21

Materials Science

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21.1 Introduction

Materials science is an interdisciplinary field dealing with the properties of matter and its applications to various areas of science and engineering. This science investigates basically the relationship between the structure of materials and their various properties. It includes elements of applied physics and chemistry, as well as chemical, mechanical and electrical engineering. With significant attention to nanoscience and nanotechnology in recent years, materials science has been propelled to the forefront [1].

The research—from a fundamental and applied point of view—is concerned with the synthesis, atomic structure, chemical element distribution and various favorable properties of materials and structures. The basic understanding and optimization of properties and structures is further supported by sophisticated computer models from the nano- to the macroscale and leads to a manifold of applications in industrial products. Prominent examples are found in the aerospace, automotive, biomedical, energy and microelectronics industries.

The interactive feedback between experiments and sophisticated computer simulations developed within the last ten 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. In this regard, two major aspects are most essential:

- the reliable determination of the **thermophysical properties** of metallic melts for industrial process design in order to understand the fundamentals of complex melts and their influence on the nucleation and growth of ordered phases, together with

- the reliable determination of the formation and selection mechanisms at microstructure scales in order to develop **new materials, products and processes**.

As a result, fresh insights into alloy solidification/processing can be gained with the potential of producing novel materials and structures, i.e., materials processed and designed in space [2, 3].

21.2 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 10 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 rapid tool for the microstructural optimization of high-quality castings, in particular where process reliability and high geometric shape accuracy are important (see, for example, Figure 21.1 exhibiting cast structural components and the temperature distribution during casting of a car engine block). Any improvement of numerical simulation results in an improved control of fluid flow and cooling conditions that enables further optimization of the defect and grain structure as well as mechanical stress distribution.

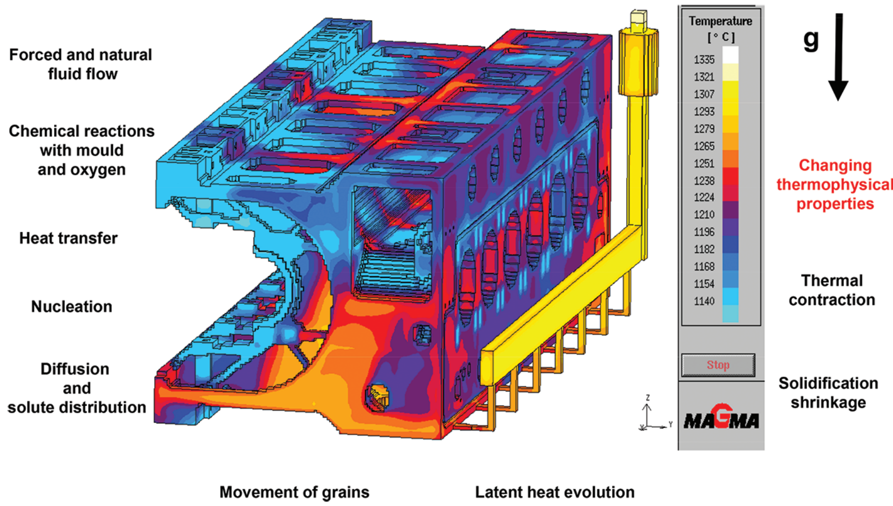


Figure 21.1 A wide range of fundamental events during casting of complex components, here a car engine with varying local temperatures.

During processing from the melt crystal nucleation and growth is in most situations the first step achieved by cooling of liquid below its thermodynamic equilibrium solidification (liquidus) temperature. Alternatively, when the formation of nuclei fails, or the growth of nuclei is very sluggish, there is formation of a metallic glass at the glass transition temperature. If the crystal nucleation rate is sufficiently low and if the growth of nuclei is sufficiently slow over the entire range/state of the undercooled liquid below the liquidus temperature, eventually the liquid freezes to a non-crystalline solid—a glass.

In particular, new metallic glasses that can be produced in large dimensions and quantities now—the so-called bulk metallic glass or super metals—are emerging as an important industrial and commercial material, superior to conventional Ti, Al- or Fe-based alloys. They are characterized by several times the mechanical strength (up to 5 GPa) in comparison with conventional materials, excellent wear properties and corrosion resistance due to the lack of grain boundaries (see Figures 21.2, 21.3).

21.3 Specifics of Low-Gravity Platforms and Facilities for Materials Science

Fresh insight into the stable and metastable undercooled liquid state and metallic alloy solidification can be gained with the potential of engineering

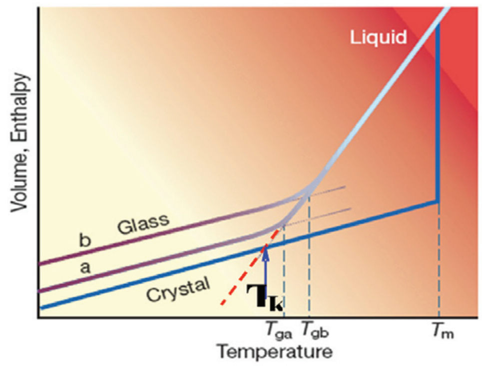


Figure 21.2 Volume and enthalpy of a glass-forming alloy as a function temperature and undercooling.

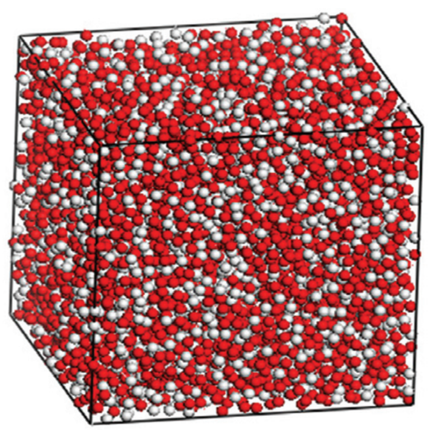


Figure 21.3 Atomic structure in an MD simulation of a Or-Cu glass [1].

novel microstructures. To perform these experiments, it is important to have access to extended periods of reduced gravity.

21.3.1 Parabolic Flights

Parabolic flights generally provide about 20 seconds of reduced gravity. For materials science experiments at high temperatures, this time is barely sufficient for melting, heating into the stable liquid and cooling to solidification of most metallic alloys of interest in a temperature range between 10,000–2,000°C. Surface oscillations can be excited by a pulse of the heating field, and the surface tension and viscosity are obtained from the oscillation

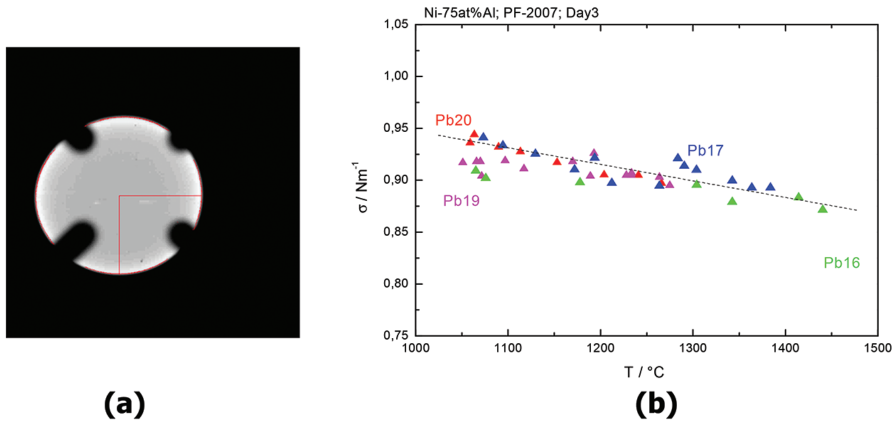


Figure 21.4 (a) Video image of a fully spherical liquid sample of a NiAl alloy in EML obtained on a parabolic flight for surface tension and viscosity measurements of liquid metallic alloys, (b) Surface tension of a drop of molten Ni-75 at.% Al.

frequency and damping time constant of the oscillations, respectively. Processing must be performed in a gas atmosphere under convective cooling conditions. Under these conditions, however, thermal equilibrium of the melt cannot be reached.

Using the Electromagnetic Levitator, surface oscillations of the liquid hot drop with diameter of 8 mm (Figure 21.4a) can be, for instance, introduced by an electromagnetic pulse and the results analyzed by a high-speed high-resolution video camera. Among the results, Figure 21.4b shows the surface tension as a function of temperature in the range 1050–1450°C of liquid Ni–75 at.% Al processed under low gravity on four parabolic flights with 10 seconds of processing time each.

21.3.2 TEXUS Sounding Rocket Processing

TEXUS sounding rockets offer a total of 320 seconds of reduced gravity which is typically split between two different experiments. As compared to parabolic flights, the microgravity quality is improved by far. Stable positioning and processing of metallic specimen with widely different electrical resistivity and density was achieved in different sounding rocket flights with an adapted electromagnetic levitation device. In Figure 21.4, the temperature-time profile of the Fe alloy processed successfully in TEXUS 46 EML-III is shown as an example. However, also under these conditions thermal equilibrium or steady-state conditions of the liquid phase cannot be attained due to the limitations in processing time.

21.3.3 Long-Duration Microgravity Experiments on ISS

A series of microgravity research is now commencing onboard the ISS in a number of multiuser facilities afforded by major space agencies, such as the European Space Agency (ESA) in the Columbus module. The short microgravity time on parabolic flights and TEXUS sounding rocket experiments necessitates forced convective cooling to solidify the specimen before the end of the microgravity time. As a consequence, long-duration microgravity measurements are needed for accurate calorimetric and thermal transport property measurements over a large temperature range. It can be expected that the following properties necessary for a full and thorough analysis of solidification processes will be performed at varying temperatures (ThermoLab-ISS program: an international effort sponsored by several national agencies including ESA, DLR, NASA, JAXA, SSO).

Furthermore, in Materials Science both directional and isothermal solidification experiments will be performed in the Materials Science Laboratory (MSL, see Figure 21.5) using dedicated furnace inserts, with the possibility of applying external stimuli such as a rotating magnetic field to force fluid low in a controlled way. The electromagnetic levitator (EML) will enable

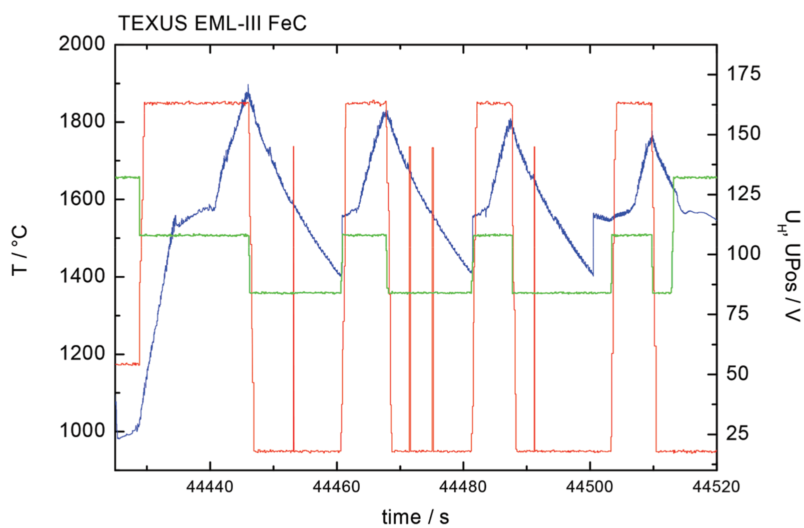
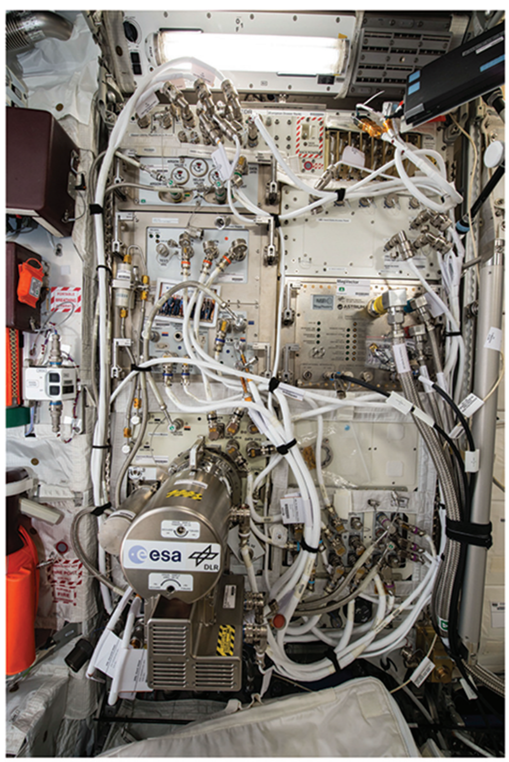


Figure 21.5 Temperature-time profile of Fe-C alloys processed on the TEXUS 46 EML-III sounding rocked flight with temperature scale (left) and heater and positioner voltage (right ordinate).

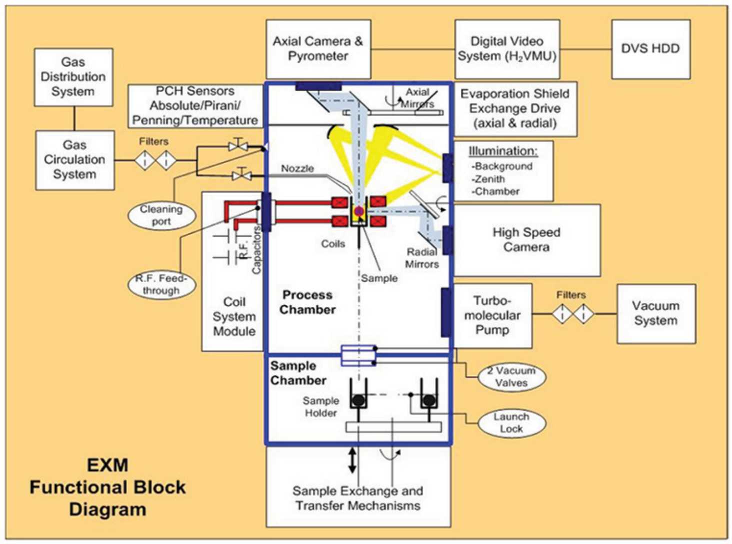
containerless melting and solidification of alloys and semiconductor samples. The EML is equipped with highly advanced diagnostic tools (Figure 21.6).

21.4 Materials Alloy Selection

For a wide range of new products in the industrial production chain, solidification processing of metallic alloys from the melt is a step of uppermost importance. On this basis, several types of alloys have been selected for the following fields of usage, for example, turbine blades for land-based power plants and for jet engines sustaining high temperatures and high stress levels, low-emission energy-effective engines for cars and aerospace, functional materials with improved performance, the so-called super metals (bulk metallic glass) with ultimate strength to weight ratio and new low-weight and high-strength materials for space exploration and future space vehicles.



(a)



(b)

Figure 21.6 Schematic presentation of (a) the Materials Science Laboratory, and (b) the electromagnetic levitator reaching temperatures up to 2200 C.

Acknowledgements

The financial support from ESA and DLR and the scientific cooperation within the International *ThermoLab Team* (MAPs and Topical Teams) is gratefully acknowledged.

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