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Smaller critical size and enhanced strength by nano-laminated structure in nickel

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ABSTRACT

Because of a shift in the dominant deformation mechanisms, the strength/hardness of metals increases with decreasing grain size down to a critical value, then decreases with further grain refinement. Here, laminated structure with low-angle grain boundaries was found to have smaller critical size and enhanced strength when compared to the equiaxed grain structure, through a series of large-scale molecular dynamics simulations. Then, the corresponding atomistic mechanisms were investigated by checking and comparing the rotations of grains and equivalent strain partitioning in grain boundary atoms. In laminated structure, grain boundary activies were found to be promoted with decreasing lamellar thickness. More importantly, when compared to the equiaxed grain structure at the same length scale (lamellar thickness/grain size), grain boundary activities were found to be inhibited by the laminated structure, which is the main reason for the enhanced strength and the smaller critical size. Besides grain boundary activities, formation of extended dislocations, formation of deformation twins, partial dislocations interacting with formed TBs, partial dislocation blocking by and even transmission through low-angle grain boundaries were also found to play important roles in plastic deformation of nano-laminated structure. The current findings should provide insights for designing stronger and more stable nanostructured metals.

1. Introduction

High strength can be achieved in metals traditionally by introducing more grain boundaries (GBs) via grain refinement or by increasing dislocation density in grain interior [1–8]. Because of a shift in the dominant deformation mechanisms from dislocation-mediated plasticity to GB-associated plasticity, the strength/hardness of metals has been found to increase first with decreasing grain size down to a critical grain size (10–20 nm), and then decrease with further grain refinement [1,2,9–15]. Moreover, a similar trend for twinboundary spacing (TBS) effect on the strength of nanotwinned (NT) metals was also found due to a transition of deformation mechanisms [16–20].

The effects of length scale (layer thickness) on the strength of bi-metal multilayered laminates have also been studied from the micrometer to the nanometer range [21–27]. The strengthening effects as a function of layer thickness can be summarized as three mechanisms: (i) the dislocation pile-up mechanism from submicron to micron range; (ii) the confined layer slip mechanism from few nm to a few tens of nm range; (iii) the interface crossing mechanism for about 1–2 nm [21,22]. The strength of bi-metal multilayered laminates increases with decreasing layer thickness in the range of the first two mechanisms and decreases with further reduced layer thickness in the range of the third mechanism. The strongest layer thickness in bi-metal multilayered laminates was found to be less than 5 nm [21,22], and this critical length scale is much smaller than the critical grain size observed for nanocrystalline metals. Recently, nanostructured metals with laminated grain structure (with aspect ratio ranging from a few to a few tens) and low-angle grain boundaries (LAGBs) could be produced by severe plastic deformation (SPD), such as accumulative roll-bonding (ARB) [3], equal channel angular pressing/extrusion (ECAP/ECAE) [4,28], and surface mechanical grinding treatment (SMGT) [29]. These nanostructured metals with laminated grain structure were observed to be ultrahard and ultrastable [3,4,28,29], while the strongest critical lamellar thickness (the length scale controlling strength) and the underlying deformation mechanisms are still open to further investigations, especially when compared to the equiaxed grain structure.

Due to the inherent limitations, the strain rate is typically high ($>10^7$/s) in MD simulations, and some deformation behaviors (such as diffusion effects) might be limited at such short deformation times at ambient temperatures. However, MD simulations with

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carefully designed model system not only have been shown to be particularly useful for studying the plastic deformation mechanism (dislocation activities, GB sliding, GB migration and grain rotation) in nanostructured metals, in which the "in-situ" deformation processes of the system and the stress and the strain distributions at atomic-level can be examined [9,17,30–36], but also have proven to be useful for investigating the size effects (grain size/TBS) on the strength of nanostructured metals [9,17]. In this regard, the focus of this paper is to find out and compare the strongest critical length scale (lamellar thickness/grain size) and the underlying atomistic deformation mechanisms for both laminated structure and equiaxed grain structure using a series of large-scale MD simulations.

2. Simulation procedures

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code was used for the MD simulations. The force interactions between atoms were described by a widely used Ni EAM potential developed by Mishin et al. [37]. In order to explore the plastic deformation process of the laminated structure with large size (the maximum investigated lamellar thickness was 25 nm with aspect ratio of 10 in the present study), it is necessary to consider simulation cells larger than those possible in fully 3-dimensional systems. Quasi 3-dimensional simulations with a columnar grain structure were considered in this regard, very similar to the configuration proposed by Yamakov et al. [30]. As indicated in the previous research [17,30], the columnar model could also be used to investigate the size effects (grain size or twin boundary spacing) on the strength of nanostructured metals although all dislocation lines are constrained to be parallel to the columnar axis. The lamellar thickness for laminated structure is noted as λ, while the grain size for equiaxed grains is noted as d here. The thickness direction (z direction) is along $[\bar{1}\,1\,0]$ and contains 12 atomic planes. The relaxed Ni samples with laminated structure (lamellar thickness $\lambda = 10$ nm) and equiaxed grains (grain size $d = 10$ nm) are shown in Fig. 1(a) and (b), respectively. The grains of 2, 3, and 4 are rotated from grain 1 about $[\bar{1}\,1\,0]$ axis with the angles of -5^0, 5^0, and 10^0 respectively for both structures, which generates low-angle boundaries for all grains. The GBs were determined by Voronoi construction in the present study (in the laminated structures, the grain shape was determined only by surrounding four seeds instead of six seeds in the equiaxed grains). Also the dash lines are indications of the orientations of the two sets of {1 1 1} slip planes in each grain. In the present study, the atoms are painted with colors according to common neighbor analysis (CNA) values. The CNA is a very useful tool used in MD simulations which allows us to determine the local ordering and the defects in a given structure. Perfect fcc atoms are painted by gray color, hcp atoms are painted by red color and green color stands for other atoms which belong to GBs, dislocation cores, free surfaces or other defects.

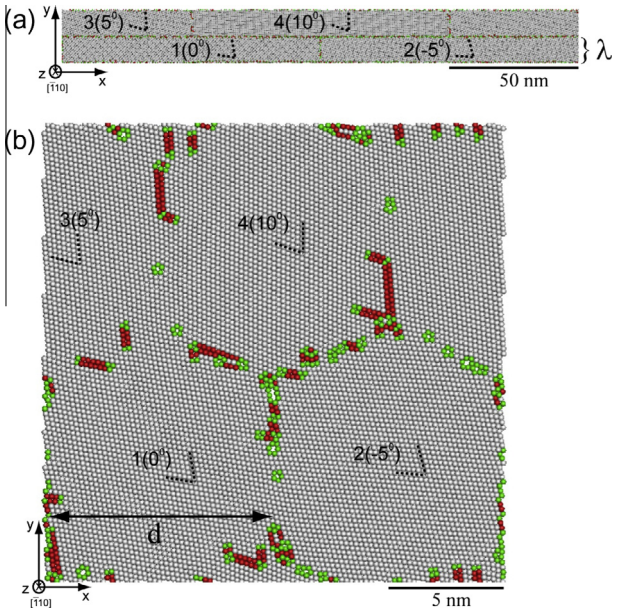

Fig. 1. (a) The relaxed Ni sample with the laminated structure ($\lambda = 10$ nm). (b) The relaxed Ni sample with the equal-axed grain structure ($d = 10$ nm).

It should be noted that the LAGBs are actually dislocation walls consisting of discontinuous dislocations due to small misorientation angles. For laminated structure, eight samples with initial lamellar thickness of $\lambda = 5$ nm, 7.5 nm, 10 nm, 12.5 nm, 15 nm, 17.5 nm, 20 nm, and 25 nm were simulated, and the aspect ratio was fixed at 10 (in the range of typical nano-laminates). The dimensions are $500 \times 50 \times 1.49$ nm^3 for the sample of laminated structure with $\lambda = 25$ nm, which contains approximately 3,500,000 atoms. For equiaxed grain structure, eight samples with initial grain size of $d = 5$ nm, 10 nm, 15 nm, 17.5 nm, 20 nm, 22.5 nm, 25 nm, 30 nm were considered. The dimensions are $60 \times 60 \times 1.49$ nm^3 for the sample of equiaxed grain structure with $d = 30$ nm, which contains approximately 490,000 atoms. When the lamellar thickness/grain size was changed, the same structure and the same crystallographic orientations of all grains were retained. Periodic boundary conditions were used in all three directions, and the tensile loading was along x direction. By the conjugate gradient method, the as-constructed samples were first subjected to energy minimization before the tensile loading, and then heated up to the desired temperature and finally relaxed by the Nose/Hoover isobaric–isothermal ensemble (NPT) under both the pressure 0 bar and the desired temperature (10 K) for 100 ps. A strain of 8% was applied to each sample (with a constant engineering strain rate of 5×10^8 s^{-1}) after the relaxation. In order to simulate the uniaxial loading, the pressures in the y and z directions were kept to zero during the tensile loading.

3. Results and discussions

In samples with equiaxed grains, the strength is determined by grain size. However, the lamellar thickness should be the controlling length scale for strengthening in samples with laminated structure (especially with large aspect ratio, such as 10 used in the present study). Fig. 2(a) and (b) shows the stress–strain curves for samples with laminated structure and equiaxed grains, respectively. Tensile stresses are observed to deviate from linear relationship with strain at a certain stress, which is an indication of onset of plastic deformation, and then gradually reach to a relatively steady-state value regardless of λ/d.

It is typically more meaningful to compare the average flow stress over a certain plastic strain interval for illustrating the effect of λ/d on the flow strength in MD simulations [9,12,17,19]. In this regard, the average flow stress from a strain of 4.5–8% is plotted against λ/d in Fig. 2(c). It can be seen that the average flow stresses of both the laminated structure and the equiaxed grain structure first increase with decreasing λ/d, reaching a maximum at a critical λ/d, and then decrease when λ/d becomes even smaller. As indicated from previous research [9,12], this behavior is due to a transition of dominant deformation mechanisms from dislocation-mediated plasticity to GB-associated plasticity. It is also observed that the critical size λ_{crit} (12.5 nm) in the laminated structure is much smaller than the critical size d_{crit} (20 nm) in the equiaxed