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Atomistic simulations of plasticity in heterogeneous nanocrystalline Ni lamella

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ABSTRACT

Atomistic simulations were performed on heterogeneous nanocrystalline (NC) Ni lamella made up of alternating NC and single crystalline (SC) layers to explore the effect of the heterogeneous microstructure on their mechanical response. It was found that the heterogeneous NC Ni lamella exhibit higher strength and better crack resistance than the pure NC Ni. After quantitatively analyzing the distribution of Von Mises shear strain in each sample, we found that the SC layer in heterogeneous NC Ni lamella can not only strengthen the whole sample following the conventional composite strengthening mechanism, but also homogenize the plastic strains in the NC layer and suppress the crack nucleation and propagation. The findings from this study can provide valuable insight into improving nanomaterial processing techniques, and have implications for the design of gradient or heterogeneous structures with superior properties.

1. Introduction

Nanocrystalline (NC) materials were extensively investigated over the past decades owing to their ultra-high strength than their coarse grained (CG) counterparts [1–4]. However, the high strength of NC materials is attained at the expense of their ductility, which is usually limited to a few percent of uniform elongation. Recently, materials with heterogeneous nanostructures, such as gradient nanograined (GNG) materials, i.e. materials with grain size ranging from tens of nanometers at surface to tens of micrometers at interior, have attracted growing attention, with their good balance of strength and ductility [5–10]. For example, Fang et al. [11] reported that the yield strength of GNG copper was twice that of its coarse grain counterpart, while its tensile uniform elongation could reach a level similar to that in the CG sample. Due to the observed grain growth on the surface layer, stress-assisted grain growth is believed to be a plausible mechanism for observed enhanced plasticity in their samples [12,13]. While a more recent experiment from Wu et al. demonstrated that GNG interstitial free (IF)-steel can also render superior combination of strength and ductility that is not accessible to conventional homogeneous materials [14,15]. Since the grain growth was suppressed by the high structural stability of IF-steel, Wu et al. proposed that the extra strain hardening extends from macroscopic strain gradients, which as a result, increased dislocation accumulation and enhanced the tensile ductility [14]. To the date, the debate still continues about the mechanism by which GNG materials retain their superior properties during tensile deformation.

As the microstructural interfaces in GNG materials migrate dynamically across the samples, rather than being stationary during plastic deformation, it has been a grand challenge to identify the characteristic features responsible for the superior properties of GNG materials through direct experimental observations. Atomistic simulation work can provide understanding for the underlying mechanisms of plastic deformation in NC materials and the appearance of particular phenomena in nano-structured materials [16–21]. In the present work, we perform the first atomistic simulations on heterogeneous NC Ni lamella, which provides a relative stationary interface from one grain structure to another and enables us to explore how the heterogeneity of grain sizes in NC materials affects their mechanical response. The findings from this study can provide valuable insight into improving nanomaterial processing techniques, and have implications for the design of gradient or heterogeneous structures with superior properties.

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2. Methodology

The heterogeneous lamella (HL) of NC Ni used in our calculation is made up of alternating NC and single crystalline (SC) layers. We constructed the HL sample shown in Fig. 1(b) by replacing half of the NC sample in Fig. 1(a) with the same thick SC layer. The SC layer had the crystallographic orientation as x-[$\bar{1}1\bar{2}$], y-[$\bar{1}11$] and z-[110]. To create stable high angle tilt grain boundaries, grains in the NC layer A-D were rotated for 30°, 60°, 90° and 120° related to the SC layer (F). Periodic boundary condition were imposed along all three directions, and the thickness in z-direction was 1.53 nm containing 12 atomic planes. The total number of atoms is about two million for the each sample. For NC layer in HL sample, eight and four grains were set in x and y directions, respectively. To study the effect of volume fraction of SC layer on the mechanical response of the HL structure, we also constructed a HL structure with quarter thick SC layer, which is named as HL1. Thus, HL 1–15 nm represents the HL structure with quarter thick SC layer and 15 nm nano grains for the NC layer. Although the exactly same microstructure presented in the current study has not been reported in previous experimental studies, this microstructure can mimic the local region near the interface between small and large grains in multimodal and bimodal nanostructured materials [5], gradient nanograined materials [11] and heterogeneous lamella materials [14] to explore the corresponding deformation mechanisms.

Large-scale Atomic/molecular Massively Parallel Simulator (Lammps) code was used to perform these calculations [22] with the embedded-atom method (EAM) potential for Ni system developed by Mishin at al [23]. Before loading, the conjugate gradient method was used to relax the system, and then the sample were equilibrated in the Nose/Hoover isobaric-isothermal ensemble (NPT) [24,25] for 50 ps to keep the temperature at 300 K, the pressure for all three directions were kept zero. After loading, uniaxial tensile was applied on the sample in x direction with a constant engineering strain rate of 5×10^8 s^{-1}. The temperature was still kept at 300 K and the pressure for z and y direction were kept zero during loading by NPT. Characterization of the system was employed multiple quantitative tools such as the Von Mises shear strain [26], common neighbor analysis method (CNA) [27], void volume fraction and plastic strain contribution from dislocation slip and grain boundary activities.

3. Comparison of the strength

Fig. 2(a) compared the engineering stress-strain curves for NC and HL samples. The stress-strain curves exhibited a relatively linear behavior and similar slopes for all samples before yielding. For those two NC samples, the yield strains were close to 2.5%, while the NC-15 nm sample carried a higher flow stress than the NC-25 nm one. That indicates the strength of NC samples used in our study still follows the regular Hall-Petch relationship, the strength in NC materials increases with the decreases of grain size, rather than the inverse Hall-Petch relationship [28]. Thus, the plastic deformation in our NC samples should not be dominated by the grain boundary (GB) activities, but the motion of dislocations [29]. Compared with the NC samples, HL samples exhibited higher strength as shown in Fig. 2(a). The average flow stress (σ_f) between 6% and 10% tensile strain of the HL structure is about 41% higher than that in the pure NC samples. So the SC layers strengthened the HL samples. Previous experiment studies on GNG metals attributed the high strength in GNG metals to the internal back stress generated in soft layers during plastic deformation [15,30–32]. Under tensile loading, the soft lamellae started plastic deformation firstly. While dislocations in soft lamellae were blocked and piled up at lamella interfaces as they were constrained by hard lamellae. That produced a back stress on dislocations in the soft lamellae to slow down or stop their motion and strengthened the soft lamellae. Furthermore, recent TEM observations revealed that dislocations can glide and pile up in NC metals, especially near the high-angle grain boundaries, that are responsible for enhanced strain hardening in those materials [33–35]. To identify whether the high strength in the heterogeneous NC Ni lamella was induced by the dislocation accumulation, we calculated the total dislocation density within the nano grains via the method developed by Stukowski et al. [36] and plotted the total dislocation density as a function of strain in Fig. 2(b). It is clear that there only a few dislocations stayed within the nano grains and the difference on dislocation densities is negligible from the HL to pure NC samples. Then the dislocation accumulation and pile-up mechanism cannot be the effective strengthening mechanism in heterogeneous NC Ni lamella. Furthermore, the analysis of the deformed microstructures in Fig. 3 demonstrates that there is no obvious difference on the grain sizes between pure NC and HL samples after deformation. Thus, the stress-assisted grain growth associated with grain boundary migration and sliding [37,38] should not be a plausible mechanism for the observed superior properties neither.

The only mechanism can be used to explain the observed high strength in heterogeneous NC Ni lamella is the conventional composite strengthening theory, which is always used to guide the design of composites composed of two or more materials that together provide properties not available when either of the individual materials is used alone [39]. For example, metal–matrix composites reinforced with silicon carbide fibers showing low density and high strength are being used in automobile engine

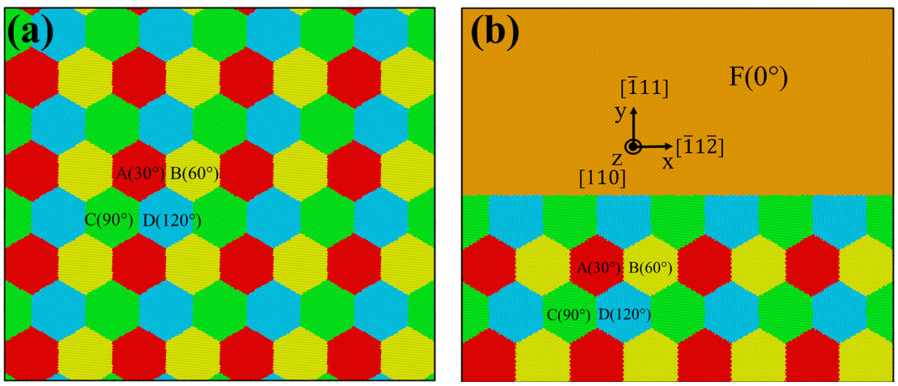

Fig. 1. Atomistic configurations of (a) pure NC Ni and (b) heterogeneous NC Ni lamella. For each grain, the atom color corresponds to the crystallographic orientation, and the crystallographic orientation of the single crystal layer were x-[$\bar{1}1\bar{2}$], y-[$\bar{1}11$] and z-[110], respectively, the other grains were rotated by certain angles around z direction.