An analytical approach to Heat Transfer in Single and Multiphase Systems

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Abstract

This paper deals main physical processes arising during phase change have been investigated. The heat exchange within a single phase, many engineering technologies involve multiphase systems. Hence the problems dealing with phase change is the movement of phase interface with the release with the absorption of latent heat at this interface. The problems are highly nonlinear and thermophysical properties are typically different on each side of the phase interface. Therefore, analytical solutions are available only for a limited class of one-dimensional problems- pure materials or fluids in infinite or semi-infinite domains. In the present paper we demonstrate phase change heat transfer in pure liquids and materials as well as multicomponent systems. The multiphase systems have (*i.e*., solid, liquid, or gas phase) including one or more components. Although the governing equations vary for each type of multiphase system (*i.e* solid-liquid, liquid-gas, etc.,), the overall features of the physical and mathematical models are analogous. Theses continuum models are based on a *mixture formulation* or an *interface tracking* formulation. In the mixture approach, the control volume consists of a homogeneous mixture encompassing both (or *all*) phases. Mixture of interface tracking formulations are demonstrated in this studies.

Key words: Interface tracking, multi-phase flow, phase interface, interfacial energy balance, scalar transport, entropy, two fluid modeling.

1   *Introduction*

A phase is considered to be any homogeneous aggregation of matter. But liquids take the shape of their container and are essentially incompressible whereas solid retain their original shape unless deformed by external forces. Moreover, gases are characterized by their low density and viscosity, compressibility, lack of rigidity and optional transparency. A *unit* cell is used to identify a geometric configuration for a grouping of atoms in the solid. *Allotropy*   refers to the existence of two or more molecular or crystal structures with the same chemical composition. Hence this group is repeated many times in space within a crystal. *Interstitial diffusion* refers to migration of atoms through microscopic openings in the lattice structure of a solid. A peritectic reaction is a reaction whereby a solid goes to new solid plus a liquid on heating and the reverse on cooling.

Briefly, a *peritectoid* explains to transforming from two solid phases to a third solid phase upon cooling. On the other hand, in a polyphase material two or more phases are present, the primary phase is the phase that appears first upon cooling. The solubility of a multicomponent mixture indicates the maximum concentration of atoms of a particular constituent that can dissolve into the mixture. Gases can dissolve into liquids. In fact the solubility increases with pressure, but decreases with temperature.

2   *Boiling and Condensation*

The phase change in boiling, vapour bubbles initially form within cavities along the heated surface. The bubbles grow when the liquid is evaporated around the bubble. Hence bubble growth with along the heated surface occurs by evaporation of a liquid *microlayer* beneath the bubble. Bubble expand due to heat transfer through the base of each bubble. Heat is also transferred from the wall around the cavity to the liquid beneath the bubble (liquid microlayer). This heat transfer leads to evaporation of the bubble above the *microlayer* and movement of the vapour – liquid interface toward the heated wall until it reaches the wall and the bubble detaches from the surface cavity. On the other hand, additional liquid comes into contact with the heating surface to sustain the boiling process. Due to its higher heat capacity and thermal conductivity, the local heat transfer rate is enhanced when liquid comes into contact with the surface.

Velocity and temperature diffusion layers at a micro-scale are formed around the surface of each departing bubble. In contrast to boiling heat transfer, condensation arises when vapour is brought into contact with a cooed surface below the saturation temperature. If a quiescent vapour comes into contact with a cooled surface, two fundamental modes of condensation can occur *dropwise* and *film* condensation. The liquid does not fully cover or wet the surface in drowse condensation, whereas the liquid film covers the entire surface in film condensation. The boiling process begins when individual bubbles form and grow along the heated surface, detailed analysis of condensation heat transfer is documented [2]. The liquid microlayer beneath a growing bubble is evaporated, leading to departure of the newly formed bubble [3][4]. This process may be approximated through a combination of liquid and vapour periods where heat conduction solutions can be applied at both successive stages [9][10]. Predictive models of bubble growth rates have been developed by various researchers, Plesset et al. [11].

The average heat flux over both periods is anticipated to have a closed dependence on the frequency of bubble departure [6]. The changing liquid layer thickness beneath a bubble is implicitly coupled with the heat conduction process in the liquid and latent heat released in the adjacent vapour phase.

A lower rate of heat transfer between the vapour and wall usually arises in film condensation, due to the added thermal resistance of the liquid film. In addition, the heat or absorbed during liquid–vapour phase change (boiling or condensation) can be represented as the amount of mass multiplied by the latent heat of vaporization such as the rate of heat transfer during boiling, q can be determined

$$\frac{q}{\dot{m}} = h_{fg} \tag{1}$$

where $\dot{m}$ and h_{fg} denotes to the mass of the liquid boiled per unit time and the latent heat of vaporization. However, a subtle correction of the right side of the Eq.(1) is observed in view of the phase change that occurs at a fixed temperature for pure (single constituent) fluids [1]. Moreover, the enthalpy of vaporization in Eq.(1) is evaluated at fixed temperature. A change of a phase (liquid or vapour) at a fixed temperature implies a constant pressure, since pressure and temperature are mutually dependent for liquid–vapour mixtures at equilibrium.

Based on an energy balance on the control volume,

$$\frac{dE}{dt} = q - \dot{m}\, h_g \tag{2}$$

The energy balance in Eq.(2) indicates the rate of energy loss by vapour carried out of the tank is equal to the heat addition minus the energy loss by the vapour carried out of the tank to maintain an isobaric process. Hence expanding the internal energy in Eq.(2) in terms of specific internal energies of the liquid and vapour phase,

$$\frac{d\tilde{E}}{dt} - \frac{d}{dt}\left(m_f \tilde{e_f} + m_g \widetilde{e_g}\right) - \dot{m_f}\tilde{e_f} + \dot{m_g}\widetilde{e_g} \tag{3}$$

Where the subscripts f and g represents the fluid (liquid) and gas (vapour) respectively. In addition conservation of mass requires that the rate of mass change within the tank balances the flow rate of escaping steam, i.e.,

$$\frac{d}{dt}\left(m_f + m_g\right) = -\dot{m} \tag{4}$$

During the phase change process, the total volume remains constant, so that

$$\forall = m_f\, v_f'' + m_g\, v_g''' \tag{5}$$

Which can be differentiated which gives us,

$$\dot{m}_f \, v_f''' + \dot{m}_g \, v_g''' = 0 \tag{6}$$

Combining Eq.(4) and (5), we obtain,

$$\dot{m}_f = -\dot{m}\left(\frac{v_g'''}{v_g''' - v_f'''}\right) \tag{7}$$

$$\dot{m}_g = \dot{m}\left(\frac{v_f'''}{v_g''' - v_f'''}\right) \tag{8}$$

Furthermore, substituting Eqs.(7) and Eq.(8) into Eq.(3) and then Eq.(2) and rearranging,

$$\frac{q}{\dot{m}} = h_g - \frac{\widehat{e_f} v_g''' - \widehat{e_g} v_f'''}{v_g''' - v_f'''} = h_{fg} + \left(h_f - \frac{\widehat{e_f} v_g''' - \widehat{e_g} v_f'''}{v_g''' - v_f'''}\right) \tag{9}$$

The enthalpy of the saturated liquid, h_f is subtracted from h_g in Eq.(1) as such that $h_{fg} = h_g - h_f$, whereas a correction of h_f involving internal energies and specific volumes was provided by the last fraction in Eq.(9).

3 *Solidification and Melting*

Solidification and melting occur in many engineering applications [2], including materials processing, ice formation on aircraft and other structures, and thermal energy storage with phase change materials (PCMs). On the other hand, the heat transfer q, due to phase change between solid and liquid phases can be written as

$$q = \dot{m} \, h_{sf} \tag{10}$$

Where $\dot{m}$ and h_{sf} refer to the rate of mass change and due to the phase transition and the latent heat of fusion, respectively. In this section we study the solid – liquid phase change have been demonstrated. Heat transfer has important effects on interfacial processes during phase change. Solidification is initiated and a planar solid liquid interface moves into the liquid over time. The boundary is maintained below the phase change temperature and remains parallel to the planar phase interface. Moreover, the Gibbs free energy G, has special importance in solid-liquid phase change such

$$G = H - TS \tag{11}$$

where *H*, *T* and *S* denotes enthalpy (extensive), temperature and entropy respectively. Again assuming component *A* in a multicomponent mixture

$$\mu_A = \left.\frac{\partial G_A}{\partial n_A}\right|_{Tp} \tag{12}$$

where the derivative is evaluated at constant pressure and temperature. We have demonstrated that uniformity of the Gibbs free energy, $dG = 0$ at thermodynamic equilibrium since no temperature and pressure gradients would exist. Furthermore, a solid and liquid separately and Gibbs free energy of each phase as it varies with temperature (below and above the phase change temperature) as

$$G^l = H^l - TS^l \tag{13}$$
$$G^s = H^s - TS^s \tag{14}$$

now the superscripts l and s represents the liquid and gas respectively. On the other hand, the change of Gibbs free energy, ΔG_{max} due to mixing of the two phases at any temperature is

$$\Delta G_{mix} = \Delta H_{mix} - T \Delta S_{mix} \tag{15}$$

At the phase change temperature $T = T_m$,

$$\Delta G = 0 = \Delta H - T_m \Delta S \tag{16}$$

In which it indicates that the entropy of fusion can be approximated, we obtain

$$\Delta S_f \approx \frac{L}{T_m} \approx R \tag{17}$$

where L denotes the latent heat of fusion (ΔH_{sf}), R~8.4 J/mol H is approximately constant.

3.1   *Nucleation*

It occurs when the probability of atoms arranging themselves on a crystal lattice is high enough to form a solid crystal from the liquid. In this case, homogeneous nucleation signifies to solidification of liquid initiated by undercooling alone. Furthermore,   heterogeneous nucleation signifies when the walls of a container or particle impurities exist to assist in providing nucleation sites for the solidifying crystal. The critical condition for the onset of homogeneous nucleation occurs when the decrease in the Gibbs free energy of the crystal becomes [3],

$$\Delta G = \sigma A + \Delta g \Delta V \tag{18}$$

Where Δg indicates Gibbs free energy difference between the liquid and solid and ΔV represents spherical volume enclosed by the crystal, hence σ denotes the specific interface energy (J/m^2). In addition, we have noticed that from the Eq.(18) indicates the decrease in the Gibbs free energy due to phase change balance the work required to keep the initial crystal bonds in the *lattice* structure

from melting back to the liquid first term plus the change in the Gibbs free energy in changing from *liquid* to *solid* phases.   Moreover, the first term of the Eq.(18) denotes the work term

required to maintain the crystal bonds together without melting, is characterized by the by the interface energy,σ and this interface energy is a property of the material, can be expressed in terms of the Gibbs-Thompson coefficient, Γ_{gt} and for metals,

$$\Gamma_{gt} = \frac{\sigma}{\Delta s_f} \approx 1 \times 10^{-7} Km \tag{19}$$

Now using Eq.(17) considering phase change at T_m , the Gibbs free energy per unit volume becomes,

$$\Delta g = \Delta h - T\Delta s = L - T\frac{L}{T_m} \tag{20}$$

Where enthalpy and entropy with temperature in the middle expression of Eq.(17) are considered to be small in comparison to the respective changes associated with the phase transformation. Again combining both terms in Eq.(20)

$$\Delta g = \left(\frac{L}{T_m}\right)\Delta T = \Delta s_f \Delta T \tag{21}$$

Where $\Delta T = T_m - T$ denotes the undercooling level, and substituting Eq.(21) into Eq.(18) with a radius r to represents a characteristic spherical volume $r = r_0$ encompassing the nucleating crystal,

$$\Delta G = (4\sigma\pi r^2) - \frac{4}{3}\pi r^3 \Delta s_f \Delta T \tag{22}$$

The critical condition for the onset of nucleation occurs when the driving force for solidifications equal to the respective force for melting. Furthermore, without particle impurities in the liquid or a rough-walled container to prematurely initiate the phase transition, the undercooling level in Eq.(25) is required to sustain the nucleation site.

3.2   *Critical Radius of a Crystal for the Onset of Nucleation*

Using the Gibbs free energy to determine the critical radius of a crystal that initiates homogeneous nucleation in the solidifying liquid; the maximized ΔG occurred when

$$\frac{d(\Delta G)}{dr} = 0 \tag{23}$$

Differentiating the expression in Eq.(22) with respect to r and substituting into Eq.(23), and solving for the resulting critical undercooling,

$$\Delta T = \frac{2\sigma}{r_0 \Delta s_f} \tag{24}$$

Eq.(24) indicates critical condition to initiate homogeneous nucleation, and in terms of critical radius,

$$r_0 = \frac{2\sigma}{\Delta T \Delta \eta_f} \tag{25}$$

The radius r_0 refers to the critical nucleation radius for homogeneous nucleation. On the other hand, the rate of nucleation is slightly undercooled liquid is less than the rate of nucleation for a material that is substantially undercooled below the phase change temperature because the former (warmer) material possesses more internal energy to possibly metals crystal back into the liquid, thereby reducing the rate of nucleation. Thus, this increase of nucleation rate with undercooling level (up to some maximum point), I_{max} can be expressed

$$I(T) = exp\left(\frac{-\Delta G_n^0}{kT}\right) \tag{26}$$

where G_n^0 and k represents the Gibbs activation energy and Boltzmann constant ($k \approx 1.38 \times 10^{-23} J/K$) respectively. In addition, for materials exhibiting a higher density in the solid phase , the *liquid* occupies a larger volume than the solid phase change temperature. But the atomic packing is greater in the solid phase, which implies that there is more freedom of movement of atoms in the liquid. Eq.(26) may be interpreted as

$$n_r = n_0 \exp\left(\frac{-\Delta G_n^0}{kT}\right) \tag{27}$$

Where n_r, n_0 denotes the average number of newly formed spherical clusters of radius r and the total number of atoms, respectively. Again, G_n^0 denotes a thermal activation barrier over which a solid cluster must pass to become a stable nucleus.

Based on equations Eqs.(25)-(27), the speed at which solid nuclei appear in the liquid denoted by $\dot{n}_{hom}$ at a given undercooling level can be better understood. Eq.(24) id rearranged to predict the critical nucleation radius, r_o required at the critical nucleation undercooling. The left hand side of Eq.(27) can be interpreted as the number of clusters reaching the critical radius r_o . Hence it is related to the speed of solid formation as

$$\dot{n}_{hom} = \dot{f}_0 \, n_r \tag{28}$$

where f_o be the frequency of adding atoms to the stable, newly formed nuclei cluster and this frequency is dependent on the interface energy, surface tension at the phase interface, and areas of the nuclei. Furthermore, the analysis is performed for heterogeneous nucleation along a flat mold wall, the critical nucleation radius analysis holds for any nucleation geometry, such as rough surfaces or solid impurities in the liquid. The initiation of heterogeneous nucleation is important in various practical instances, such as the addition of inoculants to industrial chemicals

to act as agents reacting with a component in the liquid to form a solid nucleus. Thus the effectiveness of an inoculants is dependent on the nucleation geometry, particularly θ, interface energy σ and entropy in fusion of the solidified material.

The structure of the face interface can be characterized by the nature of the surface area bonding at the interface which can be analysed by the number of sides attached to the *lattice* structure in a cube-shaped crystal. Hence the interface growth is determined by the probability that a molecule will reach the interface and remain there until it bonds to the interface. Thus the probability increases with an increasing number of neighbours in the crystal. In the Fig.(1) it is shown that a type-3 atom is halfway in the solid (three sides bonded to the solid) and halfway in the liquid (three sides exposed to liquids). A certain sequence of phase transition can then be envisioned in Fig.(1). Type 3 atoms are added until a row along the interface is completed. Then type 2 atoms (i.e. two sides bonded to the solid) are needed to start the next row, which is adjacent to the previous row at the solid-liquid interface. This requires more undercooling than a type 3 formation. Finally, an entirely new row is initiated by a type 1 atom (*i.e.*, only one side attached to the solid). Now, this formation requires the most undercooling since the remaining five sides are exposed to liquid and possible remelting.

Interfacial balance for evaporating droplets, dynamics of these momentum interactions for evaporating and oscillating droplets in a zero gravity environment [5].

Another way is that the *phase* interface can be characterized as automatically rough, yet microscopically smooth. The morphological stability affects the structure of the solid-liquid interface. Hence for a pure material, a stable interface is *columnar* whereas the unstable interface is *equiaxed*. In the stable, columnar interface, consider the onset and advancement of a wavy phase interface in the positive x direction due to solidification and heat extraction through the solid in Fig. (2). The peak and valley of the wavy interface (where the peak refers to the farthest extent into the solid) will be denoted along planes A and B respectively. The corresponding heat flows are q_A through the solid and q_B into the solid from the liquid, respectively. The temperature gradient in the liquid is higher along plane A since the phase change temperature is reached at the edge of the solid perturbation is melted and the interface remains stable which is planar.

On the other hand, the wavy interface, specifically an interface formed along the outer edge of a specifically shaped crystal that grows radially outward. In this case latent heat is released radially outward from solidified crystal into the liquid. The crystal grows radially outward until it impinges on other nuclei. The heat flows along the peak as plane A and valley as plane B of the wavy interface are denoted by q_A and q_B respectively. Moreover, the temperature gradient is again higher along the plane A, which suggests that the tip of the wavy interface rejects more heat. Furthermore, the perturbation at this tip grows faster and waviness of the interface increases (*i.e.*, unstable interface). Hence the resulting structure is the equaixed due to the sustained growth of interface perturbations along certain crystal axis directions. The morphological stability of the solid-liquid interface is affected by the presence of other constituents in the material. The solubility limit refers to the maximum concentration

of solute that can dissolve in the solvent to form a solid solution. This solubility limit affects the coupled heat and mass transfer in phase change processes. Let us consider a binary alloy that consists of lead and tin which are in both in solid and liquid phases. During phase transition, the concentration of solute (tin) in the solid remains less than that of the original mean solute composition due to the difference in solubilities of both constituents within each phase. The balance of the solute from that original concentration remains in the liquid. Entropy and second law of thermodynamics have important implications in the study of liquid – solid systems [7][8].

Interfacial Energy Balance   In this work, phase change problems, the heat balance at the phase interface largely affects the movement and position of the phase interface[12][13]. Hence in solid-liquid systems, the heat transfer from the liquid phase into the phase interface, HT_l consists of conduction and advection components:

$$HT_l = -K_l \, dA \, \frac{dT}{dn} \big|_l \, dt + \rho_l \, {}_{v_l} \, \hat{e}_l dA dt \qquad (29)$$

Where $\hat{e}$ denotes to specific internal energy and HT_s is obtained in the solid phase. Therefore, a control volume at the phase interface is selected with a thickness of *dn*. Then the change of energy that accompanies the advance of the interface arises due to the energy difference between the initially liquid volume, occupying *dAdn*, and a final solid volume, *i.e.*,

$$dE \equiv HT_l\text{-}HT_s = \rho_l \, \hat{e}_l \, dAdn - \rho_s \, \hat{e}_l dAdn \qquad (30)$$

Using Eq.(29), as well as the analogous result for the heat flux in the solid phase, and substituting those results in Eq.(3)) the following result is obtained

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$$(\rho_l \; \bar{e}^-_l - \rho_s \bar{e}^-_s) . \frac{dn}{dt} = -k_l \frac{dT}{dn} \; |_l + k_s \; \frac{dT}{dn} \; |_s + \rho_l \, v_l \, \hat{e}_s \qquad (31)$$

Also combining Eq. (32) with Eq. (31) and rearranging terms, we obtain

$$\rho_1 \, v_1 - \rho_2 \, v_2 = (\rho_1 - \rho_2) \frac{dn}{dt} \qquad (32)$$

$$-k_l \frac{dT}{dn} \; |_l + k_s \; \frac{dT}{dn} \; |_s = - \rho_s \, v_s \, \Delta \, \hat{e}_f + \rho_s \, v_i \, \Delta \, \hat{e}_f \qquad (33)$$

Where $\Delta \; \hat{e}_f = \hat{e}_l - \hat{e}_s$ denotes the latent heat of fusion and $v_i = dn /dt$ refers to the interface velocity. Eq. (33) represents the heat balance at a solid-liquid interface.

Conclusion and Discussion

In the present paper the following conclusions can be drawn as

(i)   initial numerical solution for an enhanced model of two-phase flow which includes fluid-fluid interfacial area as a primary variable.

(ii) the particular case studied, the saturation profiles show little dependency on interfacial area.

(iii) since the correct functional forms of the resistance terms used in the model are not known, hence more studies are required to assess the practical importance of the interfacial area equations to flow modeling.

(iv) now the results in the present paper represents a starting point for this more general analysis.

(v)   hence the overall significance of interfacial areas in the mathematical description of multi-phase flow in porous media, remains to be determined.

(vi)   the degree to which the governing equations can be simplified, must be explored numerically.

(vii) this requires a comprehensive and systematic approach.

(viii) the results are used to test a specific conjecture that relates average interfacial   velocity to average phase velocities.

(ix)   in particular, we conclude that the proposed *equations* in our above studies that relates interfacial velocities to phase velocities only hold under very specific conditions, like piston-like stable displacements in which trapped interfaces are neglected.

(x)   in addition, to close the extended set of equations for two-phase , which includes specific interfacial area as a primary variable, new constitutive equations need to be developed.

(xi)we can make a few observations such as

  (a) inclusion of interfacial area equations allows for direct calculations of the amount of interfacial area in the system.

  (b) equations written for the individual phases also incorporate effects on the interfaces through functional dependencies in the appropriate nonlinear coefficients .

  (c) again, inclusion of a unique relationship between P_c, s^w and a^{wn} allows hysteresis within the $(P_c - s^w)$ plane to be incorporated into the algorithm with no additional effort.

  (d) arbitrary drainage and imbibitions cycles can be simulated without redefining the constitutive curves.

  (e) this *appears* to be major advantage of this approach to multi phase flow modeling.

(f) the cost of such additional generality and flexibility is the need to identify and quantify additional parameters – as well as their functional dependencies on interfacial area.

(g) furthermore, additional equations also need to be solved compared to the traditional equations for multiphase flow.

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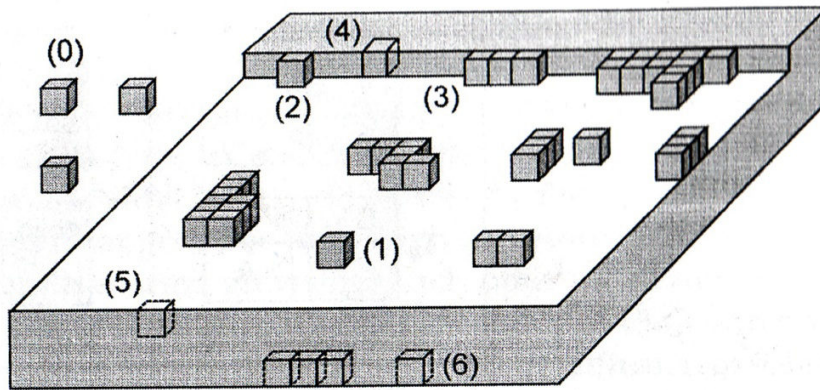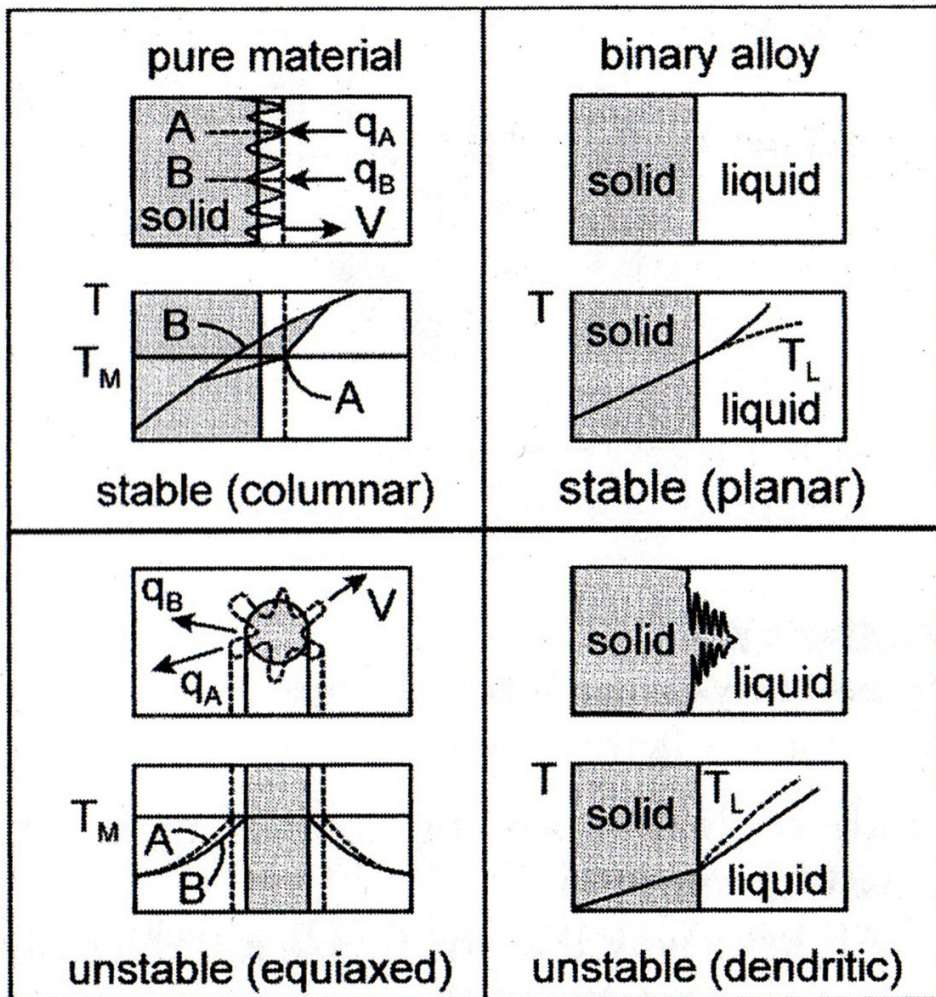
Fig. (1) Stages of crystal and solid formation.

Fig. (2) Stability of phase interface.

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