18 March 2024

PhD contract offer

Motion and packing of dendrites during solidification: modeling and scale bridging

General information

Workplace: Nancy, France
Type of contract: PhD contract
Contract period: 36 months
Expected date of employment: October 2024
Proportion of work: Full time
Remuneration: 2.100€ gross monthly salary
Desired level of education: Master's degree in mechanical engineering, physics or materials science.
Experience required: -

Missions / Activities

Background

Metallic materials are composed of crystal microstructures and their mechanical properties depend on the size, morphology, and chemical composition of these microstructures. In manufacturing of virtually all metal products, solidification processes, such as casting, welding, or additive manufacturing, are a decisive step for the formation of the microstructure. Understanding the link between process parameters and the microstructure of the product is particularly important for the improvement of properties of high-performance components with high added value, e.g., the impact toughness of steel nuclear reactor pressure vessels or the fatigue strength of turbine blades in an aircraft engine.

During the solidification of a metal alloy, the solid crystal structure often forms in the shape of dendritic grains. The dendrites, a few millimeters in size, first grow freely in the liquid and can move during their growth. They are carried by the flow and are spread across the whole solidifying piece, which can be several meters in size. They sediment, pack, and continue to grow until complete solidification. The structure of the solidified piece depends strongly on these transport phenomena.

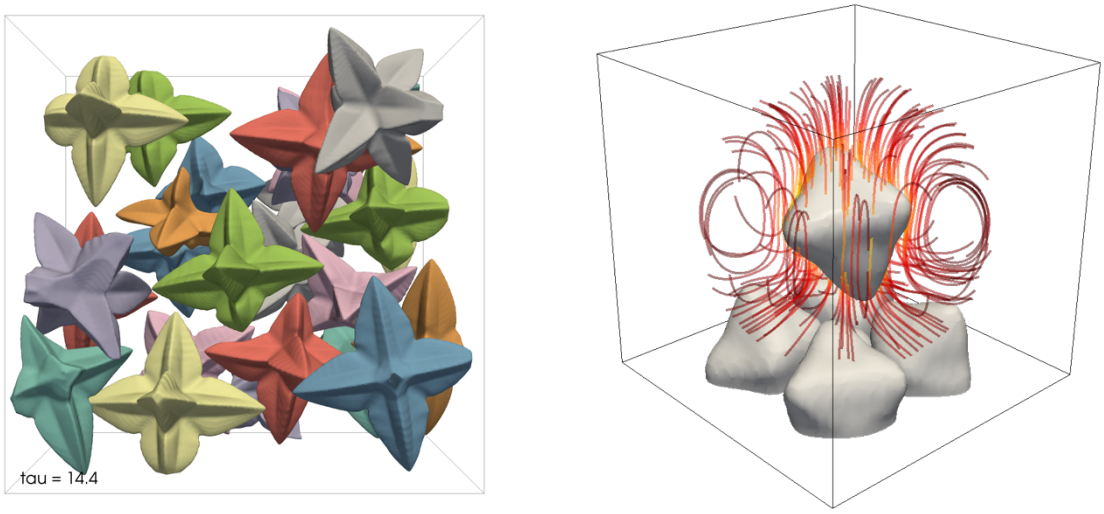

Figure 1: GEM simulations of dendritic solidification. Left: equiaxed dendrites influenced by mutual interactions. Right: Settling and packed dendrites.

Our work on the dynamics of motion of dendritic grains [1] has shown that the transition between the zone of free-floating grains and the packed layer of stationary grains occurs across a narrow zone, with the thickness of about 5 times the grain size. In this packing zone, the distance between the grains decreases rater abruptly and the coupling between the flow of the liquid, the motion of the grains and their growth leads to high variations of chemical composition and temperature. Today, a theory to describe the packing zone does not exist. The phenomena in this zone are one of the key factors for the formation of the nonuniform structure and chemical composition in castings [2].

Objectives and Methods

The objective of the PhD thesis is to answer the following questions:

- What are the principal phenomena that control the formation of the structure in the grain packing zone?
- How can we describe the packing zone at a macroscopic scale of the solidifying part in order to incorporate the description into a model for the simulation of the industrial process?

Experimental characterization of the phenomena in the packing zone is extremely difficult. However, recently developed mesoscopic models of solidification [3] can provide detailed quantitative information on the evolution of the shape and size of the grains, concentration and thermal fields, etc. They can simulate ensembles of up to a hundred grains; it is therefore possible to carry out numerical experiments and characterize all these aspects.

The Grain Envelope Model (GEM) [4–6] will be employed to investigate the growth and motion of the grains, as well as the relevant couplings in the packing zone. The GEM describes the growth of individual grains, coupled with a CFD finite-volume modeling of flow, diffusion and heat transfer and with a DEM (Discrete Element Method) model of contact between grains. The code is developed on the OpenFOAM platform. The project will consist of the following steps:

(1) An extension of the GEM will be developed to incorporate the phenomena in the packing zone into the model.

(2) Simulations of solidification in the packing zone will be performed for prototype configurations, relevant for the conditions encountered in metallurgical processes.

(3) The simulations will be upscaled to formulate constitutive laws that describe the solidification in the packing zone in macroscopic process models.

References

[1] A. Olmedilla, M. Založnik, T. Messmer, B. Rouat, H. Combeau, Packing dynamics of spherical and non-convex grains sedimenting at low Stokes number, *Physical Review E* **99** (1) (2019) 012907. https://hal.univ-lorraine.fr/hal-02381208

[2] H. Combeau, M. Založnik, S. Hans, P. E. Richy, Prediction of Macrosegregation in Steel Ingots: Influence of the Motion and the Morphology of Equiaxed Grains, *Metallurgical and Materials Transactions B* **40** (3) (2009) 289–304. doi:10.1007/s11663-008-9178-y.

[3] D. Tourret, L. Sturz, A. Viardin, M. Založnik, Comparing mesoscopic models for dendritic growth, *IOP Conf. Series: Mater. Sci. Eng.* **861** (2020) 012002. https://iopscience.iop.org/article/10.1088/1757-899X/861/1/012002

[4] Y. Souhar, V. F. De Felice, C. Beckermann, H. Combeau, M. Založnik, Three-dimensional mesoscopic modeling of equiaxed dendritic solidification of a binary alloy, *Computational Materials Science* **112** (2016) 304–317. https://hal.univ-lorraine.fr/hal-01709353

[5] A. Olmedilla, M. Založnik, H. Combeau, Quantitative 3D mesoscopic modeling of grain interactions during equiaxed dendritic solidification in a thin sample, *Acta Materialia* **173** (2019) 249–261. https://hal.univ-lorraine.fr/hal-02381280

[6] A. Olmedilla, M. Založnik, 3D mesoscopic modeling of settling and packing of equiaxed dendrites, in: *Modeling of Casting, Welding and Advanced Solidification Processes XV*, Djurönäset, Sweden, 2020. Presentation

Keywords: Solidification, Multiscale modeling, Multiphase heat & mass transfer, Fluid dynamics, Particle packing, Scale bridging

Work context

The PhD student will work under the supervision of Dr. Miha Založnik, expert on solidification and Jean-Sébastien Kroll-Rabotin, expert on multiphase fluid dynamics. She/he will be part of the *Solidification* and *Process Metallurgy* groups and will benefit from an interdisciplinary scientific environment: materials science, metallurgy, heat & mass transfer, computational modeling, experimentation and characterization at laboratory and industry scale.

Skills

Requirements for applicants:

- Master's degree in mechanical engineering, materials science or physics.
- Good notions of heat & mass transfer, fluid dynamics, numerical methods.
- Experience in numerical modeling (finite volume method appreciated).
- Proficiency in computer programming (C++, Python, OpenFOAM®).
- Proficiency in technical report writing and presentation.
- Sense of initiative, problem-solving and teamwork skills.
- Fluent in English, some knowledge of French is beneficial.

Constraints and risks

The position you are applying for is located in a sector relating to the protection of scientific and technical potential. It therefore requires, in accordance with the regulations, that your arrival be authorized by the competent authority of the Ministry of Higher Education, Research and Innovation.

About Institut Jean Lamour

The Institute Jean Lamour (IJL) is a joint research unit of CNRS and Université de Lorraine.
Focused on materials and processes science and engineering, it covers: materials, metallurgy, plasmas, surfaces, nanomaterials and electronics.
The IJL has 263 permanent staff (30 researchers, 134 teacher-researchers, 99 IT-BIATSS) and 394 non-permanent staff (182 doctoral students, 62 post-doctoral students / contractual researchers and more than 150 trainees), of 45 different nationalities.
Partnerships exist with 150 companies and our research groups collaborate with more than 30 countries throughout the world.
Its exceptional instrumental platforms are spread over 4 sites ; the main one is located on Artem campus in Nancy.

Application

To apply, send us a short statement of your interests, your CV, and full academic transcripts of the last two years of your master's studies.

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