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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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List of Contributions

1. Baidak, S.T.; Lukoyanov, A.V. Common topological features in band structure of RNiSb and RSb compounds for R= Tb, Dy, Ho. *Materials* **2023**, *16*, 242. https://doi.org/10.3390/ma16010242.
2. Xiang, G.; Luo, X.; Cao, T.; Zhang, A.; Yu, H. Atomic diffusion and crystal structure evolution at the Fe-Ti interface: molecular dynamics simulations. *Materials* **2022**, *15*, 6302. https://doi.org/10.3390/ma15186302.
3. Zheng, H.; Sun, J.; Guo, N.; Wang, M. Atomic Research on the Diffusion Behavior, Mechanical Properties and Fracture Mechanism of Fe/Cu Solid–Liquid Interface. *Coatings* **2022**, *12*, 1299. https://doi.org/10.3390/coatings12091299.
4. Lv, B.; Chen, C.; Zhang, F.; Poletaev, G.M.; Rakitin, R.Y. Potentials for describing interatomic interactions in γFe-Mn-CN system. *Metals* **2022**, *12*, 982. https://doi.org/10.3390/met12060982.
5. Fashu, S.; Huang, B.; Wang, N. Modification of Precipitate Coarsening Kinetics by Intragranular Nanoparticles—A Phase Field Study. *Metals* **2022**, *12*, 892. https://doi.org/10.3390/met12060892.
6. Kumnorkaew, T.; Lian, J.; Uthaisangsuk, V.; Bleck, W. Kinetic model of isothermal bainitic transformation of low carbon steels under ausforming conditions. *Alloys* **2022**, *1*, 93–115. https://doi.org/10.3390/alloys1010007.
7. Chen, X.; Wu, B.; Li, J.; Zhang, X.; Zuo, P.; Wu, X.; Li, J. Microstructural Evolution in Large-Section Plastic Mould Steel during Multi-Directional Forging. *Metals* **2022**, *12*, 1175. https://doi.org/10.3390/met12071175.
8. Ciepielewski, R.; Miedzińska, D. A Study of Aluminum Honeycomb Structures under Dynamic Loading, with Consideration Given to the Effects of Air Leakage. *Materials* **2023**, *16*, 2211. https://doi.org/10.3390/ma16062211.
9. Zhao, Y.; Du, C.; Wang, P.; Meng, W.; Li, C. The mechanism of in-situ laser polishing and its effect on the surface quality of nickel-based alloy fabricated by selective laser melting. *Metals* **2022**, *12*, 778. https://doi.org/10.3390/met12050778.
10. Alshoaibi, A.M. Fatigue crack growth analysis under constant amplitude loading using finite element method. *Materials* **2022**, *15*, 2937. https://doi.org/10.3390/ma15082937.
11. Ma, W.; Sun, Z.; Wu, H.; Xu, L.; Zeng, Y.; Wang, Y.; Huang, G. Buckling Analysis of Thin-Walled Circular Shells under Local Axial Compression using Vector Form Intrinsic Finite Element Method. *Metals* **2023**, *13*, 564. https://doi.org/10.3390/met13030564.
12. Lopez-Garcia, R.D.; Medina-Juárez, I.; Maldonado-Reyes, A. Effect of quenching parameters on distortion phenomena in AISI 4340 steel. *Metals* **2022**, *12*, 759. https://doi.org/10.3390/met12050759.
13. Peng, Y.; Kong, Z.; Dinh, B.H.; Nguyen, H.H.; Cao, T.S.; Papazafeiropoulos, G.; Vu, Q.V. Web Bend-Buckling of Steel Plate Girders Reinforced by Two Longitudinal Stiffeners with Various Cross-Section Shapes. *Metals* **2023**, *13*, 323. https://doi.org/10.3390/met13020323.
14. Huang, Z.; Yu, X. Numerical simulation study of expanding fracture of 45 steel cylindrical shell under different detonation pressure. *Materials* **2022**, *15*, 3980. https://doi.org/10.3390/ma15113980.
15. He, T.; Chen, Y. Influence of Mold Design on Shrinkage Porosity of Ti-6Al-4V Alloy Ingots. *Metals* **2022**, *12*, 2122. https://doi.org/10.3390/met12122122.
16. Kim, M.S.; Kim, H.T.; Choi, Y.H.; Kim, J.H.; Kim, S.K.; Lee, J.M. A new computational method for predicting ductile failure of 304L stainless steel. *Metals* **2022**, *12*, 1309. https://doi.org/10.3390/met12081309.

17. Wallat, L.; Altschuh, P.; Reder, M.; Nestler, B.; Poehler, F. Computational design and characterisation of gyroid structures with different gradient functions for porosity adjustment. *Materials* **2022**, *15*, 3730. https://doi.org/10.3390/ma15103730.
18. Liu, M.; Yan, P.; Liu, P.; Qiao, J.; Yang, Z. An improved particle-swarm-optimization algorithm for a prediction model of steel slab temperature. *Appl. Sci.* **2022**, *12*, 11550. https://doi.org/10.3390/app122211550.
19. Zhao, T.; Gao, Y.; Shi, R.; Li, Z.; Shi, Q. Structure of Randomly Distributed Nanochain Aggregates on Silicon Substrates: Modeling and Optical Absorption Characteristics. *Materials* **2022**, *15*, 4778. https://doi.org/10.3390/ma15144778.
20. Chen, Y.; Gao, Y.; Guo, C.; Guo, Y.; Guo, Z.; Liu, Y.; Liu, T. Effect of the Addition of Steel Fibers on the Bonding Interface and Tensile Properties of Explosion-Welded 2A12 Aluminum Alloy and SS-304 Steel. *Materials* **2023**, *16*, 116. https://doi.org/10.3390/ma16010116.

References

1. Rappaz, M.; Bellet, M.; Deville, M.O.; Snyder, R. *Numerical Modeling in Materials Science and Engineering*; Springer: Berlin, Germany, 2003; Volume 20.
2. Liu, H.; Xu, X.; Zhang, J.; Liu, Z.; He, Y.; Zhao, W.; Liu, Z. The state of the art for numerical simulations of the effect of the microstructure and its evolution in the metal-cutting processes. *Int. J. Mach. Tools Manuf.* **2022**, *177*, 103890. [CrossRef]
3. DebRoy, T.; Mukherjee, T.; Wei, H.L.; Elmer, J.W.; Milewski, J.O. Metallurgy, mechanistic models and machine learning in metal printing. *Nat. Rev. Mater.* **2021**, *6*, 48–68. [CrossRef]
4. Bandyopadhyay, A.; Traxel, K.D. Invited review article: Metal-additive manufacturing—Modeling strategies for application-optimized designs. *Addit. Manuf.* **2018**, *22*, 758–774. [CrossRef] [PubMed]
5. Klingenberg, W.; Singh, U.P. Further observations and review of numerical simulations of sheet metal punching. *Int. J. Adv. Manuf. Technol.* **2006**, *30*, 638–644. [CrossRef]
6. Dal, M.; Fabbro, R. An overview of the state of art in laser welding simulation. *Opt. Laser Technol.* **2016**, *78*, 2–14. [CrossRef]
7. Thomas, B.G. Review on modeling and simulation of continuous casting. *Steel Res. Int.* **2018**, *89*, 1700312. [CrossRef]
8. Sun, Y.; Li, Q.M. Dynamic compressive behaviour of cellular materials: A review of phenomenon, mechanism and modelling. *Int. J. Impact Eng.* **2018**, *112*, 74–115. [CrossRef]
9. Zhang, Z.; Wang, Y.; Ge, P.; Wu, T. A review on modelling and simulation of laser additive manufacturing: Heat transfer, microstructure evolutions and mechanical properties. *Coatings* **2022**, *12*, 1277. [CrossRef]
10. Kiran, A.; Hodek, J.; Vavřík, J.; Urbánek, M.; Džugan, J. Numerical simulation development and computational optimization for directed energy deposition additive manufacturing process. *Materials* **2020**, *13*, 2666. [CrossRef]
11. Chen, X.; Wang, C.; Ding, J.; Bridgeman, P.; Williams, S. A three-dimensional wire-feeding model for heat and metal transfer, fluid flow, and bead shape in wire plasma arc additive manufacturing. *J. Manuf. Process.* **2022**, *83*, 300–312. [CrossRef]
12. Gu, H.; Li, L. Computational fluid dynamic simulation of gravity and pressure effects in laser metal deposition for potential additive manufacturing in space. *Int. J. Heat Mass Transf.* **2019**, *140*, 51–65. [CrossRef]
13. Taghizadeh, M.; Zhu, Z.H. A comprehensive review on metal laser additive manufacturing in space: Modeling and perspectives. *Acta Astronaut.* **2024**, *222*, 403–421. [CrossRef]
14. Zhou, N.; Lv, D.C.; Zhang, H.L.; McAllister, D.; Zhang, F.; Mills, M.J.; Wang, Y. Computer simulation of phase transformation and plastic deformation in IN718 superalloy: Microstructural evolution during precipitation. *Acta Mater.* **2014**, *65*, 270–286. [CrossRef]
15. Zepeda-Ruiz, L.A.; Stukowski, A.; Oppelstrup, T.; Bulatov, V.V. Probing the limits of metal plasticity with molecular dynamics simulations. *Nature* **2017**, *550*, 492–495. [CrossRef] [PubMed]

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