Chapter 1
Introduction

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1 General

Material scientists originally devoted most of their efforts to studying the solid state of materials, their microstructure, and their mechanical and thermal properties. However, in the last 10–20 years, a change in paradigm has taken place, and the importance of the liquid phase has been recognized. In this regard, it is interesting to note that almost 100% of all metallic products are, at some stage, produced through solidification and casting processes. Consequently, this field of new materials, processes, and products constitutes a major backbone to industries worldwide.

Solidification from the melt leaves its fingerprints in the final material, and hence it is of utmost importance to understand the properties of the molten state and its solidification behavior. The prominent feature of fluids, namely, their ability to flow and to form free surfaces, poses the main difficulty in their theoretical description. The physics of fluids is governed by the Navier-Stokes equation and by the ubiquitous presence of convection. In addition, when dealing with metallic materials, the high temperatures involved lead to experimental difficulties, the most trivial but also most fundamental being the suitability of available containers.

Besides the atomic scale inherent to condensed matter and the intermediate scales associated with the solidification microstructures, fluid flow driven by gravity generally occurs in the melt at the macroscopic level so that the relevant length scales in casting are widespread from the atomic size (capillary length, crystalline defects such as dislocations, attachment of atoms, etc.) to the meter size of the ingot (fluid flow, spacing of dendrite side branches, etc.).

Accordingly, to produce materials that meet ever-higher specific requirements and performance, the solidification processing of structural and functional materials

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has to be controlled with ever-increasing precision. It can be foreseen that materials for tomorrow will be optimized in their design and underlie more efficient production conditions, availability of scarce resources, and cleaner processes.

The interactive feedback between experiments and sophisticated computer simulations developed within the last 10 years that now drives the design and processing of materials is reaching performances never been seen in the past. Thus, it becomes possible to control and optimize the defect and grain structure at critical patches of components. Here, two major aspects are most essential for the continued improvement of materials processing with increasing requirements on composition, microstructure, and service achievements, which often implies the breaking of technology barriers:

- The reliable determination of the thermophysical properties of metallic melts in order to understand the fundamentals of complex melts and their influence on the nucleation of ordered phases.
- The reliable determination of the formation and selection mechanisms at microstructure scales in order to understand the fundamentals of casting and other solidification processes (foundry, welding, brazing, atomization,...). This also requires accurate knowledge of thermophysical properties.

2 Scientific Challenges

Casting is a non-equilibrium process by which a liquid alloy is solidified. The liquid-solid transition is driven by the departure from thermodynamic equilibrium, where no change can occur. From the standpoint of physics, casting thus belongs to the vast realm of out-of-equilibrium systems, which means that, rather than growing evenly in space and smoothly in time, the solid phase prefers to form a diversity of microstructures.

Actually, the relevant length scales in casting are widespread over ten orders of magnitude. At the nanometer scale, the atomic processes determine the growth kinetics and the solid-liquid interfacial energy, and crystalline defects such as dislocations, grain boundaries, and voids are generally observed. Macroscopic fluid flow driven by gravity or imposed by a stimulus (electromagnetic field, vibration, etc.) occurs in the melt at the meter scale of the cast product. The characteristic scales associated with the solidification microstructures are mesoscopic, i.e., intermediate, ranging from dendrite tip/arm scale (1–100 μm) to the grain size (mm–cm). It follows that the optimization of the grain structure of the product and inner microstructure of the grain(s) during the liquid-to-solid phase transition is paramount for the quality and reliability of castings, as well as for the tailoring of new advanced materials for specific technological applications.

On this basis, the quantitative numerical simulation of casting and solidification processes is increasingly demanded by manufacturers, compared to the well-established but time-consuming and costly trial-and-error procedure. It provides a

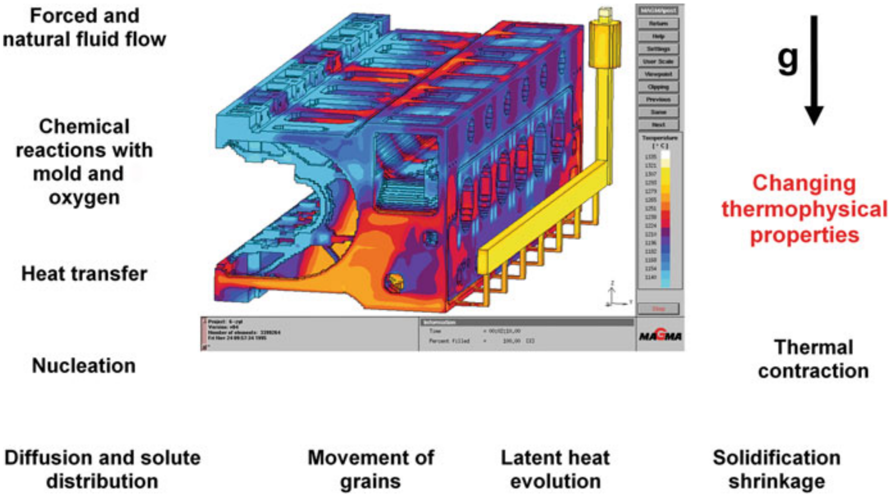

Fig. 1.1 A wide range of fundamental events during casting of complex components – here, a car engine with varying local temperatures. (Courtesy MagmaSoft)

rapid tool for the microstructural optimization of high-quality castings, in particular where process reliability and high geometric shape accuracy are important (see, e.g., Fig. 1.1 exhibiting cast structural components and the temperature distribution during casting of a car engine block). Any improvement of numerical simulation results in improved control of fluid flow and cooling conditions that enable further optimization of the defect and grain structure as well as stress distribution at critical patches of components. Through the control of unwanted crystallization events, it becomes even possible to produce completely new materials with a controlled amorphous (glassy) or nanocomposite structure.

3 Microgravity Space Conditions and Containerless Processing

The paucity of thermophysical property data for commercial materials as well as materials of fundamental interest is a result of the experimental difficulties arising at high temperatures. Some of these data can be obtained more or less accurately by conventional methods, in particular for non-reactive metals such as noble metals. High-precision measurements, however, on chemically highly reactive melts at the temperatures of interest require the application of containerless processing techniques and the use of high-precision non-contact diagnostic tools.

By eliminating the contact between the melt and a crucible, accurate surface nucleation control and the synthesis of materials free of surface contamination become possible. For highly reactive metallic melts, electromagnetic levitation

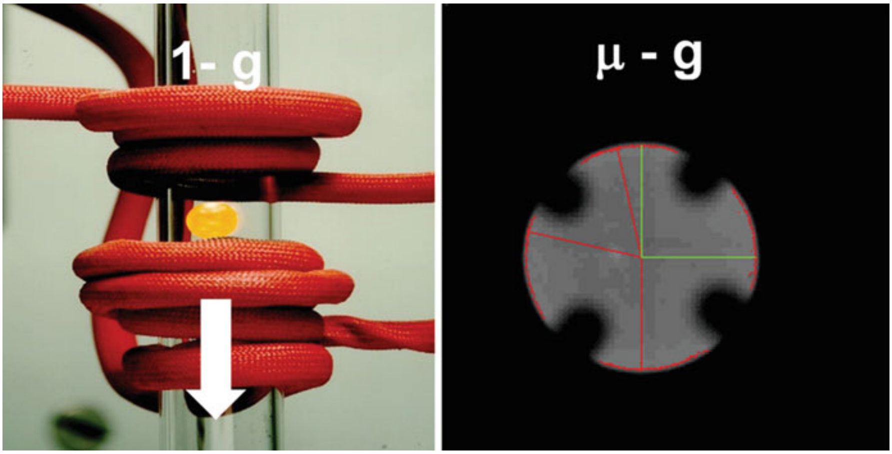

Fig. 1.2 Electromagnetic processing on the ground (left) and in microgravity (right) – the latter allowing controlled investigations of fully spherical liquid metallic samples (6.5–8 mm diameter) with a wide range of sophisticated analytical equipment. (Courtesy DLR)

(EML) is a well-developed containerless technique that offers several advantages over alternative levitation methods (electrostatic levitation, gas-phase levitation) due to the direct coupling of the high-intensity radiofrequency electromagnetic field with the sample.

Ground-based experiments using electromagnetic levitation have achieved limited success in measuring thermophysical properties of liquid alloys, since the high electromagnetic field B required to lift the sample against gravity (Lorentz force $F \propto \nabla B^2$) also causes excessive heating and turbulence due to induced eddy currents. In contrast, under microgravity conditions, much smaller levitation forces are needed since the force of gravity no longer has to be overcome. In fact, in space, only a weak positioning field is required.

This means that heating effects, magnetic pressure, melt turbulence, and asphericity of the molten drop are significantly reduced, allowing considerably more accurate results to be obtained or making such experiments possible at all. As an example, Fig. 1.2 shows a comparison between a specimen levitated in a ground-based em-levitation (left) and a liquid specimen positioned under reduced gravity conditions in an em-levitation device on board a parabolic flight (right). As compared to the specimen levitated on the ground, the specimen positioned under reduced gravity exhibits no detectable deviation from a spherical shape.

The motivation for performing benchmark experiments in the microgravity environment thus is straightforward and at a high level of scientific innovation. Firstly, in space it is possible to suppress the gravity-induced effects of fluid flow and more subtle sedimentation effects during solidification. Therefore, the contribution to fluid flow and heat transport in the melt can be investigated without the complications of buoyancy-driven thermo-solutal convection and sedimentation/flotation.

Secondly, the space environment on long time scales allows the application of containerless processing techniques, such as electromagnetic levitation. Levitated melts can be controlled effectively at temperatures up to 2200 °C, which in turn enables critical liquid parameters to be measured much more accurately and in a larger temperature range as compared to the earth laboratory.

Experience with parabolic flights (μg duration 10–20 s) and TEXUS rocket flights (μg duration ca. 180 s) already indicated that some aspects of the experiments could be successfully performed, but μg times are far too short to reach thermal equilibrium and measurements in the adiabatic regime. Expanding the experimental time-temperature window through the use of the International Space Station (ISS) opens a completely new realm of space experimentation. The main advantages in this regard can be summarized as follows:

- Avoidance of any chemical reactions with a metallic or ceramic container
- Decoupling of electromagnetic heating and positioning fields, therefore minimized levitation forces and, thus, controlled heating and reduced liquid convection in comparison with 1-g gravity conditions on earth
- Achievement of fully spherical samples
- Control of the sample environment (and cooling rate) in vacuum (better than 10^{-8} Torr) or inert gas atmosphere
- Extended periods of processing time (>10,000 s) in a temperature range between 700 and 2200 °C.
- Considerably improved accuracy of the measurements.

4 Experimental Program

The processing of metallic alloys (a combination of two or more elemental metals) through melting and casting techniques, whereby the molten material is poured or forced into a mold and allowed to harden, was invented several thousand years ago. Today, this processing is still an important step in the industrial production chain for a wide range of products. The end products often need to perform well and retain their integrity under extreme circumstances, particularly when used at high temperatures or when the product must be as light as possible in order to conserve energy. To produce these high-performance materials, the process must be closely controlled for the sake of both optimal design and efficiency of production.

The production and fabrication of alloys together with the casting and foundry industry generate a considerable amount of wealth. For example, the 10 million tons of castings produced in 1 year within the European Union is worth about 20 billion Euros. To continue generating this kind of turnover, the casting and foundry industry relies on the design and creation of advanced materials, which is accomplished by using sophisticated computer codes to control the metallurgical processes. These days everyone is looking for the next great breakthrough that leaps forward in technology that revolutionizes the way business is done. The answer may lie in a surprising place: space. In the last years, a scientific program has been established by the European Space Agency (ESA) using weightlessness as an important research tool on parabolic flights, on sounding rockets, and, most recently, on the International Space Station.

Experiments performed in microgravity enable the study of the relevant volume and surface-dependent properties free of certain restrictions of a gravity-based environment. In space it is possible to suppress gravity's effects on the flow of molten metals and on sedimentation during solidification. Without gravity's interference, it is possible to isolate other properties for investigation, such as diffusion and how it contributes to mass and heat transport in the melt without the gravity-associated complications of certain solute ingredients being more buoyant than others.

Using advanced experimental techniques to gather data on the intricate processes of melting and casting brings us closer to the design of new materials with better performance. Such advanced products can range from meter-sized objects to micrometer-sized powders, for example:

- Energy-efficient turbine components for the aerospace industry and land-based power plants.
- Powder production to improve catalytic performance of modern fuel cells and advanced combustion engines.
- High-strength metals with added functionalities.
- Precision casting of detailed shapes for electronic casings.
- Low-weight and high-strength materials for modern space vehicles within the space exploration programs.
- Medical implants.

In order to perform the necessary experiments, it is important to have access to extended periods of reduced gravity. A crucial ISS facility is the electromagnetic levitator (EML). As fantastic as it sounds, this equipment does precisely what the name implies: levitated molten metals. The EML permits containerless melting and solidification of alloy samples. Furthermore, the EML is equipped with highly advanced diagnostic tools that permit accurate measurements of thermophysical properties, as well as direct observation of the experiment during flight by high-speed videography.

As the products we make become more sophisticated, it follows that their production processes must keep up. Advancements in liquid processing techniques have enabled the industry to create products such as jet engines, spacecraft, and medical implants, but society's push for continually stronger, lighter, and more efficient products requires that next great leap.