crystals

MDPI

Editorial

Characterization and Modelling of the Deformation and Failure of Engineering Metallic Materials

Hui Wang [1,2,*], Lihong Su [3,*], Ebad Bagherpour [4,*] and Qiang Xing [1]

[1] School of Mechanical Engineering, Nantong University, Nantong 226019, China
[2] Institute of Industrial Science (IIS), The University of Tokyo, Kashiwa 277-8574, Chiba, Japan
[3] School of Mechanical, Materials, Mechatronic and Biomedical Engineering, University of Wollongong, Wollongong, NSW 2522, Australia
[4] Brunel Centre for Advanced Solidification Technology (BCAST), Brunel University London, Uxbridge UB8 3PH, UK
* Correspondence: hw737ntu@163.com (H.W.); lihongsu@uow.edu.au (L.S.); ebad.bagherpour@brunel.ac.uk (E.B.)

Metallic materials are at the heart of modern industry and infrastructure, valued for their outstanding strength, ductility, and other excellent mechanical properties [1,2]. The deformation and failure in these materials are inherently multiscale and multifactorial phenomena [2,3]. At the atom- or micro-scale, they originate from dislocation motion, twinning, phase transformation, void nucleation, etc. [1,4]. Plastic deformation and failure are strongly shaped by how different microstructural features interact with one another [4,5]. As we push for lighter structures [6–8], greater durability in harsh environments [9,10], and longer service lives [11–13], understanding how metals deform and fail has become more important—and more challenging—than ever. For this purpose, both advanced characterization techniques and numerical modelling methods have been developed.

Material characterization techniques have advanced quickly in recent decades [14,15], which offers insights into deformation mechanisms at a wide range of length and time scales. At the micro-scale, in situ mechanical testing using electron microscopy allows for the direct observation of dislocation activity [14], phase evolution [16], and crack propagation during loading [15]. Techniques like Scanning electron microscopy (SEM), electron backscatter diffraction (EBSD), and transmission electron microscopy (TEM) are widely used to reveal local crystal orientations, microstructural features, and areas of strain, offering a detailed understanding of how materials deform at the grain level [15]. At larger scales, digital image correlation (DIC) techniques offer full-field strain mapping during mechanical tests [17,18], revealing heterogeneity in strain distribution and early signs of localized deformation. Meanwhile, X-ray diffraction, particularly using synchrotron radiation, has enabled the measurement of internal stresses, lattice strains, and phase distributions [19]. Emerging techniques, such as 3D tomography, atom probe tomography (APT), and a focused ion beam (FIB), allow for the three-dimensional reconstruction of microstructures [19–22].

Numerical modelling techniques have also progressed significantly. The finite element method (FEM) remains a cornerstone of mechanical simulation. The conventional FEM relies on phenomenological constitutive models, which does not consider microstructural factors [23–25]. When crystal plasticity models are integrated into finite element simulations, crystal plasticity finite element methods (CPFEMs) can account for the orientation of crystals and the specific slip systems that operate during deformation [26–28]. The microstructure in a CPFEM can originate from EBSD data, ensuring more accurate predictions [29,30]. At a lower scale, discrete dislocation dynamics (DDD) simulations capture

Received: 30 June 2025
Accepted: 7 July 2025
Published: 11 July 2025

Citation: Wang, H.; Su, L.; Bagherpour, E.; Xing, Q. Characterization and Modelling of the Deformation and Failure of Engineering Metallic Materials. *Crystals* **2025**, *15*, 642. https://doi.org/10.3390/cryst15070642

the collective behaviour of dislocations and their interactions [31], while molecular dynamics (MD) simulations provide atomistic insights into mechanisms such as dislocation nucleation, phase transformation, and grain boundary migration [32,33]. Though computationally intensive, these numerical approaches are invaluable for exploring deformation phenomena that are difficult to observe experimentally. This Special Issue has collected works regarding the recent progress concerning on the above-mentioned topics.

Zhang et al. [34] used cavitation water jet peening (CWJP) to strengthen the surface of the 7075 aluminum alloy. The process increased surface hardness from 109.2 Hv to 144.0 Hv, with the strengthening effect extending up to 600 μm deep. In another study by Ding et al. [35], laser shock peening was also used to improve the fatigue life of 1Cr18Ni9Ti. It was found that the 3J category produced the best result due to the optimal grain refinement and residual compressive stress. Abdi et al. [36] applied twin parallel channel angular extrusion (TPCAE) to an AZ91 cast magnesium alloy to improve its hydrogen storage properties. The TPCAE process was conducted at temperatures from 340 °C to 200 °C, and the hydrogen absorption and desorption tests were measured at 250 °C, 300 °C, and 350 °C. Three TPCAE passes at 250 °C resulted in the best absorption capacity, i.e., 6.1 wt.% within a time span of 2000s. To enhance the welding quality of aluminum and steel, Zhang et al. [37] placed a copper and a nickel coating on the surface of the former and latter, respectively. This interlayer copper–nickel binary coating suppressed the formation of brittle intermetallic compounds, and the welding quality was increased by 56% compared to the uncoated aluminum–steel welding.

Chen et al. [38] conducted dry sliding tribometric tests with different loads to evaluate the mild–severe wear transition of the 2095 Al-Li alloy. The wear rate grew slowly when the load was 2–4N, grew fast at a medium load (8–16N), and grew gradually at loads from 32N to 40N. SEM mapping shows that the abrasion and oxidation were significant during the transition from mild to severe wear, and the tribo-induced plastic deformation of the substrate is the reason for this wear transition. Wang et al. [39] used multiple misorientation parameters, derived from EBSD mapping, to evaluate the plastic damage, including the grain reference orientation deviation (GROD), grain orientation spread (GOS), grain orientation spread over the grain diameter (GOS/D), and the geometrically necessary dislocation (GND). It was found that the GOS/D was a reasonable indicator for the plastic damage in 316 steels. The underlying mechanism for plastic deformation and damage is dislocation movement, and thus understanding the behaviours of dislocation movement is critically important. Chang et al. [40] used an indentation stress relaxation process to study the dislocation velocity and stress exponent in commercial pure aluminum, and this exponent was found to be 2.5 ± 0.5 for ambient temperature.

Shen et al. [30] conducted CPFEM simulations to investigate the influence of ultrafine-grained (UFG) austenite on the mechanical properties of medium-Mn steel by comparing the stress and strain between the samples with and without austenite. The 3D EBSD-scanned microstructure was modelled to ensure high fidelity, where the grain morphology, crystallographic orientation, and phase composition were preserved. The UFG austenite was found to be a main contributor to the ductility and strength of medium-Mn steel. CPFEM simulations were carried out to evaluate the sensitivity of the nanoindentation stress relaxation methodology to the dislocation velocity-stress exponent [40]. Compared to the uniform-field and mean-field methods, the full-field CPFEM requires a large amount of computation time, since homogenization is not theoretically assumed. Liu et al. [41] utilized a Submodel method to exceedingly enhance the mesh resolution in areas of interest, and the CPFEM simulations successfully captured the weak texture components and local deformation. Qin et al. [33] performed molecular dynamics simulations to systemically study the behaviours of crack propagation in the Ni-based superalloy. It was found that high-stress triaxiality promoted

brittle cracking, while low-stress triaxiality enhanced the plastic crack; the cracks grow slowly when they are located in the γ and γ' phase; the γ/γ' phase interface hinders the crack propagation when the crack is perpendicular to the γ/γ' interface.

As metal processing techniques continue to evolve, we are seeing the development of more advanced materials with increasingly complex microstructures. These advances call for equally sophisticated tools to understand how structure influences performance. This Special Issue aims to present state-of-the-art developments in this vibrant field, and to deepen our understanding of how metals deform and fail. As Guest Editors, we hope you find this Special Issue helpful and inspiring. Finally, we are deeply grateful to the authors for their publications, to the reviewers for their time and comments, and to the Editorial team for their suggestions and support.

Author Contributions: The authors equally contributed to this work. All authors have read and agreed to the published version of the manuscript.

Funding: L.S. acknowledges the financial support from the Australian Research Council (ARC) through the Discovery Early Career Researcher Award (DECRA) fellowship (No. DE180100124). H.W. was supported by the Large Instruments Open Foundation of Nantong University (KFJN2428), the Test Centre of Nantong University.

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

References

1. Singh, M.; Kumar, P.; Biswas, A. An overview of recent developments in Al metal matrix nanocomposites for strength-ductility synergy. *Mater. Today Proc.* **2022**, *80*, 168–175. [CrossRef]
2. Sohrabi, M.J.; Kalhor, A.; Mirzadeh, H.; Rodak, K.; Kim, H.S. Tailoring the strengthening mechanisms of high-entropy alloys toward excellent strength-ductility synergy by metalloid silicon alloying: A review. *Prog. Mater. Sci.* **2024**, *144*, 101295. [CrossRef]
3. Zhao, L.; Zheng, W.; Hu, Y.; Guo, Q.; Zhang, D. Heterostructured metal matrix composites for structural applications: A review. *J. Mater. Sci.* **2024**, *59*, 9768–9801. [CrossRef]
4. Wang, S.; Hu, Z.; Huang, Z.; Gao, B.; Chen, X.; Hu, J.; Zhu, Y.; Li, Y.; Zhou, H. New deformation mechanism and strength-ductility synergy in pure titanium with high density twin. *Int. J. Plast.* **2024**, *174*, 103908. [CrossRef]
5. Gupta, A.; Khatirkar, R.; Singh, J. A review of microstructure and texture evolution during plastic deformation and heat treatment of β-Ti alloys. *J. Alloy Compd.* **2022**, *899*, 163242. [CrossRef]
6. Georgantzia, E.; Gkantou, M.; Kamaris, G.S. Aluminium alloys as structural material: A review of research. *Eng. Struct.* **2021**, *227*, 111372. [CrossRef]
7. Verma, R.P.; Lila, M.K. A short review on aluminium alloys and welding in structural applications. *Mater. Today Proc.* **2021**, *46*, 10687–10691. [CrossRef]
8. Bai, J.; Yang, Y.; Wen, C.; Chen, J.; Zhou, G.; Jiang, B.; Peng, X.; Pan, F. Applications of magnesium alloys for aerospace: A review. *J. Magnes. Alloy* **2023**, *11*, 3609–3619. [CrossRef]
9. Ou, Y.; Wang, H.; Zhao, Y.; Zhou, Q.; Luo, C.; Hua, Q.; Ouyang, X.; Zhang, S. Recent advances and strategies for high-performance coatings. *Prog. Mater. Sci.* **2023**, *136*, 101125. [CrossRef]
10. Zhang, J.; Miao, J.; Balasubramani, N.; Cho, D.H.; Avey, T.; Chang, C.-Y.; Luo, A.A. Magnesium research and applications: Past, present and future. *J. Magnes. Alloy* **2023**, *11*, 3867–3895. [CrossRef]
11. Liu, H.; Yu, H.; Guo, C.; Chen, X.; Zhong, S.; Zhou, L.; Osman, A.; Lu, J. Review on Fatigue of Additive Manufactured Metallic Alloys: Microstructure, Performance, Enhancement, and Assessment Methods. *Adv. Mater.* **2023**, *36*, e2306570. [CrossRef] [PubMed]
12. Zheng, Z.; Zhan, M.; Fu, M.W. Microstructural and geometrical size effects on the fatigue of metallic materials. *Int. J. Mech. Sci.* **2022**, *218*, 107058. [CrossRef]
13. Farh, H.M.H.; Seghier, M.E.A.B.; Zayed, T. A comprehensive review of corrosion protection and control techniques for metallic pipelines. *Eng. Fail. Anal.* **2022**, *143*, 106885. [CrossRef]
14. Li, S.; Powell, C.A.; Mathaudhu, S.; Gwalani, B.; Devaraj, A.; Wang, C. Review of recent progress on in situ TEM shear deformation: A retrospective and perspective view. *J. Mater. Sci.* **2022**, *57*, 12177–12201. [CrossRef]
15. Gussev, M.; McClintock, D.; Byun, T.; Lach, T. Recent progress in analysis of strain-induced phenomena in irradiated metallic materials and advanced alloys using SEM-EBSD in-situ tensile testing. *Curr. Opin. Solid State Mater. Sci.* **2023**, *28*, 101132. [CrossRef]

16. Zhao, H.; Zhu, Y.; Ye, H.; He, Y.; Li, H.; Sun, Y.; Yang, F.; Wang, R. Atomic-Scale Structure Dynamics of Nanocrystals Revealed by In Situ and Environmental Transmission Electron Microscopy. *Adv. Mater.* **2023**, *35*, e2206911. [CrossRef]
17. Weidner, A.; Biermann, H. Review on Strain Localization Phenomena Studied by High-Resolution Digital Image Correlation. *Adv. Eng. Mater.* **2021**, *23*, 2001409. [CrossRef]
18. Janeliukstis, R.; Chen, X. Review of digital image correlation application to large-scale composite structure testing. *Compos. Struct.* **2021**, *271*, 114143. [CrossRef]
19. Guo, E.; Du, Z.; Chen, X.; Chen, Z.; Kang, H.; Cao, Z.; Lu, Y.; Wang, T. Development of magnesium alloys: Advanced characterization using synchrotron radiation techniques. *J. Mater. Sci. Technol.* **2024**, *195*, 93–110. [CrossRef]
20. Li, P.; Chen, S.; Dai, H.; Yang, Z.; Chen, Z.; Wang, Y.; Chen, Y.; Peng, W.; Shan, W.; Duan, H. Recent advances in focused ion beam nanofabrication for nanostructures and devices: Fundamentals and applications. *Nanoscale* **2020**, *13*, 1529–1565. [CrossRef]
21. Hu, R.; Jin, S.; Sha, G. Application of atom probe tomography in understanding high entropy alloys: 3D local chemical compositions in atomic scale analysis. *Prog. Mater. Sci.* **2022**, *123*, 100854. [CrossRef]
22. Baba, N.; Hata, S.; Saito, H.; Kaneko, K. Three-dimensional electron tomography and recent expansion of its applications in materials science. *Microscopy* **2022**, *72*, 111–134. [CrossRef]
23. Wang, H.; Su, L.; Yu, H.; Lu, C.; Tieu, A.K.; Liu, Y.; Zhang, J. A new finite element model for multi-cycle accumulative roll-bonding process and experiment verification. *Mater. Sci. Eng. A* **2018**, *726*, 93–101. [CrossRef]
24. Zhang, Z.; Gu, G.X. Finite-Element-Based Deep-Learning Model for Deformation Behavior of Digital Materials. *Adv. Theory Simulations* **2020**, *3*, 2000031. [CrossRef]
25. Bate, P.; Ashby, M.F.; Humphreys, F.; Sellar, C.; Shercliff, H.; Stowell, M. Modelling deformation microstructure with the crystal plasticity finite–element method. *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.* **1999**, *357*, 1589–1601. [CrossRef]
26. Roters, F.; Eisenlohr, P.; Hantcherli, L.; Tjahjanto, D.; Bieler, T.; Raabe, D. Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications. *Acta Mater.* **2010**, *58*, 1152–1211. [CrossRef]
27. Renversade, L.; Quey, R. Intra-grain orientation distributions in deformed aluminium: Synchrotron X-ray diffraction experiment and crystal-plasticity finite-element simulation. *Acta Mater.* **2023**, *262*, 119419. [CrossRef]
28. Zhou, X.; Zan, S.; Zeng, Y.; Guo, R.; Wang, G.; Wang, T.; Zhao, L.; Chen, M. Comprehensive study of plastic deformation mechanism of polycrystalline copper using crystal plasticity finite element. *J. Mater. Res. Technol.* **2024**, *30*, 9221–9236. [CrossRef]
29. Depriester, D.; Goulmy, J.; Barrallier, L. Crystal Plasticity simulations of in situ tensile tests: A two-step inverse method for identification of CP parameters, and assessment of CPFEM capabilities. *Int. J. Plast.* **2023**, *168*, 103695. [CrossRef]
30. Shen, P.; Liu, Y.; Zhang, X. Crystal Plasticity Finite Element Modeling of the Influences of Ultrafine-Grained Austenite on the Mechanical Response of a Medium-Mn Steel. *Crystals* **2024**, *14*, 405. [CrossRef]
31. Frankus, F.; Pachaury, Y.; El-Azab, A.; Devincre, B.; Poulsen, H.F.; Winther, G. Investigating the formation of a geometrically necessary boundary using discrete dislocation dynamics. *J. Mech. Phys. Solids* **2025**, *199*, 106069. [CrossRef]
32. Yuan, T.; He, N.; Ma, S.; Cheng, Y.; Jiang, Y.X.; He, L.; Chen, C.; Chen, Y.; Ye, H. Atomic structure and molecular dynamics simulation of a symmetrical tilt $[0\bar{1}1](511)\Sigma 27$ grain boundary in polysynthetically twinned TiAl crystals. *Mater. Charact.* **2025**, *227*, 115275. [CrossRef]
33. Qin, X.; Liang, Y.; Gu, J. Effects of Stress State, Crack—γ/γ' Phase Interface Relative Locations and Orientations on the Deformation and Crack Propagation Behaviors of the Ni-Based Superalloy—A Molecular Dynamics Study. *Crystals* **2023**, *13*, 1446. [CrossRef]
34. Zhang, Z.; Yang, Y.; Gao, Y.; Wang, G.; Shi, W. Performance Analysis of 7075 Aluminum Alloy Strengthened by Cavitation Water Jet Peening at Different Scanning Speeds. *Crystals* **2022**, *12*, 1451. [CrossRef]
35. Ding, X.; Ma, S.; Zhang, J.; Jiang, Z.; Li, H.; Wang, S.; Wang, C.; Zhong, J. Numerical Simulation and Process Study on Laser Shock Peening of 1Cr18Ni9Ti Material. *Crystals* **2023**, *13*, 1279. [CrossRef]
36. Abdi, M.; Ebrahimi, R.; Bagherpour, E. Improvement of Hydrogenation and Dehydrogenation Kinetics of As-Cast AZ91 Magnesium Alloy via Twin Parallel Channel Angular Extrusion Processing. *Crystals* **2022**, *12*, 1428. [CrossRef]
37. Zhang, H.; Gu, H.; Ma, D. Experimental Study on Laser Lap Welding of Aluminum–Steel with Pre-Fabricated Copper–Nickel Binary Coating. *Crystals* **2025**, *15*, 300. [CrossRef]
38. Chen, Q.; Yu, Y.; Ma, G.; Sun, X.; Lu, L. Dry Sliding Wear Behavior and Mild–Severe Wear Transition of the AA2195-T6 Alloy under Different Loads. *Crystals* **2023**, *13*, 698. [CrossRef]
39. Wang, X.; Du, Z.; Zhang, F.; Zhu, Y.; Liu, Y.; Wang, H. Plastic Damage Assessment in 316 Austenitic Steel Using the Misorientation Parameters from an In Situ EBSD Technique. *Crystals* **2022**, *12*, 1126. [CrossRef]

40. Chang, T.-Y.; Vandenbroeder, G.; Frazer, D.M.; Yushu, D.; Pitts, S.; Chen, T. Nanoindentation Stress Relaxation to Quantify Dislocation Velocity–Stress Exponent. *Crystals* **2024**, *14*, 680. [CrossRef]
41. Liu, Y.; Zhang, Q.; Ge, Q.; Wang, X.; Shen, Y. Improving Texture Prediction by Increasing Mesh Resolution in Submodel: A Crystal Plasticity FE Study and Experiment Verification. *Crystals* **2023**, *13*, 849. [CrossRef]