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Mechanistic coupling of dislocation and shear transformation zone plasticity in crystalline-amorphous nanolaminates

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ABSTRACT

The deformation behavior of crystalline-amorphous nanolaminates is explored through molecular dynamics simulations using nanolaminate models that contain columnar nanograins in the crystalline layers to more closely resemble experimentally accessible nanolaminate structures. Quantitative analysis of the plastic strain distribution among competing mechanisms and their coupling at the nanoscale is accomplished through the implementation of continuum deformation metrics. The transfer of plastic strain between shear transformation zone (STZ) and dislocation plasticity initially transpires through the emission of dislocations from STZ activity impinging on the amorphous-crystalline interface (ACI). The addition of grain boundaries biases this process to regions near the boundaries at low strains, which reduces the activation barrier for the onset of dislocation plasticity. With increasing strain, dislocations are absorbed into the amorphous layers via slip transfer across the ACI, in turn triggering the activation of new STZs. Cooperative slip transfer between dislocations and STZs suppresses grain boundary microcracking collectively with large-scale shear localization, and provides an explanation for the enhanced toughness of crystalline-amorphous nanolaminates.

1. Introduction

The mechanical behavior of nanocrystalline metals has been studied extensively over the past decade to understand the fundamental physics underpinning their remarkable strength and unusual deformation physics [1–6]. The illustrious Hall-Petch scaling law, which describes the increase in strength with grain size reduction [7,8], captures strength scaling well into the nanocrystalline regime and is a consequence of grain boundaries inhibiting the mobility of dislocations [9,10]. However, at grain sizes of about 10–20 nm, the Hall-Petch relationship breaks down [5,11,12] and classical dislocation dynamics shift to grain boundary-mediated dislocation processes [13–15]. The net accumulation of dislocations at grain boundaries during deformation often leads to grain boundary microcracking [6], which limits the ductility of nanocrystalline metals to about a few percent tensile elongation to failure [3,16].

One promising route to improving the ductility of nanocrystalline metals is using gradient nanostructures containing, e.g., bimodal nanocrystalline grain size distributions [17] or periodically modulated crystalline-amorphous patterned structures [18]. While amorphous metals also suffer from limited plastic strain prior to fracture as a result of shear localization [19–21], a number of observations have suggested that the synergistic interaction between dislocation and shear transformation zone (STZ) plasticity across the amorphous-crystalline interface (ACI) can fundamentally alter the mechanical behavior [18,22–25]. These materials represent a specific subset of metallic multilayers often referred to as crystalline-amorphous nanolaminates, and have demonstrated the sought-after combination of high strength (>1.0 GPa) and improved tensile elongation to failure (>13%) that has eluded equiaxed nanocrystalline metals for over a decade [18,22,26–31].

In light of the critical role grain boundaries play in the deformation physics of nanocrystalline metals, the introduction of incoherent interfaces (i.e. ACIs) can be expected to open up new regimes in the mechanical behavior. In equiaxed nanocrystalline Ni-W alloys, Rupert et al. [32] demonstrated that through manipulation of the interfacial state, defect sources can be limited for enhancing strength without augmenting the fundamental mechanisms accommodating plasticity. It is in this vein that ACIs have been employed to engineer sources and sinks for defects in crystalline-amorphous nanolaminates, and a pioneering example is

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found in the Cu-Cu_3Zr system studied by Wang et al. [18]. These materials exhibited exceptional ductility relative to both crystalline metallic multilayers and equiaxed nanocrystalline Cu while retaining a yield strength of ~1 GPa. Measurements of the activation volume and strain rate sensitivity were consistent with interface-mediated dislocation plasticity [27], and substantiated post-mortem transmission electron microscopy (TEM) observations.

Several additional studies have demonstrated ductility improvements in crystalline-amorphous nanolaminates citing comparisons with equiaxed nanocrystalline metals [31,33,34] while others have focused on understanding the implications of the hierarchical structure for limiting shear localization in the amorphous regions [22]. Introduction of the nanocrystalline layers inherently disrupts the continuity of the amorphous phase, which has been demonstrated to constrain shear band growth [35] and promote homogenous plastic flow [36]. Simultaneously, the inherent structural length scale defined by the thickness of the amorphous layers suppresses the onset of shear instabilities. Citing the aged-rejuvenation-glue-liquid shear band model [37], Wang et al. suggested that shear localization was inhibited when the amorphous layer thickness was less than a critical incubation length scale required for STZs to evolve into a mature shear band [18]. Despite conceptual differences in the synergistic effects of yielding in each phase, a number of studies [38–40] have substantiated the embryonic shear band argument for suppressing shear instabilities in crystalline-amorphous nanolaminates.

Significant insight has been gained on the coupling between dislocation and STZ plasticity through compression and nanoindentation experiments, which facilitate plastic strain accumulation without the onset of early fracture that results from localization in tension. By analyzing the plastic zone beneath the indents via correlative atom probe tomography and TEM, Guo et al. determined that dislocation glide in the crystalline Cu layers coincided with shear banding in the CuZr amorphous layers [24,25,41]. Microcompression testing of Cu/CuZr nanolaminates by Zhang et al. [23,42] revealed that dislocation-free nanocrystalline layers were accompanied by the nucleation of nanocrystallites within the amorphous layers. This deformation-induced partial devitrification was attributed to the transfer of plastic strain upon the absorption of dislocations across the ACI into the amorphous layers. Despite these compelling observations, assessment of the mechanistic coupling between dislocation and STZ plasticity has been largely based on inferences from post-mortem analysis of defects or other local structural changes.

Atomistic nanolaminate models are particularly convenient for direct investigation of deformation mechanisms as a function of the hierarchical structural length scales and deformation conditions (e.g. temperature, strain rate, loading direction) [43]. The triggering of STZs upon the absorption of dislocations in the amorphous layers was demonstrated in the uniaxial tensile simulations conducted by Wang et al. [18] on nanolaminates containing single crystal Cu layers. This finding was further substantiated in the simulations by Pan and Rupert [44] on bicrystals containing amorphous intergranular films, which acted as efficient sinks for dislocations that delayed the onset of interfacial cracking relative to “clean” grain boundaries. Brandl et al. [28] explored Cu-CuZr crystalline-amorphous nanolaminates comparable to the previously described simulation structures under shear deformation boundary conditions. Interfacial shear was accommodated by the emission and propagation of dislocations at the ACI, in turn facilitating co-deformation of the nanolaminate phases. Interfacial sliding has also been connected to localized STZ plasticity acting in cooperation with dislocation motion by Chen et al. [45]. Finally, the addition of free surfaces under simulated compressive loading by Arman et al. [46] revealed that dislocations, particularly of screw orientation, nucleated from the free surfaces but were subsequently absorbed at the ACIs.

The coupling between dislocation and STZ plasticity at the ACIs in crystalline-amorphous nanolaminates provides a new mechanism for accommodating plastic strain during deformation. While several pioneering experiments have demonstrated the unique combination of strength and ductility afforded by the co-deformation of the crystalline and amorphous phases, mechanistic insights have largely been inferred from post-mortem deformation structures. Molecular dynamics simulations have been successful in capturing transient coupling events between the disparate deformation mechanisms operating at the ACIs. Despite these perceptive results, a number of open questions must be addressed to bridge the deformation physics from simulations with experimental mechanical behavior measurements. Perhaps one of the most important issues is that the existing computational models employ single crystal orientations completely absent of grain boundaries, which represent a critical feature in the deformation of nanostructured metals. How will grain boundaries bias the onset of dislocation and STZ plasticity in the respective regions of the nanolaminate, and what are their implications for the interfacial deformation physics? With a better understanding of the synergistic interactions between grain boundaries, ACIs, and the mechanisms accommodating plastic strain at the nanoscale, nanolaminate architectures can be designed to expand the strength-ductility envelope in nanostructured metals.

In this paper, a new crystalline-amorphous nanolaminate model is constructed that incorporates grain boundaries through the addition of columnar nanocrystalline grains in the crystalline layers to more closely resemble experimentally accessible nanolaminate structures. Uniaxial tensile deformation is accomplished using molecular dynamics with a strain rate of 10^8 s^{-1}, and the strain distribution among competing mechanisms is quantified via continuum deformation metrics. Our results demonstrate that STZ activity at the ACI is influenced by the presence of grain boundaries and responsible for the emission of interfacial dislocations, which are absorbed collectively by grain boundaries and the amorphous layers through continued deformation. Dislocation annihilation at the ACIs combined with a reduction in grain boundary plasticity abates grain boundary microcracking, thus providing an explanation for the exceptional ductility exhibited by crystalline-amorphous nanolaminates relative to equiaxed nanocrystalline counterparts.

2. Simulation methods

Molecular dynamics (MD) simulations were carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) platform [47]. The embedded-atom method (EAM) potential developed by Mendelev et al. [48] for the Cu-Zr binary system was employed, as it provides a good representation for both Cu-Zr metallic glasses [48] and pure crystalline Cu [49]. To build the various nanolaminate configurations, a $Cu_{64}Zr_{36}$ amorphous alloy was generated by heating a single crystal Cu-Zr alloy to 2000 K for 2 ns, followed by quenching to 300 K at a cooling rate of 0.01 K ps^{-1}. The single crystal-amorphous nanolaminate (SC-NL) was then constructed by combining a 5 nm-thick layer of the quenched $Cu_{64}Zr_{36}$ amorphous alloy with a 10 nm-thick single crystal Cu layer oriented with the $[11\bar{2}]$, [110], and [111] directions along the x, y and z directions, respectively. The application of periodic boundary conditions and homogenous structure effectively resulted in this configuration requiring only 11,930 atoms to model a 5/10 (i.e. a 5 nm-thick amorphous layer and 10 nm-thick crystalline layer) single crystal-amorphous nanolaminate. The SC-NL is illustrated in Fig. 1a, and is comparable to the structure studied by Wang et al.