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Revisiting Jackson-Hunt calculations: Unified theoretical analysis for generic multi-phase growth in a multi-component system



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ABSTRACT

A straight-forward extension of the Jackson-Hunt theory for directionally solidifying multi-phase growth where the number of components exceeds the number of solid phases becomes difficult on account of the absence of the required number of equations to determine the boundary layer compositions ahead of the interface. In this paper, we therefore revisit the Jackson-Hunt (JH) type calculations for any given situation of multi-phase growth in a multi-component system and self-consistently derive the variations of the compositions of the solid phases as well as their volume fractions, which grow such that the composite solid-liquid interface is isothermal. This allows us to unify the (JH) calculation schemes for both in-variant as well as multi-variant eutectic reactions. The derived analytical expressions are then utilized to study the effect of dissimilar solute diffusivities and interfacial energies on the undercoolings and the solidified fractions. We also perform phase field simulations to confirm our theoretical predictions and find a good agreement between our analytical calculations and model predictions for model symmetric alloys as well as for a particular Ni-Al-Zr alloy.

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1. Introduction

Eutectic solidification offers interesting examples of multi-phase microstructural formation wherein two or more phases typically self-organize during growth. In binary eutectics, these microstructures range from lamella [1–7] to rods [8–10] and mixture of morphologies, depending on the volume fractions of the phases and the interfacial energies. For more than two solid phases, the number of possibilities is still larger and some of the experimental results obtained during directional solidification of three-phase growth are found in metallic alloy systems, such as, Pb-Sn-Cd [11–13], Al-Cu-Mg and Zn-Sn-Pb [14], Al-Cu-Ni [15], Bi-In-Sn [16,17], Nb-Ni-Al [18], Al-Ag-Cu [19–21]. Experimental evidence of eutectic solidification in quaternary organic alloys is reported in Refs. [22,23]. Phase-field simulations of bulk-two phase growth have also been performed in Refs. [24–26] and corresponding examples of simulations of three-phase growth can be found in Refs. [27–32]. A review of studies of multiphase solidification in multi-component alloys is presented in Ref. [33].

Theoretically, one of the interesting questions is the

investigation of steady-state eutectic growth and establishing the relationship between the undercooling, the spacings and the velocities, which is essentially a relationship between the microscopic length scale that is described by the spacing λ , and the macroscopic diffusion length scale ($2D/V$, D is the diffusivity in liquid, V is the velocity). A very nice review on the developments in the theoretical models for describing eutectic growth as well as its close counterpart in eutectoid growth can be found in Ref. [34]. In this regard, one of most applied theories for directional solidification conditions is the Jackson and Hunt theory (JH) [35], where expressions for the undercooling (ΔT) versus spacing (λ) are derived for given velocities, for both lamellar and rod configurations of growth. The operating scale of the eutectics that may arise in experiments is discussed based on the minimum undercooling spacing as a marginal stability point. Conditions for transition between rod and lamellae morphologies is also discussed. Extension of the (JH) formalism for two-phase lamellar growth in ternary alloys, has been attempted by McCartney [36] and Plapp et al. [37], while similar extensions for investigation of invariant growth in three-phase eutectics has been performed by Himemiya and Umeda [38] and Choudhury et al. [39].

The theoretical development as per (JH) firstly provides for a solution to the Stefan problem at the multi-phase solidification front with the assumption of a planar interface. Capillary effects are

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introduced using the average curvature of each of the solid-liquid interfaces that are calculated with the equilibrium slopes of the solid-liquid interface at the tri-junction point. From this, the average curvature undercooling is computed using the interfacial properties and superposed upon the constitutional undercooling in order to derive the total undercooling at the solid-liquid interface. While the system of equations as posed by Jackson and Hunt are quite generic, the authors impose certain assumptions, in order to simplify the equations and derive closed-form solutions analytically. Two of these assumptions are respectively the constancy of phase compositions as well as volume fractions with undercooling, i.e. the values are approximated from the phase diagram at the eutectic temperature.

In general however, these assumptions in the JH theory are valid for low Peclet number ($\lambda V/2D$) growth which is achieved at lower solidification velocities. For higher Peclet numbers, the phase fractions as well as the compositions of the phases change considerably from the values at the eutectic temperature, and thereby need to be accounted for. One of the first attempts in this regard has been from Series et al. [40] which provides error-estimates w.r.t to the classical Jackson-Hunt calculations using an electrical analogue to solve the solute-diffusion problem. Subsequently, Magnin and Trivedi [41] (also referred to as the TMK model) provide solutions in the high Peclet number regime for specific phase diagrams, while the more general case is studied by Ludwig and Leibbrandt [42], both of these works use the more generic analysis of the solute diffusion problem as discussed by Donaghey and Tiller [43]. In addition to higher velocities, one of the other reasons due to which phase fractions could change, are due to the different densities of the phases. This has been addressed in the work by Magnin and Trivedi [44,45], wherein one of the additional assumptions in the original JH calculations [35] that is the equality of phase undercoolings which is imposed in order to close the system of equations for determining the composition field in liquid, is relaxed.

In multi-component alloys, one of the additional reasons due to which the phase compositions may change from their equilibrium values at the eutectic temperature is due to the difference of solute diffusivities. This can result in modified phase fractions even at the same undercooling, which is in contrast to binary alloys, where the composition of the phases necessarily change only due to a increase in the undercooling. Furthermore, in multi-variant eutectic reactions, where the number of components exceed the number of solid-phases, just the equality of undercoolings at the interface does not present a closure of the systems of equations as in the classical invariant eutectic growth problem, unless certain phase diagram related assumptions are implied as in Refs. [36,37]. This is because the number of boundary layer compositions exceed the number of available equations (equality of phase undercoolings), and requires the solution to the complete solute diffusion problem. This relaxes the assumption of the constancy of the phase compositions and phase fractions with undercooling.

A couple of recent theoretical studies in this regard have been presented for two-phase mono-variant growth. The study by Catalina et al. [46] presents a linearized theory without allowing for the changes in composition in one of the solidifying phases. A more rigorous extension again for multi-component two-phase growth is provided recently by Senninger and Voorhees [47], where they take into account the composition variations of both the solid phases.

In this paper, we extend the works by Catalina et al. [46] and Senninger and Voorhees [47] and in general the classical JH theory for any given multi-phase configuration in a generic multi-component alloy. While we relax two of the assumptions in the classical (JH) theory relating to the constancy of phase

compositions as well as the phase fractions, two other assumptions of planarity of the interfaces to determine the diffusion field as well as the assumption of equal undercooling of the solid-liquid interfaces to effect closure of the equations, is retained. Further, the equality of molar volumes for the components is assumed in both the analytical calculations as well as phase-field simulations that are performed later. An influence of these assumptions are discussed at the end. Our work shares the same spirit as [46] and [47], however, one of the major differences is that we relate the deviations of the phase compositions to the departures of the diffusion potentials and temperature and thereby the functional dependence between the variations of the solid and liquid compositions is more elegantly retrieved. In addition, we verify our analytical calculations with phase-field simulations considering model symmetric alloys as well as a monovariant eutectic reaction in the Ni-Al-Zr alloy. In all the studies mentioned above, the effect of solute diffusivities in modifying the selection of solid phase fractions have not been explored. We investigate this aspect using our phase-field simulations as well as analytical calculations.

2. Analytical theory

2.1. The Jackson Hunt calculation

In order to motivate our present work let us re-visit the main results of the classical Jackson-Hunt analysis as detailed in Ref. [35], for deriving the undercooling vs spacing relationships for two-phase growth in a binary alloy. The situation is modeled by considering a repeating representative unit of two phases α and β growing in a directional solidification set-up where the imposed temperature gradient (G) at the interface traverses with a velocity V , that sets the rate of solidification. The undercooling at each interface can be written as,

$$\Delta T^v = -m_B^v \left(\tilde{c}_B^v - c_B^E \right) + \Gamma_v \tilde{\kappa}_v, \quad (1)$$

where, \tilde{c}_B^v represents the average composition in the liquid in local equilibrium with the v -th phase ($v = \alpha, \beta$) and c_B^E represents the eutectic composition. m_B^v is the liquidus slope. Γ_v and κ_v denote the Gibbs-Thomson coefficient and the interfacial curvature, respectively.

The classical Jackson-Hunt solution starts by writing the composition profiles as a Fourier series (see Eq. (2)). The solution to Fourier amplitudes (all except the boundary layer composition, or the zeroth order Fourier mode I_0) is derived as described in Sec. 2.2 such that the governing equations as well as the Stefan conditions are satisfied. A corresponding generic analysis for invariant eutectic growth in multi-component systems is laid out in Ref. [39].

A short description about the zeroth order mode which also partly sets the motivation of the rest of the paper is in order. The zeroth order Fourier mode I_0 as described by Eq. (11) for a binary alloy with solute $I = B$ reads, $B_0 = [c_B^{\alpha l} \eta_\alpha + c_B^{\beta l} (1 - \eta_\alpha)] - [c_B^{\alpha} \eta_\alpha + c_B^{\beta} (1 - \eta_\alpha)]$, where $c_B^{\alpha/\beta, l}$ represents the liquid compositions in equilibrium with the α/β interfaces, η_α is the volume fraction of the α phase. If one uses the volume fractions and compositions at the eutectic temperature (as for the other Fourier modes) for determining the boundary layer composition B_0 (far-field composition is at the eutectic) it would result in zero and the corresponding undercoolings at the interface using Eq. (1) would not be equal. This calculation, would also be physically incorrect, as the phase compositions deviate from their values at the eutectic temperature.

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