J Mater Sci (2024) 59:4723–4727

The Physics of Metal Plasticity: in honor of Professor Hussein Zbib

Preface: the physics of metal plasticity

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Published online:
27 March 2024

Plastic deformation in solids constitutes a multifaceted and intricate multiscale process that remains, to a large extent, not fully understood. Especially, in metals, plasticity is inherently related to the presence and evolution of various types of defects, profoundly affecting the observed microstructures and mechanical response. The challenges in understanding the deformation processes arise primarily from their multiscale nature and the strong coupling between the underlying mechanisms operating at different spatial and temporal scales. The mechanisms of plastic deformation are controlled by many factors such as the atomic structure of the material, the type of defects and the nature of their mutual interactions, as well as the way the thermomechanical stimuli are applied, to mention a few.

This special issue of the Journal of Materials Science is entitled "The Physics of Metal Plasticity" and is dedicated to the memory of our esteemed friend, colleague and mentor Professor Hussein M. Zbib. Professor Zbib who passed away in February 2020, left behind outstanding contributions and achievements in theoretical and computational solid mechanics. Notably, his groundbreaking work in multiscale modeling and simulations of engineering materials showcased his dedication to advancing our understanding of the microscopic facets of plastic deformation in crystalline materials. Professor Zbib's legacy also encompasses pioneering efforts in developing dislocation dynamics simulation framework that has been utilized to enhance our understanding of the microscopic aspects of plastic deformation in crystalline materials. Additionally, his extensive research spanned constitutive modeling of solids, mechanics of nanolaminates, irradiated materials, gradient plasticity, and shock-induced deformation.

Recognized for his many contributions, Professor Zbib was selected a Fellow of the American Association for the Advancement of Science (AAAS) and the American Society of Mechanical Engineers (ASME). His impact extended to the Lebanese Academy of Sciences, where he served as an executive member.

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https://doi.org/10.1007/s10853-024-09584-7

Professor Zbib received the 2003 Computational Mechanics Achievement Award from the Japanese Society of Mechanical Engineers. He was the recipient of the 2010 Khan International Award for outstanding contribution to the field of plasticity. Furthermore, Professor Zbib received research excellence awards from the Voiland College of Engineering and Architecture in 1994 and 2015 and from the School of Mechanical and Materials Engineering in 2000 at Washington State University. In 2018, he was named a Regents Professor, the University's highest faculty recognition.

This special issue features twenty-seven contributions that delve into several aspects of plastic deformation across different length and time scales. Employing several modeling, simulation, and testing methodologies, these studies offer insightful investigations into the intricate dynamics of plasticity. Notably, the role of defects on the mechanical response in pure metals, alloys, and polymers are emphasized. The contributions are sorted according to length scale, including those at which the investigation is conducted.

Topical articles focusing on recent atomistic simulation results and offering a detailed analysis of plasticity in small volumes such as nanolaminates, multilayered materials, thin films, and nanoparticles are presented [1–4]. The roles of dislocation slip, twinning, phase transformations, grain boundaries and interfaces in impact the mechanical response are explored using molecular dynamics (MD) simulations. Hasan et al. [1] investigated the mechanical response and the orientation-dependent deformation of Nb-Zr single crystals. The induced plasticity resulting from dislocation slip, twinning, displacive phase transformation and solute segregation were analyzed. Using transmission electron microscopy (TEM) and MD simulations, Wang et al. [2] studied the effects of residual stress and interface coherency on the mechanical response of nanostructured Al/Ti multilayers. In another related work [3], MD simulations were conducted to determine the factors the affect the scratch resistance of NbC/Nb nanolaminates. It was reported that the scratching response is predominantly influenced by the individual layer thickness, the scratching tool size and scratching attack angle. In another study, the strength of nanolaminated Cu with incoherent interfaces and the role of stacking-fault energy (SFE) on the dislocation core structure and its slip were explored [4]. Aquistapace et al. [5] carried out MD simulations of the nanoindentation of diamond nanoparticles. It is reported that an amorphization phase is detected and remains even during the unloading stage of the nanoindenter. Additionally, a surprising finding of dislocation density increase during unloading is observed and is associated with the formation of a large number of junctions that hinder dislocation motion.

Over the past 3 decades, the simulation of the deformation of materials at the microscopic/mesoscopic scale has seen widespread use of discrete dislocation dynamics (DDD) computations. These techniques have proven invaluable in unraveling uncertainties surrounding complex plastic flow and microstructure-evolution processes. Plastic flow is inherently coupled with the collective behavior of dislocations and their interactions with other defects. In this topic, three contributions utilized DDD computations to investigate several physical and numerical issues in simulating the behavior of large number of dislocations in single and polycrystals. Li and Khraishi [6] carried out verification and validation parametric studies for 3D DDD simulations. The effect of several parameters such as strain rate, initial dislocation density, size effects, solid solution density and the effect of stacking faults were analyzed. Martensitic steel is a high-strength steel that exhibits a hierarchical microstructure consisting of packet, block and lath boundaries. In an effort to understand the interactions between dislocations and boundaries in this material, coupled FEA/3D DDD were carried out to mimic the uniaxial loading condition in martensitic steel [7]. The interactions between the gliding dislocations and all boundaries were examined and parametric studies of the effect of the initial dislocation density, the packet and block size, as well as the lath width were conducted. The dislocation/microstructure evolution during nanoindentation is simulated using a multiscale dislocation-dynamics plasticity model [8]. The effect of the nanoindenter surface, the crystal orientation and the initial dislocation configuration were investigated. In another work that is based on phase-field methodology, the evolution of microstructural features of additively manufactured Ni-based superalloys are simulated using a surrogate model based on a Materials Knowledge System framework using data generated from phase-field simulations [9].

This special issue comprises several articles focused on continuum-modeling approaches of the deformation processes using finite element analyses (FEAs), dislocation-density-based modeling, a crystal-plasticity approach, and damage mechanics modeling. The

results of these continuum simulations were compared with the experimental results obtained from mechanical testing and microstructural characterizations. Nikravesh and Shen [10] conducted 3D FEA of the formation and transformation of wrinkles involving plastic instability in thin films. Their findings indicate that plastic yielding transforms the surface instability patterns into more localized forms that are only partially relieved upon unloading. A combined experimental and FEA of severe plasticity based on linear corrugation and straightening technique in AZ31 alloy was presented [11]. The simulations and the experimental characterizations reveal that the overall strain accumulation was highest in the regions of the specimen with the smallest grain sizes. It was also demonstrated that a relatively simple deformation model can successfully predict the formation of fine and coarse grain development in certain regions with higher and lower shear strains. Moreover, FEM showed the formation of dead zones with very small shear strains. In another study, Vattré [12] presented a 3D formulation applicable to multilayered materials with combined magneto-electro-elastic properties. It was found that stacking arrangement of a tri-layered material significantly influences the stress distribution which consequently affects the sign of the electric and magnetic profiles. Additionally, the role of interfacial defects on the mechanical and electro-magnetic behaviors were assessed. A micro–macro-modeling strategy to simulate the mechanical behavior of the thermally sprayed, AlSi-PES abradable, coating materials is developed whereby xCT scan of the microstructure is combined with a constitutive plasticity and damage models [13].

Dislocation-density-based models are utilized to investigate the texture evolution in polycrystalline metals. The synergetic effect of the grain size gradient and the initial texture on plastic deformation of gradient steel is modeled and assessed using self-consistent viscoplasticity framework [14]. An integrated experimental and dislocation-density-based modeling was used to investigate the microstructural mechanisms and defects in Inconel specimens with different precipitate volume fractions [15]. The observed mechanical response was rationalized based on the formation of short rod-shaped precipitates and the creation of significant total and partial dislocations leading to the increase in both strength and ductility. Nandi et al. [16] conducted crystal plasticity finite element simulations to explore the underlying mechanisms responsible for the observed anisotropic lateral contraction and elliptical tensile fracture surfaces of cylindrical Haynes 282 specimens. It is argued that the anomalous deformation behavior can be attributed to the presence of near single crystal texture of the initial structure.

The mechanical response and texture evolution of metallic samples subjected to equal-channel angular pressing are simulated using coupled continuum dislocation dynamics (CDD) with a crystal plasticity approach [17]. A unique grain fragmentation model was employed, and post-deformation textures were analyzed and discussed in details. Serrano et al. [18] investigated the mechanical behavior and fracture of CMT-welded AA 6061-T651 alloy using coupled continuum damage mechanics and anisotropic plasticity analysis. The predictive capability of the proposed model was verified with experimental measurements of the stress–strain diagrams of the welded samples. Alqawasmi et al. [19] studied the mechanical properties of an Inconel 718 superalloy manufactured by laser-directed energy deposition (L-DED). It was demonstrated that the mechanical properties within the manufactured samples were heterogeneous. It was shown that heat treatment of the L-DED samples, processed optimally, can lead to average properties close to the wrought counterpart.

Two contributions in this issue focused on the mechanical response of polymeric materials [20, 21]. Ghaderi et al. [20] presented a physics-based framework to describe the relationship between elastomeric network mechanics and environmental degradation. Special attention was paid to the effects of thermal aging and cyclic fatigue on the material's behavior, and the predictive capability of the framework was demonstrated. In another investigation [21], the effect of UV-aging on LDPE films and plates is studied. It was found that the stiffness of the samples remains insensitive to aging both overall and sufficiently away from plate surfaces. However, in films and superficial plate layers a significant increase in stiffness is established, which co-exists with a crack pattern that depends on the sample thickness.

In a three-part article, McDowell [22–24] presented a non-equilibrium statistical thermodynamics framework for thermally activated dislocation processes in metals and alloys. The thermodynamics foundations of internal state variables (ISV) are used to investigate the micro-mechanistic origins of dislocation reactions whereby Gibbsian incremental thermodynamics is employed to address the thermal activated reactions in a way that is consistent with ISV theory. Certain

concepts that are important to connect all relevant aspects of dislocation viscoplasticity are presented [23] such as definition of the intrinsic entropy rate produced by reactions, the evolution of internal stresses and their role in increasing the degree of correlation of reaction enthalpy barriers, within and among subsystems of the ensemble, and the interpretation of origins of the maximal intrinsic entropy production (MEP) rate principle in terms of an increasing number density of reactions. The maximal intrinsic entropy production rate or MEP heuristic is considered in the context of this framework. It is argued that maximization of the number density of likely reactions, with the configurational entropy change of pending reactions as a proxy at each step of the process, facilitates increasing correlation of enthalpy barriers within and among subsystems along the nonequilibrium ensemble trajectory, and the flow rules in common crystal plasticity models are considered to conform to fully correlated conditions of a single rate-limiting barrier strength. Moreover, the statistical thermodynamics framework is contrasted against contemporary theories that emphasize the role of configurational entropy of dislocations. The utility of atomistic simulation and DDD method in advancing our understanding of outstanding issues related to thermally activated dislocation processes are discussed [24]. In a related work [25], a thermodynamic class of crystal plasticity models is used to predict the stored energy and Taylor–Quinney coefficient of copper and aluminum single crystals as well as polycrystalline austenitic steel, 316L. The contributions of statistically stored dislocations and geometrically necessary dislocations for the stored energy prediction are analyzed.

Along with the computational and modeling methodologies discussed above, mechanical testing and microscopic characterization were used to investigate tested samples. In situ SEM tensile tests were performed to study the mechanical response of nanoscale fibrous Al–Si and Al–Si–Sr eutectic colonies and colony boundaries [26]. The strength of a single colony is found to be highly dependent on the orientation of Si nanofibers relative to the loading direction. Tensile samples with multiple colonies exhibited improved strain hardening, but the measured ductility was limited by cracking at colony boundaries. Finally, a review of the latest research progress on phase change materials (PCMs) enhanced by nanomaterials was presented [27]. The variety of nanomaterials, the synthesis of nanocomposite PCMs, the effect of nanomaterials on the thermal conductivity of PCMs, and the application of nanocomposite PCMs were summarized.

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