Why Solidification? Why Phase-Field?

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"Solidification" is a branch of pattern formation in theoretical physics. "Phase-field" is an applied tool in engineering. This strange combination of basic and applied research is reviewed against its historical background: a story of failure and success. The main achievements in both fields are highlighted, and future perspectives are briefly discussed.

INTRODUCTION

If we read the word "solidification," we might think of the compaction of the soil in geophysics. Or the coagulation in an emulsion. Metallurgists think of the crystallization of a melt. Theoretical physicists think of a self-similar transport solution and its variation, which determines the scale of the solidifying object. Of course they mean a "dendrite" (see, e.g., Ref. 1), which has a theoretical solution similar to viscous fingering in oil drilling.[2] A dendrite is the growth structure of the solid crystal during solidification, which has a morphologically unstable interface with its melt under typical solidification conditions of an alloy (as discussed in Ref. 19). The crystal forms a "tree-like" structure, from which we get the name. (See Fig. 1).

Why solidification? From the practical point of view, the understanding of dendritic growth is crucial for understanding the technical process of metal casting. "Worldwide, as many as 10 billion metallic dendrites are produced in industry every second" starts the "News and Views" article in *Nature* by Rappaz and Kurz in 1995.[3] Today, the rate will even be higher. The theoretical problem of "solidification" is settled in its principles, I will report. Good theoretical models and numerical tools are available to cope with the solidification of technical materials. These tools have found their way into practical engineering solutions that are applied on a routine basis in foundries every day around the world.

Why phase-field? The answer is simply because there is no other numerical tool for coping quantitatively with the problem of a dendrite in three dimensions. There are several other numerical techniques that have been investigated in the past, and there may be new techniques emerging in the future. It is from its numerical efficiency that phase-field won the race. In this review, I'll summarize the historical development partly from the literature, and from my own experience and from narrations—for those who are younger than me and did not have the chance to meet the pioneers—and for the pioneers to smile at the past.

PEARLITE AND THE PROBLEM OF SCALE

Pearlite is the mother of pattern formation (for a recent revisit, see Refs. 4 and 5; for the classic picture, see Refs. 6–8). In the early days of modern metallurgical research, it was found that perlitic steel becomes tougher if it is cooled more quickly from austenite. This behavior had been a mystery for a long time since pearlite was believed to be a "phase" because the fine laminate structure between the crystallographic phases ferrite and cementite, below 1 micrometer, could not be resolved by light microscopes. In a light microscope, one only observes a shiny appearance, from which we get the name "shining like a pearl."[9] Only after the invention of the electron microscope in 1932[10] were physicists able to reveal the lamellar structure of pearlite. A first explanation of the transformation process from austenite to ferrite and cementite, the so-called cooperative growth mode, was published by Clarence Zener in 1947.[6] Mats Hillert found the analytical solution in 1957.[7] The Zener–Hillert model of cooperative growth states that the supersaturation in austenite, due to the rejection of carbon from the growing ferrite, slows down growth. To remove this supersaturation, a fine lamellar width is needed, so that the carbon will have a short diffusion path to the cementite tip where it is needed to grow the cementite. A fine lamellar spacing favors growth. The second ingredient is the interface energy. For fine spacing, a large part of the driving
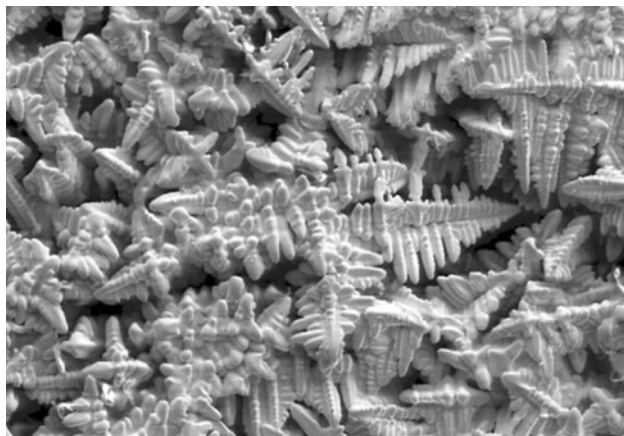
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Fig. 1. Typical equiaxed dendrites of a metallic alloy at about 20% solidification. The picture is taken from a pore where the interdendritic melt had been sucked out to preserve the dendrite. The interface branches out to form six arms for a cubic crystal, which again form secondary arms with a quite regular structure depending on the alloy and the solidification conditions.

force for the transformation is consumed by the creation of interfaces. This slows down the growth. There is an "optimum" spacing, according to Hillert's solution.

There remain basically two open questions: does this correspond to reality? If so, how does a pearlitic structure find the optimum spacing? Let me first answer the second question: it does not (in general). There was a long-lasting debate about a principle of "maximum growth" or "minimum undercooling," which would guide nature to a unique state. It is today established without doubt that such a principle does not exist, although it may be a working solution for engineering-type models. There is a full band of stable spacings around the optimal spacing, none of them being preferred over the others. This has been intensively studied for eutectic systems. Why not for the eutectoid system pearlite? This answers question one: the model is not able to make quantitative predictions for pearlite. The reason for this was already discussed by Hillert: because there is a large lattice misfit among austenite, ferrite, and cementite, which causes strong mechanical loads. To include these loads in the analytical solution of Ref. 7 was impossible and had to wait for an appropriate numerical tool. Imagine which? Let us continue first with the historical picture. Tiller in 1957 applied Zener's model to directional eutectic solidification. He formulated the picture of cooperative growth due to lateral redistribution of the solute—for eutectic solidification.[11] He got a standing ovation in October 1957 at the ASM weekend seminar held in Chicago, IL.[12] Jackson and Hunt showed in 1966[13] that the Hillert solution, originally developed for pearlite, perfectly matches their well-controlled experiments of the directional growth of a eutectic alloy. It is from that time on that Hillert's solution has been known as the

"Jackson-Hunt" solution, although these authors clearly reference the original work of Zener and Hillert. Their finding caused an "earthquake" in metallurgy. Many researchers who had been working on steel and pearlite started investigating eutectic growth, among those Wilfried Kurz and Rohit Trivedi. This was the birth of a new discipline: "solidification."

DENDRITIC SOLIDIFICATION AND THE PROBLEM OF ANISOTROPY

Solidification became the toy problem of materials scientists interested in basic physics, and of physicists interested in materials. Well-controlled experiments started to serve as benchmarks for mathematical models, which soon turned into numerical tools. In solidification, one deals with diffusion mainly in liquid: the diffusion in solid is lower than the diffusion in liquid for all substitutional elements by a factor of a 1000 and can safely be neglected. The temperatures are high, and the interface can be treated in local equilibrium for moderate solidification speeds. The interface energy anisotropy between the solid and the liquid is low for most metals. Therefore, crystallography can be neglected to first order. The only remaining problem is convection in liquid melts, but there are technical measures for coping with this problem (see below). Solidification problems can be posed in such a way that they can be correlated to theory, while in solid state not even the order of magnitude matches: the famous "factor of ten" in Hillert's pearlite solution.

Since eutectic solidification works so well, what about dendritic solidification? Here we have the "Ivantsov solution"[14] of a dendrite approximated by a paraboloid of revolution. This solution describes the growth problem in a moving coordinate system as a scale invariant, or self-similar, solution of the Peclet number $Pe = \frac{Rv}{D}$ with the growth speed of the dendrite tip v, the tip radius R, and the liquid diffusivity D. What does this mean? A slow dendrite may grow with a large radius, as well as a fast dendrite with a small radius. The transport solution does not select the scale. It was only natural to introduce the interface energy, or curvature, to fix the scale, as had been done very effectively in eutectic solidification, as described earlier. One had to subtract the energy dissipated by creating interfaces from the dissipation caused by diffusion. This idea had been introduced in 1960 by Temkin[15] and further developed by Trivedi.[16] And it failed! The isothermal dendritic growth experiments (IDGEs) by Martin Glicksman and co-workers[17,18] showed that dendrites grow with a much larger tip radius (and lower velocity) than predicted by the maximum growth hypothesis and a curvature corrected Ivantsov solution. A more than 20-year struggle to explain this phenomenon started. Steps in this struggle, all of them representing seminal scientific achievements, include the Mullins-Sekerka stability analysis of

transformation fronts,[19] the marginal stability hypothesis by Müller-Krumbhaar and Langer,[20–22] as well as space experiments under microgravity to suppress melt convection and g-jitter.*[23]

Today's accepted theory is the so-called microscopic solvability theory.[24] Briefly put, it states that the interface energy anisotropy (which is small for metals and therefore is neglected in most applications) becomes crucial for the close to self-similar problem of dendrite growth before the first-order perturbation (curvature) becomes active. The dendrite tip has a small protrusion compared with a perfect parabolic shape. This protrusion triggers the growth direction according to the crystallographically weakest interface orientation. The protrusion has to match in shape the microscopic fluxes of heat or solute parallel to the interface. This determines the scale. Has this become clear? The original paper of Ben Amar and Brener[24] presents sophisticated mathematical derivations and gives only an asymptotic solution. We would like to have a full solution. Therefore we need numerical solutions!

PHASE-FIELD AND THE PROBLEM OF ACCURACY

Numerical simulation in solidification is one of the success stories of the (relatively) new computer age. It started out with one-dimensional simulations of the heat transfer in a casting, including the latent heat. Latent heat makes the problem inherently nonlinear, and latent heat is almost 50% of the total heat content of a metallic melt poured into a mold. Nonequilibrium models of early solidification treating nucleation and kinetic control soon followed.[25] Academic software applications grew into commercially successful products. There had been many attempts to simulate dendrites in 3D by different techniques. The first promising one was by Ryo Kobayashi.[26] The simulated dendrite morphology was strikingly close to real dendrites at a time when supercomputers had less power than today's smartphones. Comparing the simulated dendrites with images from experiments, we note what is missing: the scale bar! In fact the early phase-field models for dendritic growth showed a clear dependence of scale on the choice of the interface width, which has to be taken large compared with its atomic scale.

There have been good alternative approaches, in particular in 2D: front tracking,[27] boundary integral methods,[28] and even cellular automata.[29] There is no reason in principle why these methods should not work quantitatively in 3D. Adaptive finite elements have also been applied to a good level of accuracy.[30] Most of these attempts have passed away in the last few years for practical reasons. Phase-field models with a thin interface asymptotic[31,32] won the race.
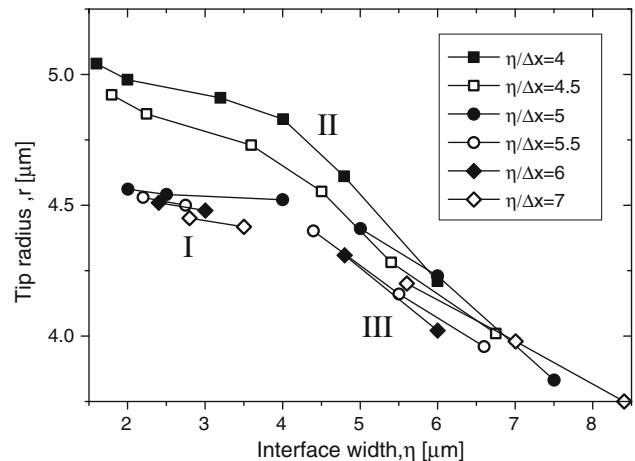

Fig. 2. Dendite tip radius in directional solidification under the conditions given in Ref. 33 versus the interface width, for different interface discretizations. Convergence is found if the interface width is smaller than the physical radius AND the numerical discretization of the interface is higher than five cells (set I). With a discretization of the interface width with fewer than five numerical cells, the evaluated radius decreases monotonically with increasing discretization (set II). For all calculations with an interface width comparable with or larger than the physical radius, the simulation results depend strongly on the width of the interface (set III). (Calculations by Mingming Zheng using OpenPhase,[35] unpublished).

Figure 2 shows a convergence study using the Karma model with a double-obstacle potential for directional solidification of an Al-Cu alloy under the conditions given in Ref. 33. The code and the conditions for this convergence study are available in Ref. 35. It clearly shows the range of appropriate numerical discretization by the independence of the predicted tip radius from numerical parameters.**

Similar studies have been performed by others. They must be good scientific standard in the future. Only then conclusive studies related to materials problems are possible. I'd like to highlight the work of Jon Dantzig and co-workers who have used additionally an adaptive mesh refinement to improve the numerical efficiency (see Fig. 3).

To conclude this section, phase-field simulations today are able to cope with the problem of scale in dendritic solidification in a quantitative manner. There is a "universal" shape of equiaxed dendrites, as shown by Karma in Ref. 31. There is a band of possible spacings in directional solidification with a critical limit of the lower spacing, as shown in Ref. 33. Needless to say, eutectic solidification can be well tackled by phase-field (e.g. Ref. 37). What is left?

BEYOND DIFFUSION CONTROL

The remaining questions concern real materials and processes. The previous examples are generic, which means they demonstrate a fundamental

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*This is the convection caused by the movement of the astronaut and other perturbations.

**The present study does not include interface preconditioning,[36] which might allow a lower discretization of the interface.
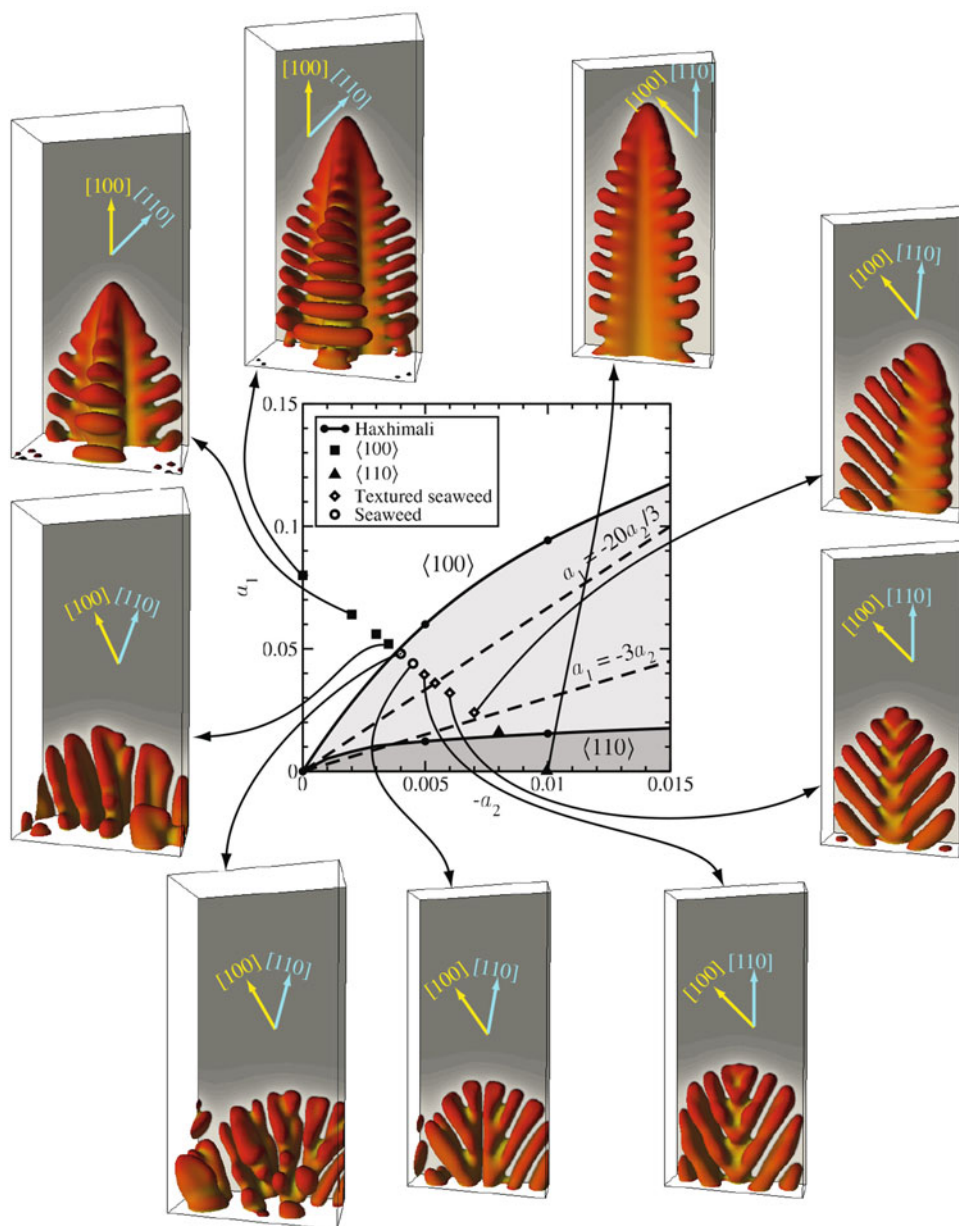
Fig. 3. Simulated microstructure development in directional solidification of Al-Zn alloys. The surface energy anisotropy as a function of the interface normal vector **n** is represented as $\gamma_{s\ell}(\mathbf{n}) = \gamma_{s\ell}^0 \left[1 + a_1\left(Q - \frac{3}{5}\right) + a_2\left(3Q + 66S - \frac{17}{7}\right)\right]$, where $Q = n_x^4 + n_y^4 + n_z^4$ and $S = n_x^2 n_y^2 n_z^2$ are the first two cubic harmonics. The figure shows the microstructure of the most favorably oriented dendrite with respect to the (vertical) pulling direction, for each pair of anisotropy parameters at the points indicated. The preferred growth direction begins as [100] for $a_2 \approx 0$, and then gradually rotates toward [110] as the parameters vary from left to right. The orientation aligns with [110] at the point where the minimum surface stiffness crosses over from [100] to [110]. Dantzig, private communication 2013. For details, see Ref. 34.

principle. The "proof of principle," in a theoretical physicist's view, is the only task. According to a materials scientist, however, it is a crucial step in model development. Having understood the universal nature of the principle, we want to apply our knowledge to material and process design problems. We want to use the numerical tools to cope with the questions of real materials and processes. There is an overwhelming body of new developments in phase-field methods (and other materials-science-related numerical methods) to be reported. A large number, probably incomplete, are quoted in recent reviews.[38–43] Please accept my apology for reporting only three examples that are related to my own research and go beyond diffusion control in phase transformations.

Rapid Solidification

Solidification is usually considered a diffusion-controlled transformation. This is due to the fast redistribution of the solute at the solidification front
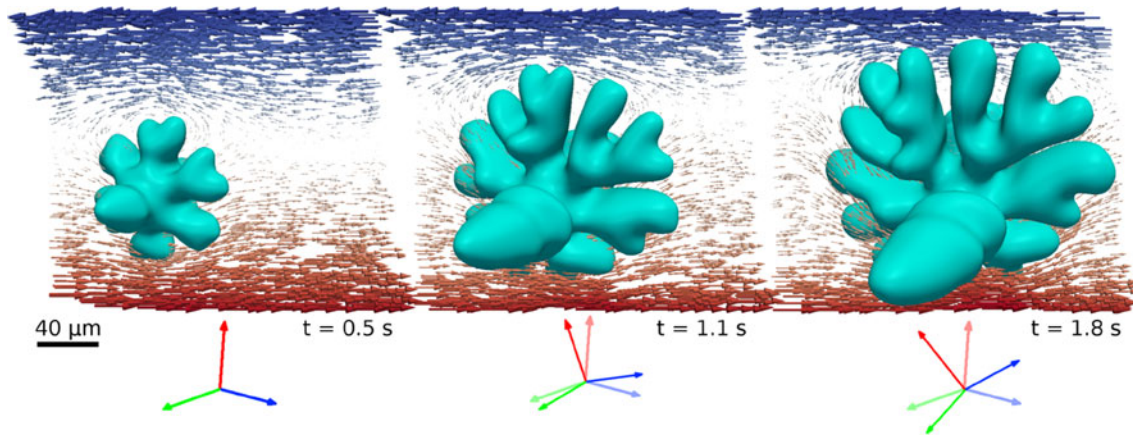
Fig. 4. Mg-Al dendrites in a shear flow imposed as a boundary condition. Due to the asymmetric forces acting on the dendrite, it rotates around all its axes in three dimensions, as indicated by the axis of abscissas (calculations by Oleg Shchyglo using OpenPhase,[35] unpublished).

at the elevated melting temperatures of metals. Then the solidification front can well be taken to be in a local thermodynamic equilibrium between the solid and the melt, corrected by the curvature undercooling. Kinetic undercooling can be neglected. Already in the early days of solidification, this picture was extended to include kinetic effects under the so-called "rapid solidification" condition.[44] Rapid solidification is either observed in strongly undercooled melts, where a solidification speed of up to $100~\mathrm{ms}^{-1}$ is reached[45] or in thin films prepared by melt spinning or splat cooling or solidification in a weld spot. No local equilibrium condition is established at the interface. Interface attachment kinetics become important[46] and solute trapping is observed: the partitioning of the solute between solid and melt decreases with increasing solidification speed. This effect is inherent in any phase-field model. A detailed study was given already by Wheeler, Boettinger, and McFaddeen in 1993.[47] Since then, it has become clear that the extent of the solute trapping depends strongly on the interface width used in the simulation. This means that a quantitative prediction of the solute trapping in a standard phase-field model is only possible if the interface width is discretized on the physical scale of the interface, which is for solidification of metals on the order of one nanometer.[†]

In one-dimensional simulations, Galenko and co-workers[48] have recently shown that a so-called hyperbolic phase-field model, which considers inertial effects within the interface, is able to predict a sharp transition to complete trapping in agreement with experiment. Here, the interface has been discretized on its physical nano-meter scale. Again, three dimensions are the challenge. Adaptive

methods (e.g., Ref. 49) may be applicable. An alternative approach is the newly developed phase-field model with finite interface dissipation by the author and co-workers.[50,51] This model is derived by coarse graining the interface region and introducing a redistribution flux between the phases that is controlled by the interface permeability introduced as an adjustable parameter dependent on the resolution on the mesoscopic scale. Adjusting this permeability in one dimension by comparison with the microscopic model[48] allows for quantitative simulation with a much reduced resolution. The details of this approach are published in Ref. 52.

Solidification and Melt Convection

Solidification has one serious problem that does not exist in solid state: melt convection. Some experiments may be well in the regime of diffusion control, but most are not. We might introduce the wording "transport-control," which means that transport in the bulk phases controls the solidification and the attachment kinetics (as described in the previous section) will be negligible. Then it is only a technical issue to consider advection in addition to diffusion. Models that have been elaborated for buoyancy driven convection, or advection driven by stirring, are available from the respective communities. The condition of "no slip" at a diffuse phase-field interface was worked out in 1999.[53] It has been shown how melt convection changes the scaling of a ripening mush[54] and how dendrites grow in forced convection in three dimensions.[39,49,55,56] It has been shown that the primary spacing of the columnar dendrites can vary by a factor of two depending on the orientation of growth relative to the direction of gravity.[57] Sedimenting dendrites have been a challenge for a long time. With today's computer facilities, this becomes a doable task. Figure 4 shows several stages of a Mg-Al dendrite in a shear flow. It turns around all its axes during growth, and it will adjust its position and

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[†]Physical solute trapping in rapid solidification and its treatment by the phase-field method should not be confused with the technique of anti-trapping for slow solidification,[32] although it is related from a technical viewpoint.
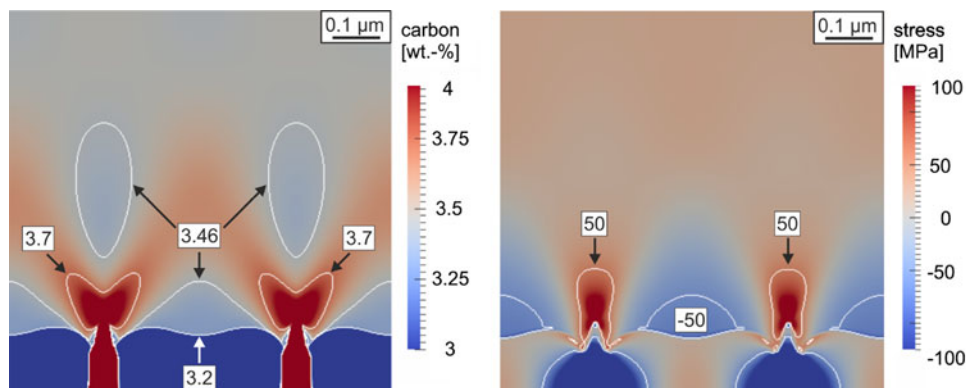
Fig. 5. Concentration (left) and stress distribution (right) at the pearlitic transformation front. Carbon forms a halo around the tip of the cementite needle. Compressive and tensile stress forms a stress dipole that drives diffusion uphill against the concentration gradient. Due to the redistribution of carbon between the compressed and expanded regions, the stress level remains below ±100 MPa, so that no plastic activity is expected (calculations by Adam Giessmann using OpenPhase,[35] unpublished).

orientation depending on the vicinity of other dendrites: a nucleated equiaxed grain in a melt will neither keep its position nor its orientation. This poses a challenge for the future.

Pearlite: Back to the Roots

In 2006, I met Rohit Trivedi, one of the pioneers in eutectic solidification, during the Euromat conference in Prague. I informed him about recent finding by phase-field simulations of pearlite formation.[58] These simulations investigate diffusion in the ferritic phase (which had been omitted in the analytical Hillert solution). The simulation showed that this contribution increases the transformation kinetics of pearlite by a factor of four (which had already been predicted by Fisher in 1950 in an analytic study[59]), but still leaving a significant gap with experiment. Rohit answered that he himself had started his career as a metallurgist working on pearlite transformation. He gave me the hint to look for strain effects in the solid state transformation. And he invited me to a symposium held in Ames in the same year, on the occasion of his 75th birthday. So I followed his advice to investigate strain effects in order to have a good story to tell. The result is striking: there is a stress dipole between the ferrite (which contracts during the transformation from austenite) and the cementite (which expands). This stress dipole produces an enormous gradient of hydrostatic stress in the austenite, which drives a strong flux of carbon against the chemical gradient. The model, as published in Ref. 4, has many shortcomings, namely, the two-dimensional approximation, the oversimplified anisotropy model for the interface between the cementite and the austenite, and the neglect of interface diffusion. Also the calculation domain is very small and no variation of spacing has been considered. Furthermore, a sound numerical study of the resolution is missing. These shortcomings led to the statement of Asta et al.,[60] who summarized the 2006

Trivedi symposium, that the model predictions should be consolidated by further experimental and theoretical investigations. Those are actually in progress. Although the full quantitative correspondence may be under debate, the principal mechanism is certain: the gradient of hydrostatic stress in the austenite, caused by the expansion–contraction dipole of the ferrite and cementite, drives carbon away from the supersaturated zone ahead of the ferrite (which is under compression) into the zone ahead of the cementite (which is under tension). There it is needed to form the carbide phase and cementite grows from a highly supersaturated and expanded austenite. This mechanism is explained in Fig. 5 (compare with a recent reconsideration of the problem in Ref. 5). The active mechanisms have been hypothesized for a long time. Phase-field is able to bring them together and herewith closes the cycle of this story.

CONCLUSION

Solidification and phase-field are tied together. Pearlite posed the challenge. Relaxing the complexity of the problem to eutectic solidification allowed quantitative verification of early transformation models by experiment. Phase-field emerged as the numerical technique for solving solidification models, whether eutectic, dendritic, or others, in three dimensions. It combines numerical efficiency with rigorous theoretical derivation by coarse graining a microscopic thermodynamically consistent principle.[43] Today we are able to attack new challenges: solid state transformations and transformations in general with more than one single dissipation mechanism. Modern phase-field models are combined with advanced models for transport in bulk: multicomponent diffusion with cross-effects, transport by advection, strain-driven diffusion, and plastic activity.[61,62] Such advanced models will be able to cope with the challenges of real materials and will be

used as predictive tools for material and process optimization.

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