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A review of dendritic growth during solidification: Mathematical modeling and numerical simulations

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ABSTRACT

Dendritic growth is one of the most common microstructures in metal and solution solidification. The subject of dendritic growth has received much attention from both scientific and industrial points of view. On the one hand, dendritic growth has become a deeply investigated subject in non-linear dynamics field. On the other hand, its understanding became essential for some engineering applications, mainly in metallurgy and latent thermal energy storage where phase change materials are used. Therefore, understanding and modeling the mechanisms which result the dendritic structures has been the objective of much research over the last decades. In order to understand the formation of dendrites, it is essential to understand the physical mechanisms on the interface separating the two phases. This paper reviews and discusses the available theories of dendritic growth, and then introduces the Gibbs-Thomson condition which has to be taken into account to handle all interfacial effects. Based on the Gibbs-Thomson condition, a complete mathematical model describing the dendritic growth problem for pure substances is formulated. This model includes the heat equation in both liquid and solid phases, the heat conservation equation at the interface separating these two phases, and the proposed Gibbs-Thomson equation. In order to solve this complex non-linear problem, several numerical methods have been developed. Hence, in its last section, the paper reviews these numerical methods distinguishing between two major classes involving the explicit and the implicit tracking of the moving interface.

1. Introduction

The formation of patterns in nature is largely found everywhere [1,2], some examples are cloud formation [3], bacterial colonies [4], and grain structures in metals [5] or rocks [6]. Dendritic crystal growth is one of the most spontaneous pattern formations. For instance, snowflakes have various types of complex and fascinating shapes, although they are formed in almost uniform circumstances.

Further, dendritic structures are also commonly forms of microstructure, being present in all macroscopic castings, ingots, and welds.

During a cooling process, if care is taken and in the absence of perturbations, it is possible that the material remains in its liquid state, even below its solid-liquid equilibrium temperature. Thus supercooled liquid may appear [7]. Such a state is thermodynamically metastable [8–10]. Then the solidification can occur either homogeneously [11,12] after sufficient cooling or heterogeneously by placing for example a solid seed in the supercooled liquid [13–15]. Furthermore, once the solid is nucleated through the supercooled liquid, the subsequent growth of the solid from the seed may not to be stable and a dendritic crystal may form, depending on several factors, mainly the degree of supercooling. “Dendrites are a prototypical system evolving from homogeneous starting conditions into complex spatio-temporal patterns far from equilibrium” [16].

The descriptive term ‘dendrite’ comes from the Greek word ‘dendron’ which means tree [17]. Like a tree, the dendrite has a highly branched, arborescent structure (see Fig. 1 [103]). Due to the interface instabilities, a dendritic crystal consists of a primary stem, secondary branches, and eventually higher order branches evolving, all growing in selected crystallographic directions.

The evolution of the dendritic pattern has received much attention from both scientific and engineering points of view for its intricate pattern selection mechanisms and useful industrial applications, mainly in metallurgy and thermal energy storage fields. On the one hand, dendrites in metallurgy establish the initial microstructures of cast metals and alloys. These microstructures, in turn, strongly influence the mechanical, physical, and chemical behaviors of the material. Otherwise, they determine the qualities of the solidified raw material and often the finished product. Thus, the understanding of

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Nomenclature

T	Temperature [K]	ΔT_O	Initial supercooling [K]
T_i	Initial temperature [K]	L	Latent heat of fusion [J kg^{-1}]
T_m	Equilibrium temperature [K]	λ_c	Cutoff wavelength [m]
T_n	Nucleation temperature [K]	T_f	Interface temperature [K]
T_c	Coolant temperature [K]	γ	Surface tension [J m^{-2}]
δ	Perturbation amplitude [m]	κ	Twice of mean curvature [m^{-1}]
δ_D	Diffusion length [m]	L_v	Volumetric latent heat [J m^{-3}]
δ_C	Capillary length [m]	v_n	Normal velocity [m s^{-1}]
Pe	Péclet number	υ	Kinetic mobility [m K^{-1} s^{-1}]
v_t	Tip velocity [m s^{-1}]	c_v	Volumetric heat capacity [J m^{-3} K^{-1}]
r_t	Tip radius [m]	θ	Interface orientation [rd]
α	Diffusivity [m^2 s^{-1}]	k	Thermal conductivity [J m^{-1} K^{-1} s^{-1}]
Δ	Dimensionless supercooling	t	Time [s]
c	Heat capacity [J kg^{-1} K^{-1}]	ω	Pulsation [rd s^{-1}]
		ρ	Density [kg m^{-3}]
		$\vec{n}$	the normal vector at the interface

these dendritic microstructures formation is technologically important in order to produce better casts and pattern formation for advanced materials. On the other hand, the dendritic growth is a very important phenomenon in the process of solidification of materials used to transfer energy. The applications can be for installations in which the crystallization is required as the latent heat energy storages and the use of phase change materials (PCM) [18,19], the distribution of energy through diphasic liquid-solid heat transfer fluids [265], but also installations where this crystallization needs to be avoided as it is the case during the transport of liquid fluids in pipes [266,267]. The end of the supercooling phenomenon and the beginning of the solidification of the whole region are shown in Fig. 2 for a pure material. In fact, during the propagation of dendrites through the supercooled liquid, the liquid temperature returns to its equilibrium temperature of solidification. This is due to the latent heat absorbed by the supercooled liquid, which is released from the interface during this phase. Hence, one would like to understand how the dendritic growth is driven or guided, in order to improve the solidification processes by controlling or preventing it.

Furthermore, apart these engineering applications providing its technical importance, dendritic growth also represents a pattern formation phenomenon, which in recent years has become a deeply researched subject in non-linear dynamics field.

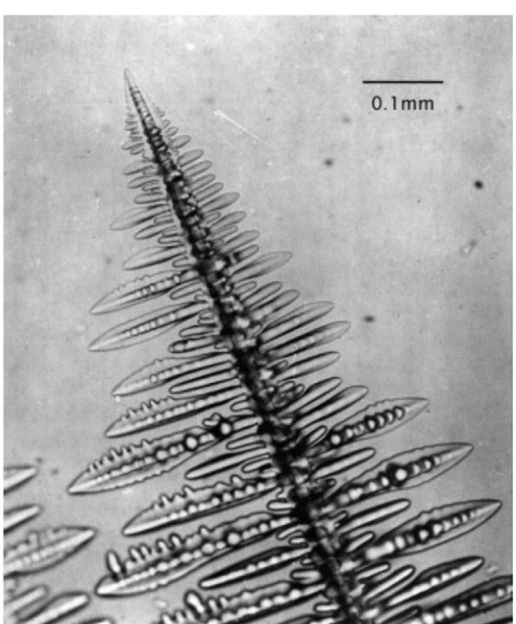

Fig. 1. Dendrite growing into a supercooled melt of pure succinonitrile [103].

The problem of dendritic growth has had a long and somewhat tortuous history [20,21]: In 1611, even before the atoms were discovered, Kepler drew attention to the shapes, numbers, and geometric similarities exhibited by the six fold symmetry of snowflakes [22]. The last 50 years have seen a renaissance of interest in this problem focusing on the dynamics of crystal growth and how the liquid-solid interface evolves during this phase, and it could be said that many of the basics behind this behavior have reached a good level of understanding to the satisfaction of researchers working on both experimental and numerical aspects of this subject.

The essential purposes in the present review paper are first, to show the available theories of dendritic growth in a simple manner to provide the reader who is interested in this problem a good and complete point of understanding and second, to present the different numerical methods used to resolve this complex problem. Thus, the paper is organized in five sections. In the second section, the dendritic growth theories starting from the Mullins-Sekerka instability as well as the history/evolution of the Gibbs-Thomson condition - which is used to calculate the interface temperature which is different than the equilibrium temperature due to the interfacial instabilities – are presented. When Gibbs-Thomson equation is appropriate, it can be coupled with the heat transport equations to give a complete understanding of the dendritic problem. The third section introduces the mathematical governing equations of the problem including the last presented Gibbs-Thomson condition at the interface. The fourth

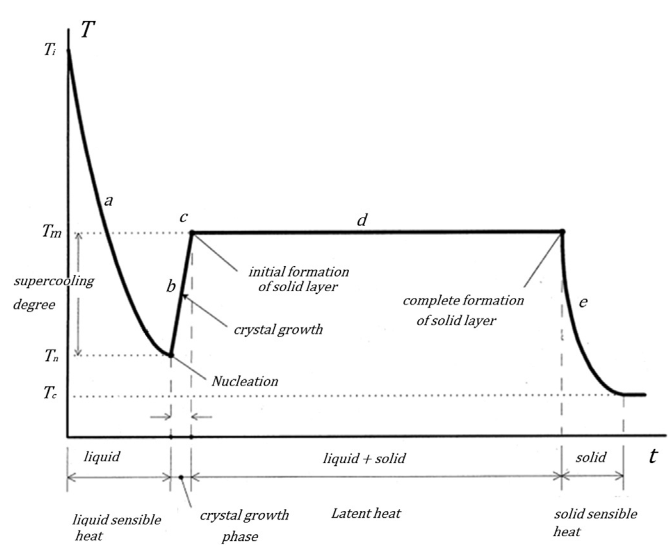

Fig. 2. Variation of the temperature (at the centre of a sample) in time, during solidification process of a supercooled liquid. Phase b concerns the crystal growth.