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Strength and plastic deformation behavior of nanolaminate composites with pre-existing dislocations

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ABSTRACT

Pre-existing dislocations (PED) are ubiquitous inside crystalline lattices which in turn affect the yield stress and the process of plastic deformation. Hence, understanding the onset of dislocations motion and interaction is critical in modifying or designing new materials with advanced properties so that their mechanical behavior approach realistic conditions. One such family of new materials is the ceramic/metallic nanolaminates. In this work, we have investigated the effect of pre-existing dislocations on the mechanical behavior of NbC/Nb nanolaminates using molecular dynamics simulations. Upon unloading at different strains from stress-strain curve of 3 nm NbC/7 nm Nb sample, we were able to generate structures with various pre-existing dislocation densities inside the layers. Uniaxial loadings parallel to the interface at two different temperatures (10 K and 300 K) were performed on each structure. Also, the yield locus was determined at 300 K by applying biaxial in-plane loading and fitted with a general flow potential to be used in macroscale analysis. Finally, the tension-compression asymmetry (TCA) was investigated for the structures with pre-existing dislocations along two different in-plane loading directions.

1. Introduction

Ceramic/metallic nanolaminate (CMN) composites exhibit high flow strength which is a fraction of theoretical limit, and considerable amount of ductility when the ceramic layer thickness is just a few nano-meters. Combining metals with good ductility and ceramics with high strength and refractory capabilities, leads to novel promising properties and improved performances especially at harsh environments under high pressure and high temperature working conditions. Besides, high corrosion and radiation damage tolerance of CMNs make them unique candidates for coating applications on oil pipelines and nuclear reactors [1–3]. For the above mentioned reasons, the study of the mechanical behavior of CMNs has attracted increasing attention during the recent years [4–6].

Interfaces in nanolaminate composites play an important role in controlling the governing deformation mechanisms and mechanical properties since they act as barriers and sinks to dislocations glide. This role becomes dominant when each individual layer thickness is less than 10 nm due to the very high volume fraction of interfaces [7,8]. In case of coherent interfaces (commensurate) [9] atomic arrangement and slip systems are nearly continuous across the interface [10–12] such that the interface is very strong and allows for dislocation transmission if the coherency stresses (usually of order of GPa), resulting from lattice mismatch, are overcome by the applied stress [13–16]. On the other hand, in semicoherent interfaces (incommensurate), misfit dislocations are formed on the interface that result in reduced interfacial strengths but stronger barriers for incoming dislocations [11,13,17].

Several studies in the literature are focused on the effect of the individual layer thickness and thickness ratio on the mechanical behavior of CMNs. The results revealed a plastic co-deformation behavior of CMNs when the ceramic layer thickness is less than 5 nm. In fact, although ceramics are brittle, at layer thicknesses below 5 nm, dislocations nucleation has been suggested in the ceramic layer without evidence of cracking [7,18–20]. The transition from brittle to ductile has been attributed to the high resolved shear stress caused by the interaction of the dislocations in the

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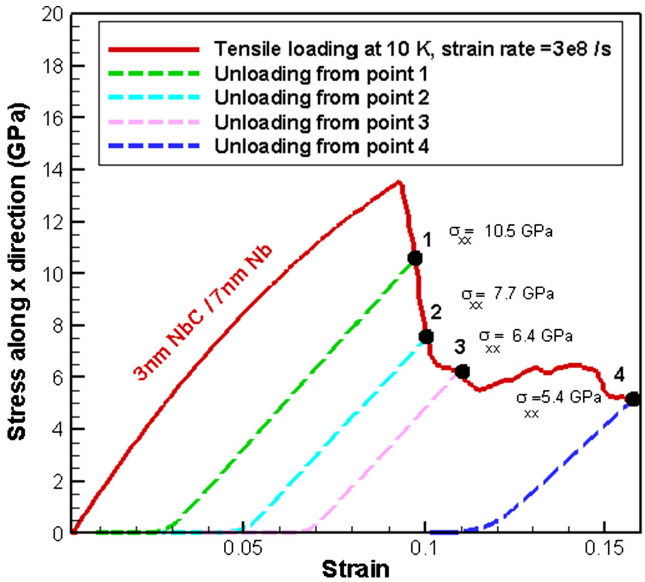

Fig. 1. Stress-strain curve of 3 nm NbC/7 nm Nb nanolaimate under uniaxial tension parallel to the interface unloaded from four different points with different dislocation densities.

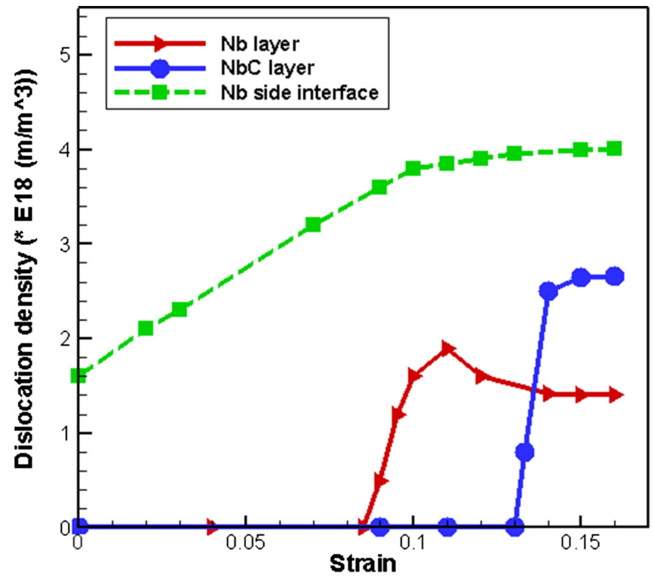

Fig. 3. Dislocation density evolution for 3 nm NbC/7 nm Nb under uniaxial tension with strain rate of 3×10^{8}/s and temperature 10 K.

interfaces of the adjoining layers that facilitates dislocation transmission across the interface [21]. Moreover, by decreasing the ceramic layer thickness, the stress field of nucleated dislocations in the softer layer becomes higher than the interfacial shear strength. That in turn results in the shearing of the interface such that dislocation transmission becomes energetically favorable [22,23].

Various experimental and atomistic efforts have studied the deformation mechanisms and mechanical behavior of CMNs under compression and nanoindentation [3,24–26]. The results showed that the strength and hardness increased as the layer thickness decreased. The mechanical behavior of Ti/TiN under compression were shown to have the same trend at different temperatures implying that deformation mechanisms were not temperature dependent. However, the yield stress was shown to be temperature dependent as the shear stress needed for dislocation nucleation was reduced at elevated temperature [27]. Molecular dynamics (MD) simulation of Cu/SiC nanocomposites showed that the deformation mechanisms depend on the interfacial strength and the volume fraction of each phase plays a key role to the mechanical properties [28]. However, the majority of the previous studies examined the structures under uniaxial loading only. The mechanical behavior of CMNs under biaxial in-plane loading has not received much attention so far, even though in the majority of potential applications the structures will operate under biaxial loading. Furthermore, the presence of pre-existing dislocations on the yield surface of CMNs has not been considered so far.

For cases where incipient of plasticity is dominated by the nucleation of dislocations, such as in well-annealed nanocrystalline materials [29–33] where density of pre-existing dislocations are extremely low or in nano multilayers where the activation stress of threader dislocations is high [3,34,35], in previous work [20] we studied the mechanical behavior of NbC/Nb nanocomposites without pre-existing dislocations within the layers using MD simulations. The results from these MD simulations show high yield stresses which correspond to dislocation nucleation. It was shown that the high stresses are not only due to the typical high strain rates in the MD simulations, which was in turn justified using nucleation theory, but also due to the lack of pre-existing dislocations in the layers which can affect the yield stress and plastic deformation behavior considerably. In this paper, the

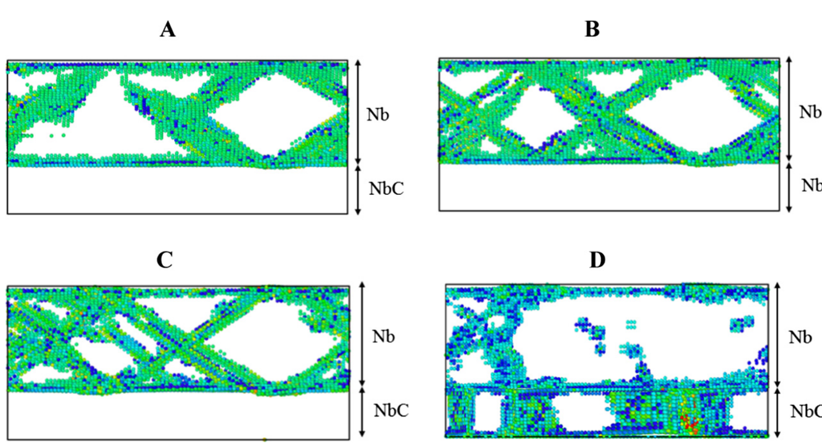

Fig. 2. Structures with pre-existing dislocations created by loading-unloading process at different strains: A, B, C, and D structures above unloaded from points 1, 2, 3, and 4 in Fig. 1 respectively. Total dislocation length in structures A, B, C, and D is 44527.1 Å, 51536 Å, 63904.6 Å, and 82457.6 Å respectively. Snapshots are colored based on *CSP*. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)