{S0}}{\partial z_+^2} \right) = 0 \end{cases} \quad (20)$$

with the boundary conditions:

as $z_+ \to \infty$, $\tilde{T}_{L0} \to 0$ (21)

as $z_+ \to \infty$, $\tilde{T}_{L0} \to 0$

as $z_+ = -\infty$, $\tilde{T}_{S0} \to 0$ (22)

as $z_+ = z = 0$, $\tilde{T}_{L0} = \tilde{T}_{S0} - \Delta G_1 \tilde{h}_0$ (23)

$$\tilde{T}_{S0} = k_0^2 \frac{\partial^2 \tilde{h}_0}{\partial x_+^2} - G_{1S} \tilde{h}_0 - C^{-1} M \sigma_0 \tilde{h}_0 \quad (24)$$

$$k_0 \left(\frac{\partial \tilde{T}_{L0}}{\partial z_+} - k_T \frac{\partial \tilde{T}_{S0}}{\partial z_+} \right) + \sigma_0 \tilde{h}_0 = 0 \quad (25)$$

where $\Delta G_1 = G_{1L} - G_{1S}$. The above system (20)~(25) has regular solution:

$$\begin{cases} \tilde{T}_{L0} = \hat{A}_{L0}\mathrm{e}^{ix_+ - z_+} \\ \tilde{T}_{S0} = \hat{A}_{S0}\mathrm{e}^{ix_+ + z_+} \\ \tilde{h}_0 = \hat{D}_0\mathrm{e}^{ix_+} \end{cases} \quad (26)$$

In general, the amplitude function $\{\hat{A}_{L0}, \hat{A}_{S0}\}$ can be a slow variable function, $\hat{D}_0$ can be a function of $\{x,t\}$. But as the first approximation is the result, they can be set to a constant. Substituting (26)into the (23)~(25), we have

$$\begin{cases} \hat{A}_{L0} = \hat{A}_{S0} - \Delta G_1 \hat{D}_0 \\ \hat{A}_{S0} = -k_0^2 \hat{D}_0 - G_{1S}\hat{D}_0 - C^{-1}M\sigma_0\hat{D}_0 \\ -k_0(\hat{A}_{L0} + k_T\hat{A}_{S0}) + \sigma_0\hat{D}_0 = 0 \end{cases} \quad (27)$$

This is a linear equation set about $(\hat{A}_{L0}, \hat{A}_{S0}, \hat{D}_0)$, and the necessary and sufficient condition for the existence of nonzero solutions is: the value of the coefficient determinant is zero. Namely

$$\begin{vmatrix} 1 & -1 & \Delta G_1 \\ 0 & 1 & k_0^2 + G_{1S} + C^{-1}M\sigma_0 \\ -k_0 & -k_0k_T & \sigma_0 \end{vmatrix} = 0$$

After simplification, it can be derived that

$$\sigma_0\left[1 + C^{-1}M(1+k_T)k_0\right] = -k_0\left[(G_{1L} + k_TG_{1S}) + (1+k_T)k_0^2\right] \quad (28)$$

This formula is the dispersion relation between frequency and wave number.

CONCLUSION

The stability of the planar interface in undercooled pure melts relies on the sign of the frequency σ. When σ is positive, the system has a growth model solution, the interface is instable; when the σ is negative, the system has a decay mode solution, the interface tends to be stable; when the σ is zero, the system has a neutral mode solution. Since the latter term of the asymptotic expansion of σ is much smaller than the previous one, the value of σ is mainly determined by σ_0. From (12),(17),(21), we know that k_0 is positive real number(otherwise the perturbation solution will tend to infinity) and all terms in the left bracket of the equation are positive in (28). Therefore, the positive and negative of σ_0 depends on the sign of (29).

$$F = G_{1L} + k_TG_{1S} + (1+k_T)k_0^2 \quad (29)$$

If $G_{1L} + k_TG_{1S} > 0$, then $F > 0$, for any wave number, the system will always be stable. If $G_{1L} + k_TG_{1S} < 0$, the stability of the system depends on the value of the wave number k_0. In particular, if $k_L = k_S$, then $k_T = 1$. Substituting $G_{1L} = -1$, $G_{1S} = 0$ into (29), we have

$$F = -1 + 2k_0^2 \quad (30)$$

Therefore, when $k_0 > 1/\sqrt{2}$, the system has the attenuation model solution, which is consistent with the condition of the short wave disturbance is attenuated, the liquid-solid interface tends to be stable; When $0 < k_0 < 1/\sqrt{2}$, the system has the growth mode solution, which is consistent with the condition of the long wave disturbance is growth, the liquid-solid interface is instable.

This paper considers kinetic undercooling of the crystal growth on the liquid-solid interface, makes the asymptotic expansion for the perturbed solution of the governing equations, and derives the dispersion relation of unsteady solidification system with asymptotic method, then proposes the discrimination condition of the stability under the straight interface solidifying, reveals the mechanism of the liquid solid flat interface to the cellular crystal interface during the solidification process, which has offered theoretical foundation for theoretical research of crystal growth and experimental work.

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