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Editorial

Material Modeling in Multiphysics Simulation

Francesco De Bona [1,*], Francesco Mocera [2] and Jelena Srnec Novak [3]

[1] Department Polytechnic of Engineering and Architecture, University of Udine, Via delle Scienze 208, 33100 Udine, Italy
[2] Department of Mechanical and Aerospace Engineering (DIMEAS), Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy; francesco.mocera@polito.it
[3] Faculty of Engineering & Centre for Micro- and Nanosciences and Technologies, University of Rijeka, Vukovarska 58, 51000 Rijeka, Croatia; jsrnecnovak@uniri.hr
* Correspondence: debona@uniud.it; Tel.: +39-0432-558269

1. Introduction

Virtual prototyping techniques, generally based on numerical methods, are widely used in the process of designing an industrial product [1,2]. In recent decades, the demand for strong improvements in terms of productivity, reliability, and cost reduction have been fundamental considerations in this form of design, often requiring more than one simultaneously occurring physical field (thermal, mechanical, electrical, metallurgical, etc.) to be taken into account. At present, a huge amount of commercial code and a huge number of new algorithms have been developed for performing multiphysics simulations [3,4]; nevertheless, the availability of a suitable material model often presents a bottleneck in obtaining reliable results. For example, see [5,6]. The Special Issue is thus aimed at investigating metallic material modeling techniques for virtual prototypes, with an emphasis on both the theoretical aspects and experimental identification and verification. The simulation of additive manufacturing techniques is paid special attention as an emerging field [7]. Nevertheless, more traditional metal-forming processes, continuous casting in particular [8], still require new approaches given increases in the casting speed and in the dimensions of the final products. A wealth of other topics could benefit from multiphysics simulations, in particular metal forming [9,10], joining techniques [11], the thermal treatment of metals [12,13], and manufacturing processes [14]. This Special Issue collates papers that provide state-of-the-art knowledge on material modeling for multiphysics simulations and in which the above-mentioned topics are developed and applied to relevant engineering case studies.

2. An Overview of the Published Articles

Additive manufacturing (AM) techniques for metals constitute a fascinating challenge in materials science and engineering. Firstly, AM techniques offer the possibility of manufacturing unique geometries, which is not possible in traditional metallurgical processing. Even more promisingly, AM processes enable local control over the microstructure and properties. It must be pointed out that it is possible that manufacturing particular geometries could cause a clash with the accuracy of the techniques used, and this requires accurate calibration of the process parameters. In (contribution 1), the distortion of thin-walled structures obtained using the laser power bed fusion (LPBF) process is thermo-mechanically analyzed. In particular, a variety of thin-walled components are printed using LPBF with different wall thicknesses and building-heights. Different open and closed shapes are compared, and a 3D scanner is used to measure their actual warpage. This experimental scheme facilitates the calibration of an FE model of the AM process. In particular, the adopted numerical strategy is based on the inherent strain method. The inherent strain tensor is assumed as a user-defined material parameter depending on the material and process characteristics. Its value was obtained experimentally. This numerical tool was also

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used to define a structural optimization strategy to mitigate the warpage of the thin-walled parts printed using LPBF. Another promising possibility offered by the AM process is the possibility of attaining local control over the microstructure and properties; nevertheless, such an approach is quite difficult in practice due to the complex multiscale relationships between the material parameters and processing conditions. This aspect is considered in (contribution 2), where coupled modeling of the process, microstructure, and properties was investigated using three different numerical strategies. The time–temperature history of the AM raster patterns from a computational fluid dynamics module serves as the input to multilayer simulations of the grain structure using cellular-automata-based code. Finally, a crystal plasticity finite element model is used to simulate the micromechanical response and properties. The aim is to assess the grain size and texture as a function of the number of layers, as well as the influence of heterogeneous nucleation.

While AM techniques are still in the development phase, nevertheless, other processes have largely been consolidated, and their set-up seems to be well defined in most cases, for instance, the continuous casting process of steels. However, even in this case, since the production requirements are becoming increasingly demanding, new strategies for overcoming the complexity of process simulation must be adopted. In particular, solidifying steel follows highly nonlinear thermo-mechanical behavior depending on the loading history, temperature, and metallurgical phase fraction calculations (liquid, ferrite, and austenite). Because most process events (e.g., solidification, segregation, defect production) are temperature-driven, formulating a tool for analyzing the thermal field is a fundamental preliminary objective in the development of an accurate material model. Theoretically, to describe such a process, a three-dimensional approach would be required. In this case, the computational cost of obtaining results is often unreasonably resource- and time-intensive. To overcome these issues, a faster bidimensional approach known as the traveling slice approach was developed and is now frequently utilized. Although this modeling strategy is frequently encountered in literature reviews, an assessment of its limitations remains lacking, especially within the current context of increases in casted product sizes, which may call into question the validity of this modeling technique. In (contribution 3), the traveling slice model is compared to a non-approximated analysis, notably using large-dimension products. The traveling slice approach can be considered a proven modeling technique for describing continuous casting processes. In (contribution 4), a numerical model with a computationally challenging multiphysics approach is used in high-performance computing to generate sufficient training and testing data for subsequent deep learning. It has thus been demonstrated how innovative sequence deep learning methods can learn from multiphysics modeling data on a solidifying slice traveling in a continuous caster and correctly and instantly capture the complex history and temperature-dependent phenomena in test data samples. The use of machine learning techniques to support multiphysics and multi-phase simulations of continuous casting processes is also proposed in (contribution 5), where an industrial contactless vertical casting process has been modeled using evolving domain and dynamic mesh techniques. In particular, an augmented genetic algorithm machine learning approach enables the implementation of an accurate material. It was thus possible to increase the accuracy and flexibility of the process simulations while limiting the required computational time and resources. The technique is sufficiently flexible to implement using mainstream commercial solvers for material processes.

Many other technological processes in metal production can benefit from material modeling, as is the case for ultrasonic treatment. Cavitation, caused by high-intensity ultrasonic treatment, is used in a wide range of industrial applications and becomes more and more pertinent to metallurgy and foundry processes. It can be used as an effective method for modifying a material's microstructure and improving its mechanical properties, especially in the context of the treatment of aluminum alloys. In (contribution 6), the capabilities of computational fluid dynamics to model the formation and dynamics of acoustic cavitation in an aluminium alloy are investigated. Among the different metal-

forming techniques, hot metal extrusion is generally preferred when the final product is characterized by a high aspect ratio—for example, turbine blades. This process induces higher plastic deformation in comparison to forging. Thus, finer process parameter tuning is required to avoid unwanted microstructural effects. A typical failure occurring during hot metal extrusion is the formation of surface cracks. Numerical modeling could thus be a useful tool to more deeply investigate the influence of the process parameters on the final characteristics of the product. In (contribution 7), an FE-based multiphysics numerical model of the extrusion process for a superalloy component was devised. In parallel, a series of experimental tests were designed and carried out to examine the extrusion of pre-heated Inconel 718 billets, thus allowing for comprehensive validation of the numerical model and its respective results. The validated model was then used to perform parametric analyses in order to pinpoint the ranges of the processing conditions that avoid the formation of unwanted features. In particular, the microstructure evolution can be simulated using a semi-empirical model, taking into account both the recrystallization (dynamic and static) and grain growth, providing the average grain size and the fraction of recrystallized grains.

Numerical simulation can also profitably support the fine-tuning of thermal treatment. In (contribution 8), a simulation procedure for predicting the influence of the carbon content and quenching process parameters on the phase composition and hardness distribution after heat treatment is proposed. Experiments applying quenching in the form of high-pressure gas quenching and quenching oil were employed to validate the computational results. In particular, careful set-up of a carbon diffusivity model incorporating the influence of the alloying elements was undertaken in this research. Thermal data such as thermal conductivity and heat capacity also required adjustments; therefore, experimental data were used. The material model must also take into account phase transformations, which, depending on the cooling rate, can be classified as diffusion-controlled or diffusionless. The Johnson–Mehl–Avrami–Kolmogorov model was adopted to describe the kinetics of the isothermal phase transformation, during which diffusion is the governing phenomenon, according to the nucleation and growth of the new phase. Martensitic transformation is a diffusionless transformation that occurs upon rapid quenching of the austenite phase. As martensitic transformation is athermal, that is, is not controlled by the thermal history of the material, the volume fraction of the transformed phase is calculated based on an equation incorporating the degree of undercooling of the material. To describe the transformation kinetics, a Koistinen–Marburger model was used. Finally, the Maynier model was adopted for hardness calculations. In (contribution 9), the isothermal decomposition of austenite in steel is mathematically modeled and computer-simulated. This research has significant implications in the field of the thermal treatment of steels. In fact, the isothermal decomposition of austenite implies the steel is quenched from the austenite range to the temperature of isothermal transformation, where all of the austenite decomposes at a constant temperature. The microstructure composition and mechanical properties of the steel considered can thus be optimized and controlled. The proposed mathematical model was verified experimentally, confirming that the characteristic parameters included in the model of ferrite, pearlite, and bainite transformation can be successfully evaluated.

Furthermore, joining techniques often require a multiphysics approach. In (contribution 10), a mathematical model of induction soldering for waveguide assembly components was developed, which could help with testing and calibrating the induction soldering process for the thin-walled aluminum waveguides found in spacecraft. To verify the developed models, simulations were compared with experiments, confirming the prediction accuracy.

Finally, in (contribution 11), fundamental research on metals was shown to potentially better our understanding of how a material model can be more accurately predicted and interpreted. In particular, the temperature dependence of resistivity over a very wide temperature range is explained according to free randomly moving electrons scattering due to electronic defects, accounting for the thermal energy exchange between phonons and free randomly moving electrons.

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