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Editorial

Numerical Modelling on Metallic Materials

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1. Introduction

Numerical modelling of metallic materials has emerged as a pivotal research area in modern materials science and engineering [1]. With the advancement of computational power and the development of sophisticated modelling techniques, numerical simulation has become an indispensable tool for studying the microstructural evolution, enhancing process understanding and optimisation, and predicting the mechanical properties of metallic materials [2–9]. By employing accurate mathematical models and efficient computational methods, researchers can simulate the complex behaviours of real-world materials in a virtual environment. This approach not only reduces experimental costs and boosts research efficiency, but also uncovers physical phenomena that are challenging to observe directly through experiments [10–15].

This Topic is dedicated to the "Numerical Modelling on Metallic Materials" and presents a curated collection of twenty cutting-edge research papers in the field. These studies span multiple scales, from microstructural evolution to macroscopic mechanical behaviour, and explore the response of various metallic materials under diverse processing and service conditions. At the microscopic level, numerical modelling is applied extensively to explore phase transformations, diffusion behaviours, and microstructural evolution in metallic materials. At the mesoscopic and macroscopic levels, numerical simulations are employed to predict the mechanical properties and failure mechanisms of metallic materials, offering insights into performance and durability. The studies featured in this collection highlight the vital role of advanced modelling techniques, including finite element analysis (FEA), molecular dynamics simulations (MDS), computational fluid dynamics (CFD), discrete element method (DEM), and phase-field (PF) and other modelling techniques, in optimising engineering designs, predicting material performance, and improving manufacturing processes.

Additionally, this Topic also showcases emerging numerical modelling approaches, such as topology optimisation and the applications of various other optimisation algorithms, in metallic material simulations. These innovative approaches, when combined with traditional physical modelling techniques, extend the capabilities of numerical modelling to encompass intelligent computation and multi-scale analysis. Such advancements pave the way for more efficient and effective strategies for the design and optimisation of future materials.

2. Outline of This Topic

This Topic includes twenty technical papers contributed by the authors working in the field and is organised into three main sections, each offering a comprehensive exploration

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of numerical modelling applications in metallic materials. The three sections comprise atomic-scale and microstructural evolution modelling, meso- and macro-scale mechanical behaviour simulations, and emerging computational techniques and advanced applications in metallic materials research. These contributions are summarised and listed below.

2.1. Atomic-Scale and Microstructural Evolution Modelling

Baidak, S.T. et al. (contribution 1) analysed the electronic band structures of intermetallic compounds and their topological characteristics using an ab initio method. Xiang, G., et al. (contribution 2) investigated the diffusion of atoms and crystal structure evolution at the Fe-Ti interface through MDS. Zheng, H., et al. (contribution 3) employed MDS to examine how different orientations, temperatures, and strain rates influence the diffusion behaviour and mechanical properties of the Fe/Cu solid–liquid interface. Lv, B., et al. (contribution 4) developed computational interatomic potentials for accurately modelling the behaviours of multi-component metallic systems. Fashu, S., et al. (contribution 5) explored the impact of intragranular nanoparticles on precipitate-coarsening behaviours in metallic alloys based on PF modelling. Kumnorkaew, T., et al. (contribution 6) presented a kinetic model for predicting bainitic transformation kinetics in low-carbon steels under different thermomechanical treatments. Chen, X., et al. (contribution 7) investigated how multi-directional forging (MDF) at 1150 °C affects the microstructure of SDP1 steel and compared it to traditional forging methods.

2.2. Meso- and Macro-Scale Mechanical Behaviour Simulations

Ciepielewski, R., et al. (contribution 8) investigated the energy-absorbing properties of aluminium honeycomb structures, particularly focusing on the impact of entrapped air within the cells during dynamic loading conditions. Zhao, Y., et al. (contribution 9) developed a model combining CFD with DEM and investigated the mechanism of laser polishing and its influence on the surface finish of additively manufactured nickel alloys. Alshoaibi, A.M., et al. (contribution 10) applied FEA to predict fatigue crack growth behaviours under cyclic loading conditions. Ma, W., et al. (contribution 11) modelled the buckling and post-buckling behaviours of thin-walled structures under axial loads. Lopez-Garcia, R.D., et al. (contribution 12) studied how quenching parameters influence distortion and residual stresses in high-strength steel components. Peng, Y., et al. (contribution 13) examined the effectiveness of different stiffener geometries in enhancing the stability of steel girders. Huang, Z., et al. (contribution 14) simulated fracture expansion behaviours in steel cylindrical shells subjected to explosive loads. In addition, He, T., et al. (contribution 15) analysed the effects of mould design on shrinkage porosity in titanium alloy casting.

2.3. Emerging Computational Techniques and Advanced Applications

Kim, M.S., et al. (contribution 16) introduced a novel constitutive model to predict ductile fracture initiation and progression. Wallat, L., et al. (contribution 17) explored computational methods for designing gyroid-based porous structures with tuneable mechanical properties. Liu, M., et al. (contribution 18) enhanced the accuracy of temperature prediction for steel slabs in industrial heating processes using an optimised particle swarm algorithm. Zhao, T., et al. (contribution 19) modelled and analysed the optical properties of nanochain aggregates on silicon surfaces. Chen, Y., et al. (contribution 20) used smooth particle hydrodynamic simulation to examine how steel fibre reinforcement enhances the tensile and bonding properties of explosion-welded aluminium–steel composites.

3. Concluding Remarks

This Topic is intended for researchers, engineers, and graduate students engaged in metallic materials research. Through these research papers, readers will gain valu-

able insights into the latest advancements in numerical modelling, explore cutting-edge computational techniques, and discover diverse applications of numerical modelling and simulation in materials science and engineering. This Topic serves as a comprehensive reference for both academic research and industrial practice, advancing the field of metallic materials.

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