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Editorial

Numerical Modelling of Mechanical Properties for Metallic Materials

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1. Introduction

The reliable identification and prediction of mechanical characteristics of metallic materials remain the main challenges in the material engineering and computational mechanics fields. The complex loading conditions of metallic structures, including possible temperature changes, residual stresses, cyclic conditions, creep, fatigue, and fracture, represent possible states where conventional material characterisation is often insufficient for robust structural analysis and lifetime prediction. Constitutive models and numerical simulations, together with carefully designed experiments, are combined to describe the material response.

This Special Issue, "Numerical Modelling of Mechanical Properties for Metallic Materials", collected recent findings in computational and experimental mechanics for the characterisation, modelling, simulation, and prediction of mechanical properties in metals. Particular attention was devoted to finite element (FE) simulations, identification of material parameters, constitutive modelling, hardening and damage functions, advanced computational mechanics techniques, and continuum damage mechanics. The contributions published in this Special Issue show how computational mechanics methods can support material optimisation, identification of material parameters, fracture prediction, residual stress assessment, and lifetime estimation.

A total of five peer-reviewed articles were published. They cover a wide range of metallic materials and engineering problems, including high-entropy alloys, aluminium alloys, austenitic stainless steel, cast iron pistons, and ferritic–martensitic steel. Despite the diversity of materials and applications, all contributions share a common methodological feature: the integration of experimental characterisation with numerical simulation to improve the predictive capability of models used for metallic materials.

2. Overview of the Published Articles

In Contribution 1, Li et al. investigated the simulation and optimisation of the shot peening process for a CoCrFeNiAlx high-entropy alloy system. The study addressed the need to improve the surface and mechanical properties of high-entropy alloys, for which conventional shot peening may not always produce a sufficiently effective strengthened layer. The authors considered dry and wet shot peening processes and analysed the resulting changes in surface behaviour, plastic deformation, stress transfer, and grain refinement. Through the experiments and process optimisation, they identified favourable shot peening parameters, showing that wet shot peening can enhance the surface state and

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promote grain refinement. This work provides a useful contribution to the modelling and optimisation of surface treatment processes for metallic materials.

In Contribution 2, Bai and Liu proposed an inverse methodology for estimating the yield stress and hardening index of aluminium alloys based on indentation curves and the projected area of the contact zone. The approach combined indentation experiments, FE simulations, dimensionless analysis, and a genetic algorithm. Four dimensionless parameters were derived from load–displacement curves, while an additional parameter was obtained from the projection area of the contact region. The method was validated on 5052, 6061, and 7075 aluminium alloys, with predicted results showing good agreement with uniaxial tension tests. This contribution is particularly relevant for practical material characterisation, since it demonstrates how indentation-based testing, supported by numerical simulation and optimisation algorithms, can be used to identify plasticity material parameters.

In Contribution 3, Dunić et al. presented an experimental characterisation and phase-field damage modelling approach for ductile fracture in AISI 316L stainless steel. A phase-field damage model was implemented in an in-house FE code and coupled with von Mises plasticity. The model employed a work-density-based criterion with a threshold, allowing damage initiation and evolution to be controlled through physically meaningful parameters. The authors validated the simulation results against compact tension (CT) specimen tests, comparing force vs. crack-mouth opening displacement and crack-tip opening displacement responses. The numerical predictions showed good agreement with the experimental results, with a maximum discrepancy of approximately 8%. This study illustrates the potential of phase-field modelling for ductile fracture prediction and structural integrity assessment of metallic materials.

In Contribution 4, Yang et al. studied the dynamic evolution of residual stress during the manufacturing process of cast iron pistons. Instead of analysing casting, machining, or heat treatment separately, the authors proposed a continuous multi-process simulation framework covering the full manufacturing sequence. The numerical model was applied to a marine diesel engine piston and was validated through residual stress measurements. The results showed that shakeout can remove a significant portion of residual stress, machining leads to stress redistribution and partial stress release, and subsequent heat treatment further reduces the residual stress level. This contribution demonstrates the engineering value of integrated process simulation for low-stress manufacturing and for improving the performance and reliability of critical metallic components.

Finally, in Contribution 5, Bucciarelli et al. developed a constitutive modelling framework for creep–fatigue interaction in 1Cr-1Mo-0.25V steel under hold-time loading conditions. The work was motivated by high-temperature applications in power generation, where creep–fatigue interaction may compromise the integrity of rotating equipment and pressure vessels. The proposed approach combined a fatigue damage-based constitutive law with creep deformation and damage modelling. Model parameters were identified using low-cycle fatigue and creep relaxation tests, and the model was validated through simulations of fully reversed axial loading with tensile hold times. The predicted lifetime values showed good agreement with experimental data, confirming the suitability of the approach for industrially relevant lifetime assessment problems.

3. Conclusions

The published works in this Special Issue demonstrate several important trends in the field.

The combination of experiments and simulations is essential for credible prediction of the material response. Whether the problem involves indentation-based parameter identification, phase-field fracture modelling, residual stress evolution, or creep–fatigue lifetime assessment, the experimental validation remains necessary for establishing confidence in numerical simulations.

The identification of reliable material parameters continues to be a key challenge. Several contributions show that inverse methods, optimisation algorithms, and advanced testing procedures can significantly improve the characterisation of plasticity, hardening, fracture, and damage parameters.

The modelling of manufacturing processes and surface treatments is becoming increasingly important. Residual stresses, surface deformation, and microstructural refinement strongly influence the performance of metallic components, and numerical simulation offers a powerful tool for process optimisation.

Finally, advanced damage and lifetime prediction models are essential for the safe and efficient design of metallic structures operating under complex loading conditions. Phase-field damage modelling and creep–fatigue constitutive frameworks represent promising directions for future research, especially when extended to complex multiaxial loading and variable temperature histories.

Future developments in this field are expected to integrate FE simulations, multiscale modelling, data-driven parameter identification, uncertainty quantification, and experimentally validated digital workflows. Such integration will support more accurate predictions of metallic material behaviour and will contribute to safer, more efficient, and more sustainable engineering design.

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Conflicts of Interest: The authors declare no conflicts of interest.

List of Contributions

1. Li, X.; Gou, G.; Jiang, C.; Xu, J. Simulation and Optimization of Shot Peening Process for CoCrFeNiAlx High-Entropy Alloy. *Metals* **2023**, *13*, 1537.
2. Bai, Y.; Liu, C. Estimation of Mechanical Properties of Aluminum Alloy Based on Indentation Curve and Projection Area of Contact Zone. *Metals* **2024**, *14*, 576.
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5. Bucciarelli, F.; Guazzini, A.; Grossi, T.; Macoretta, G.; Monelli, B.D. Constitutive Modeling of Creep–Fatigue Interaction in 1Cr-1Mo-0.25V Steel for Hold-Time Testing. *Metals* **2025**, *15*, 1014.