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Editorial

Multi-Scale Simulation of Metallic Materials (2nd Edition)

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1. Introduction

Metallic materials are some of the most important engineering materials. Current developments in our society are leading to an increasing demand for diverse novel metallic materials with desirable properties. Furthermore, there is an urgent need for these metallic materials to be manufactured in an environmentally friendly way with low energy costs, in addition to a demand for the sustainable recycling of metallic scrap/waste which contains a rich variety of impurities [1]. To reach such goals, the use of both experimental and theoretical tools to obtain comprehensive knowledge regarding metallic materials on scales ranging from the atomic-, micro-, meso- to macroscopic-level is essential.

Great efforts have been made to design novel ferrous metals and light metals including Al and Mg from, e.g., metallic scraps [2]. Moreover, improving the mechanical performance of metallic materials is a big challenge for their application. Among the major alloy-strengthening mechanisms, the uniform dispersion of nanoscale secondary phase precipitates is particularly effective. Ceramic materials have been added into metal matrices to produce nanocomposites that exhibit excellent mechanical performance [3,4]. In addition to this, new types of metallic materials, such as multicomponent high-entropy alloys [5], have been intensively explored.

Recent progress in computational capability and modeling techniques has promoted the application of multiscale simulation techniques in metallic materials [6]. Multiscale simulations which combine existing and emerging methods are currently being employed to incorporate a wide range of time and space scales that are inherent to various disciplines. Moreover, combining experimental observations and multiscale modeling provides us with a comprehensive understanding of the engineering processes and physical properties of metallic products.

Considering this, this Special Issue aims to improve our understanding of the structural, microstructural, and physical properties of complex metallic materials via multiscale approaches, including thermodynamics, finite element methods, and ab initio molecular dynamics simulations.

2. Overview of the Contributions

Zabojszcza and colleagues contributed a paper entitled 'Verification of Numeric Models of Steel Bar Coverings Using Experimental Tests—Preliminary Study' (Contribution 1). Construction failures causing damage in load-bearing structures made of steel are considered some of the most severe structural failures, not only in terms of material loss but also in terms of potential human casualties. The mitigation of these occurrences is decisive in the design of steel roofs. This work aimed to verify and assess the accuracy of a macroscopic numerical model of a metal bar roof by conducting experimental studies. The structure covered by the metal bar roof was characterized by a strongly nonlinear static response;

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ignoring these nonlinear effects leads to large computational errors. The authors performed a series of repeatable experimental tests on the structure model to determine the path of static equilibrium and the form of stability loss of the steel covering using the relation between the load and the displacements of nodes. The displacements of the nodes were verified using precise triangulation laser sensors and electronic sensors. For a low-rise bar covering, the inclusion of imperfections is particularly important, which significantly affects the local and overall stability of the structure. The obtained information helps us to understand the accuracy and reliability of numerical models. In turn, it contributes to the development of improved methods for the analysis of metal bar roof structures in future works.

Quan et al. presented their work 'A Characterization of the Powder Yield Behaviors During a Hot Isostatic Pressing Process' (Contribution 2). It has been well-established that temperature plays a crucial role in determining material properties during the hot isostatic pressing of powders. It is therefore essential to account for its effect on the yield model parameters in order to accurately and reliably describe the densification evolution of powders. The authors developed a mesoscopic, particle-scale, high-temperature uniaxial compression model based on the discrete element method. The predicted relations between strain and stress and corresponding densities in the high-temperature uniaxial compression simulations were verified via experiments. The authors analyzed the strain evolution during the uniaxial compression process and discovered the relationship between the parameters of the Shima–Oyane model and temperature. Based on the obtained parameters, they created a yield stress map for the nickel-based alloy to act as an example. The accuracy/reliability of the model was verified by comparing the experimental results with the finite element method (FEM) simulations. This study contributes to a more reliable prediction of densification behavior in the thermally driven isostatic pressing of metallic materials.

Jacobson and colleagues provided their recent work entitled 'Extending Density Phase-Field Simulations to Dynamic Regimes' (Contribution 3). Grain boundaries play a crucial role in determining the physical properties of metallic materials. Density-based phase-field (DPF) methods have emerged as a technique for simulating grain boundary thermodynamics and kinetics. Compared to the classical phase-field, DPF gives a more physical description of the grain boundary structure and chemistry. It bridges the gap between CALPHAD databases and atomistic simulations and it thus has potential applications in grain boundary and segregation engineering. The authors generated a generic DPF free energy functional which was used to carry out a series of equilibrium and dynamic simulations of grain boundaries, producing relations such as grain boundary width vs. gradient energy coefficient, grain boundary velocity vs. applied driving force, and spherical grain radius vs. time. These relations are compared with analytical solutions and the behavior of physical grain boundaries and are used to assess the validity of the coupled DPF model. A good agreement was reached between the tested quantities and established theories of grain boundary behavior, which indicated that coupling density fields with traditional order parameters in DPF simulations is an excellent approach for making DPF simulations dynamic and for improving the simulation's performance and accuracy.

Andersson and Lundbäck provided their work 'Modeling the Evolution of Grain Texture during Solidification of Laser-Based Powder Bed Fusion Manufactured Alloy 625 Using a Cellular Automata Finite Element Model' (Contribution 4). In additive manufacturing, the materials are added through a layer-by-layer method. Then, by subsequently melting the added material with a heat source, it is fused into a solid structure. The grain texture of the as-printed material evolves during the laser-based powder bed fusion (PBF-LB) process. The resulting mechanical properties depend on the obtained grain texture and the chosen

process parameters, including scan velocity and laser power. The researchers developed a coupled 2D Cellular Automata and Finite Element model (2D CA-FE) to predict the evolution of the grain texture during solidification of the nickel-based superalloy 625 produced by PBF-LB. The finite element (FE) model predicted the temperature history of the building and the CA model made predictions of nucleation and grain growth based on the temperature history. The 2D CA-FE model captured the solidification behavior observed in PBF-LB, such as competitive grain growth plus equiaxed and columnar grain growth. Three different nucleation densities for heterogeneous nucleation were investigated. The optimized nucleation density was found to give the best result as compared to the existing EBSD data in the literature. With the selected nucleation density, the predicted aspect ratio and grain size distribution of the simulated grain texture agreed well with the observed textures from EBSD in the literature.

Bin Abd Rahim et al. published the paper 'Assessing Fatigue Life Cycles of Material X10CrMoVNb9-1 through a Combination of Experimental and Finite Element Analysis' (Contribution 5). The authors combined experiments and theoretical modeling for investigating fatigue crack initiation and propagation of the material X10CrMoVNb9-1 (P91) steel under cyclic loading at room temperature. The Voronoi tessellation method was implemented to generate an artificial microstructure model at the microstructure level; following this, the finite element (FE) method was applied to identify different stress distributions. The stress distributions for multiple artificial microstructures were analyzed by using the physically based Tanaka–Mura model to estimate the number of cycles for crack initiation. For the prediction of macro-scale and long-term crack formation, the Paris law was utilized in this research. Experimental work on fatigue life with this material was performed, and good agreement was found with the results obtained in FE modeling. The number of cycles for fatigue crack propagation attains up to a maximum of 40% of the final fatigue lifetime with a typical value of 15% in many cases. This physically based two-scale technique significantly advances fatigue research, particularly in power plants, and paves the way for rapid and low-cost virtual material analysis and fatigue resistance analysis in the context of environmental fatigue applications.

Zeng and colleagues presented their results 'Crystal Plasticity Finite Element Simulation of Tensile Fracture of 316L Stainless Steel Produced by Selective Laser Melting' (Contribution 6). In the current work, the authors employed a combination of experimental observations and numeric modeling approaches to investigate the elective laser melting (SLM) of 316L stainless steel. The influence of building direction and grain boundary strength on the fracture parameters of SLM 316L stainless steel was studied using electron backscatter diffraction (EBSD) experiments which characterized the microstructure of the specimens. A representative volume element (RVE) model reflecting the microstructure of SLM 316L stainless steel was established based on a combination of the crystal plastic finite element method (CPFEM) and UMAT subroutine technology. The crystal plasticity parameters were obtained by means of analyzing the results of tensile tests. Cohesive elements were employed and inserted at the grain boundaries of the polycrystalline RVE to simulate the intergranular fracture behavior of SLM 316L stainless steel under uniaxial tensile loading. The damage and fracture mechanisms of the material at the microscale were analyzed. The simulated tensile stress–strain curves were in good agreement with the experimental results; hence, the combined CPFEM model is suitable for characterizing the mechanical response and fracture behavior of the steel. The results revealed that cracks initiate at stress concentration sites and propagate along grain boundaries with increasing external load, ultimately leading to rupture. Moreover, the building direction influences the location of microcracks and their propagation significantly.

Fang and Fan present their work 'Crystal Chemistry at Interfaces Between Liquid Al and Polar SiC{0001} Substrates' (Contribution 7) in the Special Issue. Silicon carbide (SiC) has been widely added into light metals, e.g., Al and Mg, to enhance their mechanical performance and corrosion resistance. SiC particle-reinforced metal matrix composites (SiC-MMCs) exhibit low weight/volume ratios, high strength/hardness, high corrosion resistance, and thermal stability. They have potential applications in aerospace, automobiles, and other specialized equipment. The macro-mechanical properties of Al/SiC composites depend on the local structures and chemical interactions at the Al/SiC interfaces at the atomic level. Moreover, the added SiC particles may act as potential nucleation sites during solidification. The present authors investigated local atomic ordering and chemical interactions at the interfaces between liquid Al (Al(l) in short) and the polar SiC substrates using ab initio molecular dynamics (AIMD) methods. The simulations reveal a rich variety of interfacial interactions. Charge transfer occurs from Al(l) to C-terminating atoms ($\Delta q = 0.3$ e/Alon average), while chemical bonding between interfacial Si and Al(l) atoms is more covalent with a minor charge transfer of $\Delta q = 0.04$ e/Al. The prenucleation at both interfaces is moderate with three to four recognizable layers. The information obtained here helps increase understanding of the interfacial interactions at Al/SiC at the atomic level and the related macro-mechanical properties, which is helpful in designing novel SiC-MMC materials with desirable properties and optimizing related manufacturing and machining processes.

Führer et al. published the paper 'Experimental Investigation of the Interplay Between Al-, B-, and Ti-Nitrides in Microalloyed Steel and Thermodynamic Analysis' (Contribution 8). The primary objective of this study was to accurately describe the microstructural evolution in the Fe-Al-B-Ti-C-N system using the Calphad approach, with special emphasis on correctly predicting the dissolution temperatures of nitrides. The authors built a multicomponent database through the incorporation of available binary and ternary descriptions, employing the Calphad method. The experimental findings regarding the solvus temperature of the involved nitrides were employed to validate the accuracy of the thermodynamic database. The findings offered a comprehensive understanding of the relative phase stabilities and the associated interplay among the involved elements Al, B, and Ti in the Fe-rich corner of the system. The type and size distributions of the stable nitrides in micro-alloyed steel have been demonstrated to exert a substantial influence on the properties of the material, thereby rendering accurate predictions of phase stabilities of considerable relevance.

3. Summary and Outlook

The second edition of this Special Issue of *Metals* was supported by various research groups and a final book of eight high-quality peer-reviewed articles (Multi-scale Simulation of Metallic Materials (2nd Edition) | Metals | MDPI). The success of this special issue will be followed by an. other special issue (Advances in the Study of Metal Crystals) to accept global contributions from the metal community.

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List of Contributions

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