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Modeling for Environmentally Conscious Manufacturing

Ch. Charbon and Richard A. LeSar*

Abstract

This is the final report of a one-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The goal of this project was to begin development of tools needed for the creation of an integrated simulation tool to help the development of environmentally benign advanced manufacturing. The specific manufacturing process chosen as our first example in this project was casting. The objective was to develop better models for the solidification process and to couple those into heat/fluid flow codes as the first step in the development of an advanced casting-simulation tool. There were a number of accomplishments in this project, each focused on a different aspect of solidification and its connection to manufacturing processes: (a) development of a coupled microstructure/heat flow model for equiaxed eutectic solidification, (b) development of a coupled microstructure/heat flow model for quiescent crystallization of semicrystalline polymers, (c) development of a model of the directed light fabrication process, and (d) direct modeling of dendritic growth.

1. Background and Research Objectives

This project was focused on creating an integrated simulation tool for environmentally benign advanced manufacturing. The specific manufacturing process chosen as our first example in this project was casting. The objective was to develop better models for the solidification process and couple those into heat/fluid flow codes as the first step in the development of an advanced casting-simulation tool. The ultimate goal was to develop simulation tools that would help create manufacturing methods to yield very tightly controlled materials properties (distortion, residual stresses, etc.) for materials that (may) include effects of grain orientation and anisotropy (texture) while minimizing the time and (environmental) cost associated with materials development. Thus, the simulation tools must be based on microstructural descriptions of materials properties.

The ability to control that microstructure in a manufacturing process is often critical in terms of overall materials quality, efficiency, and cost. For example, manufacturing of many materials must be done with extremely tight control of final shape and surface finish,

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alloy composition and uniformity, porosity, residual stresses, and strength, and crystal grain size distribution and morphology. The traditional approach to developing new materials and manufacturing processes, involving many trials and measurements, is unacceptable. There are too many processing parameters and the environmental cost of each trial is often too high. The coupling of advanced process modeling with the materials development process, both manufacturing and experimental verification, is thus essential.

Casting and solidification of molten metals and metal alloys is often a critical step in the production cycle, as it provides a means to create near-net-shape parts, thus avoiding machining with its additional waste stream. However, major problems with the quality of cast parts can arise because of the difficulty of preventing variations in the alloy content, the generation of porosity or poor surface finish, and the loss of microstructure-controlled strength and toughness resulting from the poor understanding and design of the mold filling and solidification processes.

The use of modeling to study solidifying materials is reasonably well developed, at least at the level of predicting what region of a sample is solid and what is fluid. However, we cannot yet predict what the final-state microstructure (distribution of defects, grains, etc.) of a solidified material will be. Yet that microstructure largely determines the properties of a material. Development of processes that yield a desired microstructure may require many trials, with consequent waste. Avoiding such trials is essential. In this project we worked on one specific part of that problem, namely the modeling of solidification processes in complex fluid and heat flow.

2. Importance to LANL's Science and Technology Base and National R&D Needs

This work will have an impact for both the future weapons complex and for industry. Development of environmentally conscious manufacturing is largely dependent on the use of simulations and modeling to greatly reduce the number of trials in the development process. This project will aid in the development of such predictive tools for metals casting. The type of manufacturing investigated in this project is critical to the development of the Advanced Design and Production Technology (ADaPT) program and is specifically called out for in the Accelerated Strategic Computing Initiative (ASCI) program plan. Industry has long faced the problem of casting materials with well-controlled properties. Our LDRD work is helping put Los Alamos in a leadership position in the area of materials process modeling. Linking microstructural-level models to continuum codes is a critical technology and a major goal of the recently formed virtual Center for Materials Process Modeling.

This project supports three of the Los Alamos core technical competencies. There is an obvious connection to the theory, modeling, and high-performance computing core competency. The project is also closely linked to the nuclear weapons science and technology core competency. The results of this work also support the nuclear and advanced materials core competency through more efficient and better materials processing.

3. Scientific Approach and Accomplishments

There were a number of accomplishments in this project, each focused on a different aspect of solidification and its connection to manufacturing processes.

A. *Equiaxed Eutectic Solidification*

We developed a model of equiaxed eutectic solidification that couples the microstructural level (nucleation, growth and impingement of the grains) with the macroscopic level of heat flow. A Finite Difference Method (FDM) is used at the macroscopic scale to compute the temperature field of a solidifying part. At the microscopic scale, individual grains are modeled and their evolution is tracked as a function of time. A strong coupling between the two levels is insured by the fact that the temperature field drives the nucleation and growth of the grains. The growth of the grains, in turn, releases latent heat which modifies the thermal field.

As an example, we consider the simple case of a rectangular (i.e., two-dimensional) sample that is insulated on the top and sides and cooled from the bottom. We consider the solidification of an alloy that solidifies with an equiaxed eutectic microstructure. We introduce a macroscopic mesh and solve the heat flow equations in the usual way at the mesh nodes. How our calculations differ from the usual approaches is in how we deal with solidification, where we have a microstructurally-based approach. We introduce possible solidification nucleation sites randomly throughout the sample. These sites are triggered (i.e., a solid nucleated) when the undercooling at these sites reaches a critical value. The critical undercooling for each site is chosen randomly such that the population of sites follows an empirical nucleation law. The grains then grow in a circular way. Eventually grains impinge on their neighbors. Growth stops at the points of contact, leading to noncircular grains in the final microstructure. The growth affects the heat flow due to the latent heat released on solidification. We connect the microstructural level to the macroscopic heat-flow mesh by apportioning the heat released in the solidification to the surrounding mesh nodes with a bilinear interpolation. The net heat flow equation is given by

$$\text{div}(\kappa \text{ grad} T) = \rho c_p \frac{dT}{dt} - L \frac{df_s}{dt} , \quad (1)$$

where κ is the thermal conductivity, T is the temperature, ρc_p is the volumetric specific heat, t is the time, L is the volumetric latent heat and f_s is the volumetric fraction of solid.

The principal outputs of the model are: temperature field, solid fraction field, and detailed picture of the microstructure. The detailed picture of the microstructure (Figure 1) enables us to analyze any microstructural parameter of interest such as grain density, grain size distribution, and grain asymmetry. This work is described in detail in two publications [1,2].

B. Quiescent Crystallization of Semicrystalline Polymers

We developed a multiscale model for the crystallization of polymers [3-5]. This model accounts for heat diffusion at the macroscopic scale, grain nucleation, growth and impingement at the mesoscopic scale and fibrils growth at the microscopic scale. The model is based on a front-tracking method coupled with a cellular discretization to track the microstructure evolution. The model can predict not only the shape and size distribution of the spherulites in the sample, but also the shape of the lamellae within each of the spherulites. It is also the first model that accurately models the impingement between spherulites and inclusions for a macroscopic sample.

The heat flow equation governing this solidification process is the same as for metals (Eq. 1). What differs is the way the solids grow, leading to different solidification microstructure. Instead of the simple equiaxed growth that we modeled in the solidification of the eutectic alloy (discussed in section A above), in semicrystalline polymers the dominant microstructural features are spherulites, which are aggregates of crystalline plate-like lamellae that grow radially from a nucleation center. We developed a microstructural method, similar to that for metals, to track the growth of the spherulites and that considers individual lamellae. However, we found that the use of a front-tracking procedure greatly increased the efficiency of our calculations. The front tracking method assumes that the interface between the spherulite and the melt grows normal to itself with a velocity given by the local temperature at each position along the interface. This is equivalent to Huygens's principle in optics.

A simulation proceeds in a somewhat similar way to that discussed above for equiaxed grain growth in metals. We introduce three distinct length scales: a coarse grid

for heat diffusion, a fine grid for tracking the solid fraction evolution, and an unstructured grid for tracking the shape of individual spherulites and the lamellae within them (Figure 2). A key to the method is that the meshes are independent of each other. The shape of the spherulite is found from the front tracking method (Fig. 2c). If the center of a cell lies within the growing spherulite, it is considered solid. From the state (solid or liquid) of each cell, the solid fraction can be easily determined. Information (latent heat, temperature) is passed from the small mesh to the coarse, heat-diffusion, mesh through a bilinear interpolation (Fig. 2b). At the beginning of the calculation, nucleation sites are distributed randomly in space throughout the melt. These nuclei are triggered when the undercooling reaches a critical value and a small, circular, spherulite is generated at that site. The spherulites grow and eventually impinge. The critical undercooling for each site is chosen randomly such that the population of sites follows an empirical nucleation law.

The principal outputs of the model are: temperature field, solid fraction field, and a detailed picture of the microstructure. In Figure 3, we show an example of the prediction of microstructure for a simple solidification geometry. In Figure 4, we see the microstructure resulting from the growth of a spherulite around a rectangular obstacle, where we compare experiment with our modeling results. The radial lines are the lamellae. The lines perpendicular to the obstacle are the contour of the spherulite at different time intervals. On the right of the obstacle, we reproduce precisely the occurrence of an intrinsic grain boundary produced by the impingement of the two parts of the same spherulite coming from two different sides of the obstacle.

C. Modeling of the Directed Light Fabrication process

An important new manufacturing technique developed at Los Alamos involves directed-light fabrication, in which a computer-guided laser melts a powder in a series of strips of a defined shape, slowly building up to a prescribed final shape. Many materials can be used in this process. The advantage is that there is little waste and the final part is near net shape. This is a new method, and much is left to understand about the thermal distribution within the growing part.

We developed a thermal code with an adaptive mesh that accounts for heat flow (laser input, radiative and convective losses, conduction) and mass deposition at the top of the sample. The model predicts the thermal field within the growing part, enabling one to compute the cooling rate and the thermal gradient, factors that dictate the microstructure size. The work is described in publication [6].

D. Direct modeling of Dendritic Growth

We developed a model that reproduces the growth of solutal dendrites. The solid-liquid interface evolves as a free boundary, constrained only by solute diffusion and curvature. The model reproduces qualitatively the destabilization of a spherical nuclei into a dendritic grain with primary, secondary and tertiary dendrite arms. This work is ongoing.

Publications

1. Ch. Charbon and R. LeSar, "A 2D Micro-Macro Model of Equiaxed Eutectic Solidification," accepted in MSMSE, (1996).
2. Ch. Charbon and R. LeSar, "A 2D Fully Coupled Model of Equiaxed Eutectic Solidification," JIM '95 Fall Annual Meeting, "Solidification and Processing," I. Ohnaka and D. M. Stefanescu, editors, (TMS, Warrendale, PA, 1996).
3. Ch. Charbon and S. Swaminarayan, "A Multiscale Model of Polymer Crystallization, I Growth of Individual Spherulites," submitted to Polymer Engineering & Science (1996).
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5. Ch. Charbon and S. Swaminarayan, "Modeling the Microstructure Evolution of Thermoplastic Composites," submitted to Materials Science and Engineering (1996).
6. D.J. Thoma, Ch. Charbon, G.K. Lewis and R.B. Nemec, "Directed Light Fabrication of Iron-Based Materials," Advanced Laser Processing of Materials - Fundamentals and Applications, MRS, Pittsburgh, to appear, (1996).

Figure 1. Simulated microstructure at different times during the equiaxed eutectic solidification of gray cast iron. The dashed line indicates the position of the equilibrium eutectic temperature.

Figure 2. Schematic representation of the three levels of discretization used in the study of polymer solidification: (a) a coarse grid for heat diffusion, (b) a cellular grid (shown as fine lines) for microstructural evolution, and (c) an unstructured grid (shown as open circles) for shape evolution of individual spherulites. The latent heat is calculated by mapping the shape of the spherulite onto the cellular grid as gray cells in (b) and (c). The coupling between the different length scales (required for the calculation of the temperature at the solidification front and the distribution of the latent heat released at the cellular level among the four surrounding heat diffusion nodes) is achieved by means of a bilinear interpolation and is shown by the arrows in (b).

Figure 3. Final microstructure of a solidified plate showing the shape and nucleation centers of the spherulites. The size of the plate is 20 mm x 10 mm. The gray border on three sides of the plate indicates adiabatic boundaries.

Figure 4: The microstructure resulting from the growth of a spherulite around a rectangular obstacle. The top figure is from experiment and the bottom from our simulation results. The radial lines are the lamellae. The lines perpendicular to the obstacle are the contours of the spherulite at different time intervals. Note that on the right of the obstacle, we reproduce precisely the occurrence of an intrinsic grain boundary produced by the impingement of the two parts of the same spherulite coming from two different sides of the obstacle.