

## BOOK REVIEW

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*Thermomechanics of evolving phase boundaries in the plane*, by Morton E. Gurtin.  
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019-853694-1

The theory of solidification and crystal growth is mathematically complex and technologically vital. It is based on partial differential equations and numerical computation, with geometric measure theory, differential geometry and calculus of variations playing useful roles as well. Every industry from semiconductors to steel must predict and control solidification processes, providing a wide range of applications for mathematical modelling and numerical analysis.

Gurtin's book provides clear, thorough derivations of basic results in the mathematical modelling of solidification processes, with only elementary real analysis and thermodynamics as prerequisites. More advanced results would require substantial background in PDE, numerical or asymptotic analysis, so the scope of the book is well chosen. References are given to further work in PDE related to solidification but not to numerical or asymptotic analysis.

Specific quantitative models of solidification come in three flavors: sharp interface, phase field and lattice models. We briefly compare the three classes of models, though Gurtin discusses only the first.

**Sharp interface models** consist of equations of motion for the solid-liquid interface, which is idealized as a curve or surface of zero thickness. The equations of motion involve the geometry and thermodynamics of the interface and the *phases* (solid or liquid) on each side. Laplace and Young studied surface tension in liquid drops with sharp interfaces in 1805, creating a theory reformulated by Gauss twenty-five years later. It was 1892, however, before Gibbs constructed the general thermodynamics of sharp interfaces which forms one of the main threads of the book.

**Phase field models** combine two ideas. First, the solid-liquid interface is smeared into a smooth transition zone. In 1830, Laplace's protégé Poisson studied such a smooth transition of density across a liquid surface, which had been neglected in the Laplace-Young theory. About 1892, Rayleigh and van der Waals constructed a complete general theory of interfaces with nonzero thickness, reformulated by Cahn and Hilliard [3] in 1958. Second, a "phase field" or "order parameter" indicating smooth changes from solid to liquid is added to the thermodynamic variables, a device popular in statistical physics under the name of "Landau-Ginzburg theory" and due in this context to Fix [8]. Recently, phase field models have been derived

by Penrose and Fife [14] for solidification of pure substances, by Wheeler et al. [17] for isothermal alloy solidification, and by Chapman et al. [4] for superconductivity.

**Lattice models** (such as the Ising model) are usually directed towards microscopic analysis of static interfacial structure, though dynamic lattice models have been used to study scaling properties of solidification in e.g. Derrida et al. [5].

Extracting experimentally verifiable results from any of these models involves formidable analytical and computational difficulties, so no single class of models has yet dominated the field. Practical stability criteria come mostly from sharp interface models, but there are difficulties in proving well-posedness and tracking complex interfaces numerically. Phase field and lattice models are conceptually simpler to solve but harder to translate into physical results.

Thus consider a sharp interface  $C(t)$  between a two-dimensional solid crystal and the liquid melt from which it grows.  $C(t)$  is a curve at each time  $t$ , moving along its normal vector with velocity  $V(t)$  defined on the interface. One sharp interface model differs from another in the dependence of  $V(t)$  on the location, geometry and history of  $C(t)$  and on external fields such as the temperature or concentration, which may in turn depend on the interface. Part I of the book is devoted to model-independent consequences of the geometric relations between  $C(t)$  and  $V(t)$  such as kinematics and conservation laws for curvature and length. This is useful material relevant to any two-dimensional moving boundary problem.

The remainder of the book is devoted to two special sharp interface models, **anisotropic motion by curvature** and the **generalized Stefan model**. Gurtin derives the fundamental equations for each model and analyzes some of their consequences. He begins from a framework of rational continuum thermodynamics, introduces kinematics, balance laws and the second law, and then constitutive relations for specific materials which are compatible with the second law. Gurtin also presents a thorough discussion of the equilibrium theory for motion by curvature, introducing classical concepts such as the Frank diagram and the Wulff crystal. (This equilibrium theory is rigorously derived from the Ising model by Dobrushin et al. [6].)

Motion by curvature, the subject of Part II, has  $V(t)$  a local function of curvature  $K$  and the unit normal vector  $n = (\cos \theta, \sin \theta)$  defined by

$$(1) \quad b(\theta)V = (f(\theta) + f''(\theta))K - F$$

where  $b > 0$ ,  $f > 0$  and  $F$  are given. This model (with  $b = f = 1$  and  $F = 0$  so  $V = K$ ) was introduced by Mullins as a model for grain growth in the late stages of solidification [13]. Physicists, geometers and analysts have studied similar models in many contexts [1, 10, 7].

If the coefficient  $g(\theta) = f(\theta) + f''(\theta)$  of  $K$  in (1) is strictly positive, a parametrization of  $C(t)$  satisfies a moving boundary problem for a nonlinear parabolic equation. Gage and Hamilton [9] and Grayson [10] used this “heat equation” to prove that smooth curves shrink to circular points and disappear in finite time when  $V = K$ .

In most models for solidification, however,  $g(\theta)$  changes sign, so the problem becomes *backward* parabolic for some intervals of the normal angle  $\theta$ . This mathematical complication causes many real-world crystals to form faceted shapes composed of smooth pieces joined at corners—a highly nonparabolic phenomenon. The corners allow  $\theta$  to skip over the backward parabolic regions and thus ensure well-posedness.

Part II concludes with a brief introduction to fully faceted (polygonal) interfaces, what one normally thinks of as crystals, which occur when  $f$  is not smooth and  $g$  has jumps. The study of such interfaces dates from Wulff's 1901 analysis of the equilibrium shape. The dynamical theory is more recent and involves "infinitesimally wrinkled interfaces" reminiscent of geometric measure theory.

Real-world solidification problems involve many further complications, the simplest being heat flow, solute diffusion, convection in the liquid, rotation, magnetic fields and so forth. These complications are employed to stabilize the interface so larger purer crystals can be grown faster. Tiller gives a thorough technological introduction in [16], while a more mathematical viewpoint can be found in Kurz and Fisher's text [11].

Part III adds thermodynamics to motion by curvature, yielding generalized Stefan-type models where heat flow competes with geometry. The heat flow makes these models nonlocal:  $V(t)$  depends on the entire history of the interface  $C(s)$  for  $0 \leq s \leq t$ , as well as initial and boundary conditions for the temperature field. This nonlocality makes analysis and numerical calculations much more difficult. Anything beyond the linearized stability theory of a flat interface moving with constant speed requires many further approximations. Nonetheless, practical stability criteria have come mostly from these models.

The simplest of these models consists of the heat equation

$$u_t = \Delta u$$

for the temperature field  $u$  at points not on  $C(t)$ , coupled with two boundary conditions on  $C(t)$ : the balance law

$$[u_n] = V,$$

where  $[u_n]$  is the jump in the normal derivative of  $u$ , and the generalized Gibbs-Thomson relation

$$(2) \quad u = (f(\theta) + f''(\theta))K - b(\theta)V.$$

Clearly if  $u$  is a constant  $F$  on  $C(t)$ , the "isothermal interface", then the Gibbs-Thomson relation (2) becomes motion by curvature, while in general the interfacial velocity  $V(t)$  depends nonlocally on  $C(t)$  and its history. Recently Luckhaus [12] and Almgren and Wang [2] proved global existence and uniqueness theorems for this model, using PDE and geometric measure theory plus a variational formulation. Numerical solution of this problem is difficult but popular (for example, see Sethian and Strain [15]).

This book does the field a great service by presenting important foundational material in a clear, accessible form. It illustrates very well the role of rational thermodynamics and elementary real analysis in modelling of a vital technological topic. It would make an excellent text for a topics course on the subject.

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JOHN STRAIN  
UNIVERSITY OF CALIFORNIA, BERKELEY