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Interface Behavior

Understanding mechanical behavior of interfaces in materials

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The response/performance of technologically relevant materials to mechanical loading environments in various applications is influenced and characterized by the presence and evolution of various interfaces. The fundamental understanding of the links between various characteristics of the interfaces (structural, chemical) and the mechanical response is a critical challenge in exploiting and tailoring new physical properties of materials for next-generation applications. The review papers and topical articles in this "Special Issue on Interface Behavior" emphasize the latest advances and also identify open questions and longer-term needs in the understanding of the mechanical behavior of interfaces in several thematic areas of materials research. The articles highlight the current experimental, theoretical and computational capabilities and limitations to understand various interface dominated phenomena and deformation mechanisms that determine the microstructural evolution and/or properties/behavior of materials across multiple scales. The various contributions through the review and topical articles are summarized below.

The review article by Clayton [1] discusses the current capabilities of mesoscale modeling methods based on the representation of interfaces on predicted deformation and failure phenomena using continuum mechanics frameworks. This review emphasizes the effects of the description of grain boundaries, twinning and failure processes using a variety of continuum mechanics models.

An "atomistically informed interface dislocation dynamics (AIDD) model" that incorporates the atomic-scale characteristics of dislocation nucleation,

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interactions and reactions at interfaces using a "geometrical interface classifications" (GIC) method is reviewed in the article by Shao et al. [2]. This framework provides an approach to map correlations between the structure and the deformation behavior of interfaces in nanolaminate microstructures and shows promise toward predictive modeling of materials behavior across multiple scales.

The recent experimental, theoretical and computational studies related to the deformation behavior of nanolayered composites comprising of metal/ceramic interfaces are reviewed by Li and Liu [3]. In particular, the review provides details of atomic-scale deformation mechanisms as observed during in situ TEM straining for the Al/TiN, Al/AlN and Cu/TiN interfaces and that predicted using density functional theory and dislocation dynamics simulations.

The current experimental insights in the deformation behavior of biphase interfaces and the capabilities and limitations of current mesoscale methods discrete dislocation dynamics and Peierls–Nabarro models for slip transfer are highlighted in the review article by Hunter et al. [4]. The review emphasizes the advances in the "phase field dislocation dynamics (PFDD) method" to model the mechanisms of slip transfer in FCC/FCC interfaces and also identifies the critical challenges in mesoscale modeling of microstructural evolution of BCC and HCP metals comprising of surfaces and voids.

The characterization capabilities and advances of the deformation behavior of metal/ceramic interfaces are discussed in the review article by Damadam et al. [5]. This review highlights the role of thickness and structure of interface layers on the atomic-scale mechanisms of nucleation and interaction of dislocations as predicted using classical molecular dynamics (MD) simulations of deformation of Nb/NbC and Ti/TiN multilayer composites.

An array of research highlights in the field of bone tissue engineering that identify the factors in the design of new biomaterials for implantable scaffolds based on concepts of cellular mechanotransduction that are critical to make and regenerate bone are reviewed by Assanah and Khan [6]. The review emphasizes the use of mechanical forces to evoke a cellular response that varies with the types of cells and the type of environment supporting the cells. Such insights are invaluable for the design of biomaterial-based constructs for regeneration of bone.

The state-of-the-art modeling capabilities to describe phonon effects in materials are emphasized in the review article by VanGessel et al. [7]. The review highlights the capabilities and limitations of the Boltzmann transport equation, lattice dynamics and MD simulation methods relevant to surface and interface effects as compared to that in bulk materials.

Several topical articles demonstrate the capability of "classical molecular dynamics simulations" to extract atomic-scale mechanisms that influence the deformation response. These include: deformation behavior of Ni/NiAl Kurdjumov–Sachs (KS) interfaces at various strain rates and temperatures by Choudhuri et al. [8]; temperature effects on deformation behavior of grain boundaries in a polycrystalline microstructure by Smith and Farkas [9]; deformation behavior of various grain boundaries in bicrystal microstructures of yttria-stabilized tetragonal zirconia (YSTZ) by Zhang et al. [10]; Hugoniot of CuZr metallic glasses for various impact velocity compositions of the microstructure by Wen et al. [11]; structure and deformation mechanisms at the Kurdjumov–Sachs interface using a newly developed embedded atom method interatomic potential for Mg–Nb by Yadav et al. [12]; and shock deformation and spallation failure behavior in a nanocrystalline Cu matrix as influenced by the size and distribution of nanoscale Cu/Ta interfaces by Chen et al. [13].

Several other topical articles highlight modeling methods to investigate the deformation behavior of interfaces. These include: steered MD simulations by Kim et al. [14] to investigate the exfoliation behavior of graphene oxide sheets due to the interactions with ethanol, methanol and water; a "phase field modeling method" that combines anisotropic interfacial energy and elasticity effects to predict critical conditions for surface roughening of SiGe thin films on Si for various orientations by Zhang et al. [15]; a "dislocation density-based crystal plasticity finite element framework" to predict transgranular and intergranular fracture based on dislocation density evolution models for transmission and pileup processes by Bond et al. [16]; a "multiphysics phase field modeling method" that incorporates heat conduction and elastic loading to model microstructural evolution of powder particles during sintering by Biswas et al. [17].

In addition, topical articles highlighting current experimental characterization capabilities include: deformation behavior of Si nanosprings comprising

of various morphologies to evaluate their potential as compliant interface layers by Antartis et al. [18] using nanoindentation and SEM characterization; debonding mechanisms, i.e., crack nucleation and propagation at the interface between an epoxy fiber and the glass matrix interface by Chu et al. [19] to test the strength of the interface under dynamic loading conditions using high-speed synchrotron X-ray phase-contrast imaging; oxidation-based strengthening behavior in nanolaminate structures of Zr and Nb by Monclús et al. [20] using nanoscale mechanical testing and analytical electron microscopy; and effects of nanofiller reinforcements on the deformation and fracture behavior in layered ceramic–polymer composites by Livanov et al. [21] using in situ optical microscopy and post-fracture electron microscopy.

A few notable reviews (not included in this special issue) on properties and performance of materials related to mechanical response include: mechanical behavior of interfaces in 2D materials by Akinwande et al. [22] and by Liu and Wu [23]; strain engineering of 2D materials by Ahn et al. [24]; experimental characterization of mechanical behavior of interfaces and interphases by Kalidindi et al. [25]; modeling methods across multiple scales by McDowell [26]; mechanical behavior of biomaterials by Meyers et al. [27]; the mechanical behavior of metallic glasses by Trexler and Thadhani [28]; and high-strain rate response by Gray III [29]. A few notable topical articles (not included in this special issue) discuss the capabilities and limitations of current methodologies/techniques to understand the behavior of materials under a variety of environments including: high-strain rate experimental methods [30]; in situ experimental techniques by Singh et al. [31]; coarse-graining-based methodologies [32, 33]; ICME by Panchal et al. [34]; and machine learning methods [35].

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