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Molecular dynamics study of creep mechanisms in nanotwinned metals

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ABSTRACT

Nanotwinned structures have shown great promise as optimal motifs for evading the strength–ductility trade-off. In this paper, we present a study of high temperature creep in polycrystalline nanotwinned face-centered cubic metals using molecular dynamics. The simulations reveal that the nanotwinned metals exhibit greater creep resistance with decreasing twin boundary spacing over a large range of applied stresses. The findings also indicate that the presence of twin boundaries entails higher stress for the onset of power-law creep compared to the nanocrystalline counterparts. Nanotwinned metals with very high density of twin boundaries exhibit a new creep deformation mechanism at high stresses governed by twin boundary migration. This is in contrast to nanocrystalline and nanotwinned metals with larger twin spacing, which exhibit a more conventional transition from grain boundary diffusion and sliding to dislocation nucleation.

1. Introduction

There is compelling evidence for the critical role of twin boundaries (TBs) in imparting the extraordinary combination of strength and ductility to nanotwinned metals [1,2]. This is in stark contrast to nanocrystalline materials, which exhibit a loss of ductility, and grain stability with decreasing grain size, thereby dampening the initial enthusiasm generated by their very high yield strength (see [3] for review). It is now well-documented that the twin boundaries strengthen by serving as effective barriers for arresting dislocation motion while simultaneously enhance ductility by absorbing dislocations onto the twin planes and accommodating plasticity. With the emerging potential of nanotwinned structures as optimal motifs for the design of high strength high ductility materials, the prospect of their creep response is of vital concern, one that would determine their true practical utility for structural applications. Although creep mechanisms in nanocrystalline materials have been investigated extensively through experiments and analytically, the topic has been relatively unaddressed in the context of nanotwinned metals, which is the focus of the present study.

The deformation mechanisms associated with creep in conventional polycrystalline metals at different ranges of applied stresses, temperatures and grain sizes are well-described by the unified Bird–Dorn–Mukherjee relation [4] given by

$$\dot{\epsilon} = \frac{AD_0Gb}{k_BT}\left(\frac{b}{d}\right)^p\left(\frac{\sigma}{G}\right)^n \exp\left(-\frac{\Delta Q}{k_BT}\right) \quad (1)$$

where $\dot{\epsilon}$ is the strain rate, A is a dimensionless constant, D_0 is a frequency factor, G is the shear modulus, b is the magnitude of the Burgers vector, k_B is Boltzmann's constant, T is the absolute temperature, d is the grain size, p is the inverse grain size exponent, σ is the applied stress, n is the stress exponent, and ΔQ is the activation energy for a particular mechanism. The Nabarro–Herring creep mechanism [5,6] that involves vacancy flow through the lattice is characterized by a $1/d^2$ dependence on the grain size, whereas Coble creep [7] that involves vacancy diffusion along the grain boundaries, exhibits a $1/d^3$ dependence. Both these mechanisms are characterized by a linear dependence on the applied stress ($n \sim 1$). Furthermore, it is well-accepted that grain boundary sliding is necessary to accommodate this diffusional transport in order to maintain compatibility of the adjoining grains and hence occurs simultaneously with diffusional creep [8]. Although at low stresses, the diffusion is rate limiting, some studies have shown analytically that at intermediate stresses, the strain rate is controlled by grain boundary sliding which is manifested in a stress exponent $n \sim 2$ [9]. $n > 4$ indicates the onset of power-law creep and is associated with dislocation-climb mediated mechanisms that become dominant at higher stresses [10].

A number of experimental studies have been carried out on creep of nanocrystalline metals at low and moderate homologous temperatures (*viz.* $T/T_m < 0.7$, T_m is the melting point) and have demonstrated various atomistic mechanisms [11–16]. Several

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molecular dynamics studies have also been performed to elucidate the atomistic mechanisms underpinning the creep response of nanocrystalline metals at elevated temperatures [17–19]. Creep mechanisms including grain boundary diffusion, grain boundary sliding, and dislocation nucleation have been identified under different levels of applied stress as intra-granular dislocation activity, especially dislocation climb, is severely limited by the small grain sizes. A few studies on nanotwinned metals have reported that nanotwinned Cu and Ag are much more structurally stable and retain their hardness than their nanocrystalline counterparts during microindentation creep tests and cyclic loading at room temperature [20,21]. Sanders et al. [14] have also noted the presence of a high density of twin boundaries in their as-prepared nanocrystalline Cu samples, and they believed these twins and low angle grain boundaries to play a role in the low strain rates observed in their creep tests. In the present study, molecular dynamics (MD) simulations of creep in polycrystalline nanotwinned Cu have been performed over a wide range of applied stresses to elucidate the role of coherent twin boundaries in governing the rate-controlling creep mechanisms. We emphasize that all MD simulations are inherently limited by high strain rates (of the order of 10^8 s^{-1}) and very short time scales (of the order of a few nanoseconds) that are accessible to these conventional atomistic methods. To partially circumvent this limitation, our simulations have been performed at high homologous temperatures at which the GB-mediated creep mechanisms are identifiable on the time scale of MD, and previous simulation results have shown agreement with phenomenological models and experimental data [22].

2. Simulation method

Simulations were performed on three-dimensional nanocrystalline (NC) and nanotwinned (NT) Cu specimens containing 16 randomly oriented grains in body-centered cubic distribution created by Voronoi construction [23]. The NC specimen had an overall size of about 21.8 nm × 21.8 nm × 21.8 nm consisting of 836,450 atoms. The NT specimen had an overall size of about 20.6 nm × 21.4 nm × 20.2 nm consisting of 712,335 atoms. The shape and size of the grains were kept uniform in order to avoid grain growth at the high temperatures considered in this study [17]. The grain size in NC samples was about 10.8 nm (Fig. 1(a)). Four NT samples were constructed with a twin boundary (TB) spacing of 0.6 nm, 1.2 nm, 2.5 nm, and 5 nm and a grain size of 10.3 nm. Fig. 1(b) shows the relaxed configuration of nanotwinned Cu with twin lamella thickness of 0.6 nm. Periodic boundary conditions were applied in the x, y, and z directions. Inter-atomic interactions were modeled using the embedded atom method (EAM) potential for Cu developed by Mishin et al. [24]. The samples were first equilibrated at a given temperature using the NPT ensemble for 200 ps. In order to investigate the creep response of both NC and NT samples, a constant stress was applied along the x direction for another 200 ps, while maintaining the other two directions stress-free and the resulting evolution of the strain was obtained. Creep was studied at different levels of uniaxial stress ranging from 0.05 GPa to 3.5 GPa and different temperatures, specifically, 720 K, 960 K, and 1080 K which correspond to 0.5, 0.7, and 0.8 homologous temperatures respectively. All simulations were performed using LAMMPS [25], and the atomistic structures were visualized based on common neighbor analysis using OVITO [27].

3. Results and discussion

Fig. 2(a) shows the evolution of strain with time for NC Cu and NT Cu with twin spacing of 0.6 nm subjected to different levels of stress at 960 K. All the curves exhibit a short elastic regime for the first few picoseconds, and then enter the creep stage as indicated by the change in slope. As our focus is on the analysis of steady-state creep, the creep curves only show the first two stages of creep. Therefore, for applied stress lower than 1 GPa, the simulations end at 200 ps, whereas for applied stresses above 1 GPa, the simulations are terminated at much earlier times, consistent with the simulations of Wang et al. [19] on NC Cu. As expected, all specimen exhibit larger deformation with increase in the applied stress. At all stress levels considered here, the NT specimen shows a lower creep rate when compared to its NC counterpart. Moreover, the difference in their strain curves increases steadily with the increase in the applied stress until 1 GPa. Fig. 2(b) shows the creep results for the same NT and NC specimen at 0.6 GPa under varying temperatures. All specimen exhibit increasing strain rate with increasing temperatures as expected. Comparing the response of NT and NC specimens, we observe similar trends as in Fig. 2(a) with the NT specimen exhibiting lower deformation and strain rate compared to the NC specimen at all temperatures. Fig. 2(c) shows the strain versus time plots for NT samples with different twin spacings at an applied stress of 0.5 GPa. Fig. 2(d) shows the variation of the creep rate as a function of the TB spacing at an applied stress of 1 GPa. The results reveal that the creep resistance of NT metals improves with decreasing twin spacing in comparison to the NC metals of the same grain size.

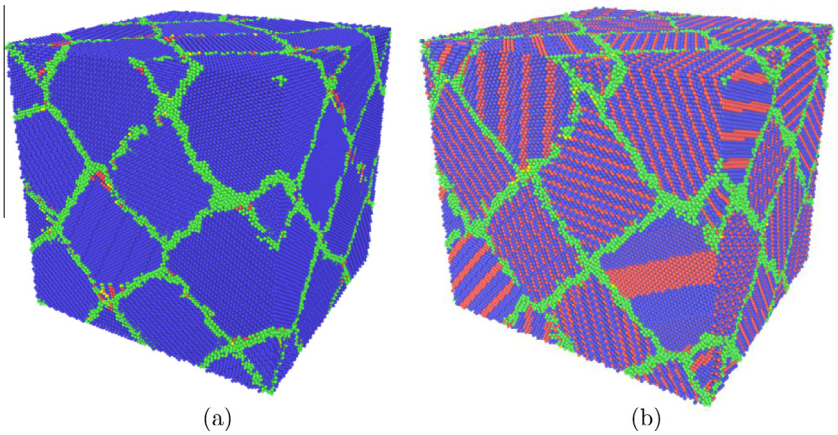

Fig. 1. Simulation specimen after thermal equilibration visualized by common neighbor analysis [26] (Blue: FCC, Red: HCP, Yellow: BCC, Green: Others) using Ovito [27]: (a) nanocrystalline (NC) Cu, (b) nanotwinned (NT) Cu with twin boundary (TB) spacing of 0.6 nm. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)