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Role of grain boundary on the sources of size effects

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ABSTRACT

The present paper investigates the effects of grain boundary (GB) on the sources of size effects. Up to now, several studies have been conducted to address the role of GBs in size effects from the atomistic point of view. However, a study which addresses the effects of GB on different governing mechanisms of size effects as the sample length scale varies has not been presented yet. Here, samples with different length scales are studied to capture the role of GB in size effects as the grain size changes. The response of single and bi-crystal Ni thin films with two different sizes are studied during nanoindentation experiment using large scale atomistic simulation. Various symmetric and asymmetric tilt GBs are incorporated to study the effects of GB geometry on the response of samples during nanoindentation. The sources of size effects are analyzed in each sample using the atomistic information obtained from the simulations. The results show that the size effects mechanism influenced by GBs changes from dislocation nucleation and source exhaustion to the forest hardening mechanism as the grain size increases. In the case of small bi-crystal samples, dislocation nucleation and source exhaustion govern the size effects. The GB contributes to the dislocation nucleation beneath the indenter which reduces the strength of sample by providing required dislocations to sustain the imposed plastic deformation. Also, the GB itself is the source of defects which can affect the sample strength depending on the indentation depth at which the dislocation is nucleated from the grain boundary. Increasing the indentation depth, some of the dislocations are blocked by the GB. However, there is no noticeable additional hardness due to the dislocations blockage by GB. Furthermore, the results show that the coherent twin boundaries shows the best performance during the nanoindentation. In the case of large bi-crystal samples, the GB does not influence the size effects at lower indentation depths where the source exhaustion is the controlling mechanism of size effects. However, at higher indentation depths, the dislocation interaction with GB contributes to the forest hardening mechanism and induces some hardening. It is observed that the dislocations are firstly absorbed by the GB. Increasing the indentation depth, some dislocations start dissociating into the next grain. However, it is observed that more dislocations are nucleated in the upper grain. The results show that the main role of GB at larger length scale is to change the pattern of dislocation structure in a way that the dislocations are piled up near the GB which increases the hardness.

1. Introduction

The mechanical properties of crystalline metals are usually governed by grain size and grain boundary (GB) properties [1–3]. The GB effects on the strength depend on several factors including the grain size, GBs geometry, mechanical and crystallographical structure of metal, strain rate, and temperature [1–3]. These factors define the deformation mechanisms in crystalline metals. Several numerical and experimental studies have been conducted to unravel the role of GBs in crystalline metals [1–3]. In the case of large grains, i.e. grain sizes of more than 1 μm, the strength increases as the grain size decreases which is commonly described by the Hall–Petch relation. The enhancement in strength is justified using the dislocation pile-up mechanism [1–3]. By decreasing the grain size, the pile-up model and consequently the Hall–Petch relationship break down at some grain size which is of the order of nanometers [4]. Other mechanisms such as GB sliding, GB rotation, and GB dislocation creation and annihilation have been proposed to describe the grain size dependency of strength in nanocrystalline metals [1–3].

Molecular dynamics (MD) simulation is a powerful tool [5–8] to model the effects of grain size and GB properties on the strength of nanocrystalline metals from the atomistic point of view. Van Swygenhoven et al. [9,10] incorporated the atomistic simulation and showed that below a critical grain size, the GB sliding is a

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dominant mechanism using molecular dynamics. In the cases of grains larger than 10–12 nm, they observed some intra-grain deformation mechanism such as partial dislocations [9,10]. Yamakov and coworkers [11–14] also conducted several atomistic simulation to study the effect of grain size on the deformation mechanisms of nanocrystalline fcc metals. It was observed that as the grain size decreases, the deformation process changes from a dislocation-based to a grain-boundary-based mechanism [11–14]. Derlet et al. [15] summarized the limitation of MD in the case of nanocrystaline metals simulation. They stated that the atomic deformation mechanisms can be successfully extracted from the MD simulation [15]. However, when it comes to the extrapolation of the obtained MD results to the experimental observations, one should consider the temperature, size, and rate at which the simulation is conducted [15].

The interaction of the dislocations with GBs has been investigated using atomistic simulation to understand the underlying deformation process. De Koning et al. [16] performed 2D and 3D MD simulations to study the various mechanisms of dislocation absorption, transmission, and reflection by incorporating both symmetric and asymmetric Σ11 tilt GBs. Hasnaoui et al. [17] simulated the nanoindentation experiment using MD simulation to study the interaction between dislocations and GBs. It was observed that the GBs can act as a sink for dislocations, reflect or emit dislocations [17]. Jang and Farkas [18] incorporated MD simulation and studied a bi-crystal nickel thin film with $\sum 5\ (210)[001]$ GB during the nanoindentation. It was shown that the GB induced some resistance to the indentation due to the stacking fault expansion [18]. Kulkarni et al. [19] compared the response of coherent twin boundary (CTB) with that of $\sum 9\ (221)$ tilt GB during nanoindentation using atomistic simulation. They stated that unlike the $\sum 9\ (221)$ GB, the CTB does not considerably reduce the strength of the sample. However, unlike Jang and Farkas [18], they did not observe noticeable enhancement in strength [19]. Tsuru et al. [20] studied the effects of coincidence site lattice (CSL) grain-boundaries on the incipient plasticity using MD. They changed the distance of indenter with respect to the GB and monitored the incipient plasticity. They concluded that the GBs with lower energies have higher mean pressures at the onset of plasticity. Stukowski et al. [21] compared the uniaxial response of nanotwinned Cu and Pd nanocrystalline samples with those without twin boundaries using large scale atomistic simulation. They showed that the effects of twin boundaries depend on the unstable stacking fault and twin boundary migration energies, and it can increase or decrease the strength of the material [21]. Sangid et al. [22] measured the energy barriers of CSL grain boundaries of slip–GB interactions using MD. It was observed that the energy barrier has an inverse relationship with GB energy in a way that the GB with lower energy has the higher energy barrier [22]. Zhang et al. [23] incorporated the atomistic simulation to investigate the response of symmetric and asymmetric $\sum$ 5 GBs during uniaxial tension experiment. They studied the effect of inclination angles on the mechanical response of copper bi-crystal [23]. Sainath and Choudhary [24] simulated the Cu nanopillars with and without twin boundaries under uniaxial tension using MD. It was shown that the GB changes the deformation mechanism and increase the strength of the simulated nanopillar [24].

The interaction of dislocations with each other and with GBs governs the size effects in bulk metals which is termed as the forest hardening [25,26]. Decreasing the sample size to the order of nanometers, however, the forest hardening model is not the governing mechanism. The size effects in nanoscale metallic samples are described using three models of source exhaustion hardening, weakest link theory, and source truncation [26–29]. Dislocation starvation, mechanical annealing, and source shut down reduce the number of sources in nanoscale samples in a way that the reduced mobile dislocation density is insufficient to handle the imposed deformation. Consequently, the applied stress should be increased to sustain the plastic deformation. The induced hardening due to the lack of sources is termed exhaustion hardening [30,31]. In the case of metallic sample of confined volumes, since the double-ended dislocation sources are close to the free surfaces, they transform into the single-ended sources. Consequently, the strength is increased due to the reduction in characteristic length of dislocation sources which is commonly termed as source truncation [32,33]. The last mechanism is the weakest link theory in which the strength of the weakest slip plane increases by reducing the sample size which enhances the strength [34,35]. Tucker et al. [36] investigated the effects of GBs on the size effects of nanowires under uniaxial compression using MD. It was shown that both GB and free surfaces can be the favorable dislocation nucleation sites [36]. Recently, Yaghoobi and Voyiadjis [37] studied the sources of size effects in nanosize single crystal Ni thin films during nanoindentation using large scale atomistic simulation. They showed that the dislocation nucleation and source exhaustion are mainly responsible for size effects during the nanoindentation of Ni samples of confined volumes at lower indentation depths [37].

In the current study, the effects of GBs on the sources of size effects are investigated. The nanoindentation response of single and bi-crystal Ni thin films are investigated by incorporating large scale atomistic simulation. Here, samples with two different sizes and various symmetric and asymmetric tilt GBs are studied to capture the role of GB in size effects as the grain size changes. Furthermore, the sources of size effects are analyzed in each sample using the microstructural information obtained from the simulations. In order to study the size effects controlling mechanisms, the total dislocation length of each sample is studied during the nanoindentation. The obtained results are then compared to the variation of hardness versus the indentation depth to unravel the contribution of GBs to the sources of size effects as the sample length scale changes. The dislocation visualization is also incorporated to study the dislocation nucleation and evolution patterns for bi-crystal and single crystal samples of different sizes.

2. Simulation details and methodology

To investigate the effects of grain size on the sources of size effects, two different sizes of Ni thin films with the dimensions of 24 nm × 24 nm × 12 nm (S1) and 120 nm × 120 nm × 60 nm (S2) are generated and simulated using the classical molecular dynamics. The total number of atoms in the samples are around 650,000 for S1 and 79,000,000 for S2. The periodic boundary conditions are applied to the surrounding surfaces. The free boundary conditions are selected at the bottom of the sample. The selected boundary conditions ensure that the dislocations do not bounce back from the sample bottom. To prevent the whole domain from translational movement, at each step, the total force is divided by the number of atoms and then applied in the opposite direction to all atoms [38–41]. Voyiadjis and his coworkers [37,40,41] has previously shown that the chosen boundary conditions type can successfully capture the nanoindentation response and microstructural information such as dislocation structure and length. The velocity Verlet algorithm with a time step of 2 fs is selected. The parallel MD code LAMMPS is used [42]. Seven different types of GB including four symmetric tilt boundaries of $\sum 3\ (111)[1\bar{1}0]$ ($\theta = 109.5^\circ$), $\sum 11\ (113)[1\bar{1}0]$ ($\theta = 50.5^\circ$), $\sum 3\ (112)[1\bar{1}0]$ ($\theta = 70.5^\circ$), and $\sum 11\ (332)[1\bar{1}0]$ ($\theta = 129.5^\circ$), and three assymetric tilt boundaries of $\sum 11\ (225)/(441)$ ($\varphi = 54.74^\circ$), $\sum 3\ (112)/(\bar{5}\bar{5}2)$ ($\varphi = 19.47^\circ$), and $\sum 3\ (114)/(110)$ ($\varphi = 35.26^\circ$) are selected to study the effects of GB properties on the size effects, where θ and φ are the interface