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Nature of creep deformation in nanocrystalline Tungsten

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ABSTRACT

Because of Tungsten's (*W*) use in high temperature and stress environments like next generation fusion reactors, exploring the creep deformation mechanism in this material is very essential. In this work, for the first time, nature of creep in nanocrystalline (nc) Tungsten and factors that govern the creep mechanism like grain size, temperature, and applied stress are studied through atomistic simulations. Applied stress is varied from 2.5 to 5.5 GPa on the metallic sample while the temperature is varied in the range of 1600–2200 K. Stress and temperature variance are repeated for average grain sizes of 2.38 nm, 2.86 nm, 3.57 nm, and 4.76 nm. From the simulations, it has been found that the creep mechanism in nanocrystalline Tungsten is contingent on the applied stress as the creep mechanism varies from lattice diffusion to grain boundary diffusion creep even up to dislocation-creep. Moreover, temperature and grain refinement seem to aid the creep phenomenon at nanoscale. For very large value of stress and temperature, the power-law fails to define the creep in nc-Tungsten. In order to quantify the propensity and mechanism of creep in nanocrystalline Tungsten, stress and grain size exponents are observed in addition to the time evolution of strain and mean square displacement. Finally, atomistic features of deformation are analyzed which evince the simulation results.

1. Introduction

Nanocrystalline metals and alloys have many unique mechanical properties that enable their uses in different structural applications [1,2]. Strength of these nanocrystalline materials is contingent on the grain size and the temperature these are exposed to [3–5]. Usually, in the coarse grained materials, refining the grains leads to strengthening of the structure. However, in nanocrystalline materials grain refinement actually increases strength after reaching a critical grain size. This effect is known as inverse Hall-Petch effect [6–10]. The grain size at which this transition occurs is normally 10 nm [8]. Grain size and distribution also influence the creep properties of nanomaterials [11,12]. Creep experiments are expensive and time consuming. Hence, to understand the underlying physics of creep many researchers resort to atomistic simulations nowadays [13–15]. However, atomistic simulations are limited by the requirement of large amount of time for creep simulation. To circumvent this problem, usually atomistic simulations on creep are done at a high temperature and stress conditions [16,17].

Previous studies on creep used MD simulation as a tool to identify the underlying atomic processes and governing mechanism of creep. These studies indicate that grain size, temperature, and applied stress concomitantly affect creep deformation in materials. Relation of these three parameters with steady-state creep rate is expressed by Bird-Dorn-Mukherjee equation [18] as,

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

where $\dot{\epsilon}$ is the steady-state creep rate (SSCR), A is a dimensionless constant, D_0 is the diffusion coefficient, G is the shear modulus, b is the Burgers vector, k_B is the Boltzmann's constant, T is the absolute temperature, d is the grain size, σ is the applied stress, ΔQ is the activation energy for thermal-activated process, p and n are the grain size and stress exponents, respectively. Molecular dynamics study on pure metals corroborates the idea of Eq. (1). Keblinski et al. [19] identified Coble creep as the governing creep mechanism in polycrystalline silicon under relatively high tensile stress. Yin et al. [20] observed shift in creep mechanism in nanocrystalline *Ni* depending on temperature it is exposed to. Karanjgaokar and Chasiotis [21], in their experiments, observed that nature of creep in *Au* films is controlled by the temperature it is exposed to. A combined experimental and computational study on *Cu* shows that the nano-twinned *Cu* offers greater creep resistance [14] compared to the twin-free nanograined *Cu* indicating a role of grain boundaries in controlling the creep. Similar outcome was also obtained by Jiao and Kulkarni [22]. Wang et al. [13] found a critical stress level after which the grain size exponent decreases for higher stress. They argued that presence of dislocation in the initial structure and their interaction with grain boundaries give rise to such anomaly. Transition in creep mechanism was observed in

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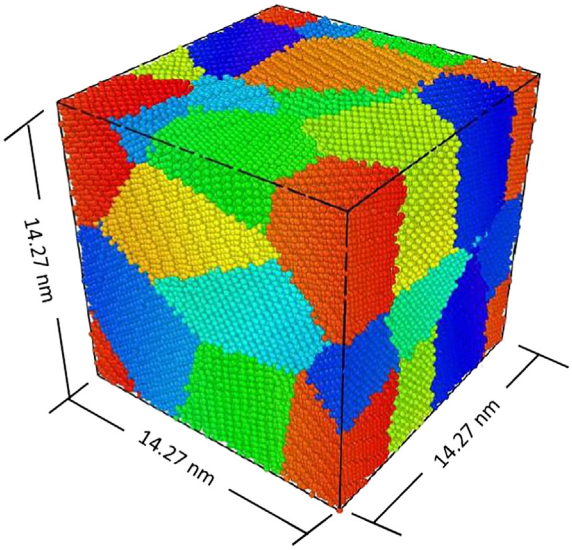

Fig. 1. Schematic diagram of the cubic sample of Tungsten nano-crystal. Grains are colored using the grain-ID. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

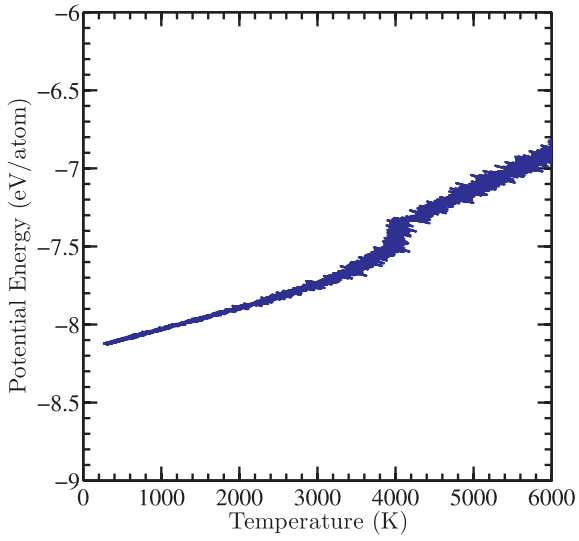

Fig. 2. Variation of potential energy per atom with temperature using EAM potential of this work.

nanocrystalline *Cu* depending on the temperature and applied stress [23]. Nie et al. [15] observed similar transition in creep mechanism in nanocrystalline *Ni* as the temperature and stress were increased. Studies on other metals and metallic alloys suggest impact of temperature, stress, and grain size on creep mechanism of materials [24–27]. However, there is no significant study on creep behavior of Tungsten at nanoscale using atomistic simulation to date. Experimental studies suggest applied stress controls the creep rate of pure tungsten albeit the power-law creep is not necessarily sufficient to describe creep phenomenon [28]. Robinson and Sherby [29] divided creep studies on Tungsten in two categories-high temperature (above 2000 °C) and low temperature creep (below 2000 °C). The low temperature creep showed stress exponent $n = 7$ which indicates breakdown of power-law relation. Using molecular simulation one can observe exact reasons of such anomaly. This makes the analysis more important.

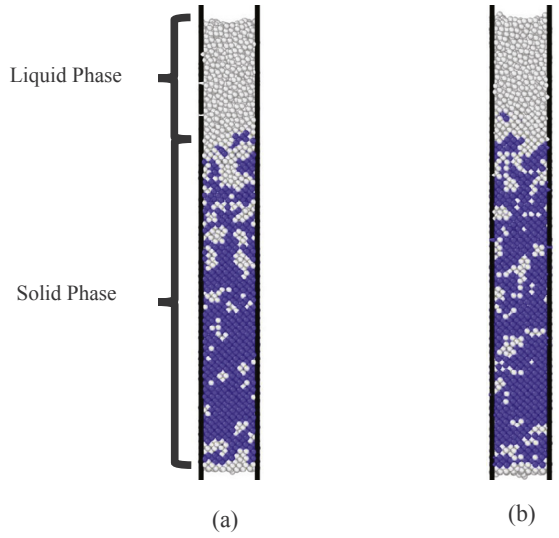

Fig. 3. Atomistic configurations of the sample of Tungsten nanomaterial at the (a) beginning of the equilibration, and (b) after 25 picoseconds at $T = 3750$ K. We can see stable two phases (liquid and solid) in the image co-existing. Atoms are colored using Centro symmetry parameter. White atoms denote the liquid phase while blue ones represent perfect bcc structure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
Variation of yield strength (in GPa) of different nanocrystalline samples of *W* with grain size and temperature.

Grain size (nm)	Temperature (K)			
	1600	1800	2000	2200
4.76	14.24	13.94	13.57	13.23
3.57	14.19	13.85	12.30	11.93
2.86	12.79	12.15	11.90	11.80
2.38	12.06	12.12	11.48	10.45

In this study, impact of grain size, temperature, and applied stress on the creep mechanism of nanocrytsalline Tungsten is analyzed using molecular dynamics technique. A cubic sample of Tungsten nanocrystal is considered and the applied constant stress ranges from 2.5 to 5.5 GPa. For analysis, temperature is varied from 1600 K to 2200 K while grain sizes considered are 2.38 nm, 2.86 nm, 3.57 nm, and 4.76 nm.

2. Computational method

A polycrystalline cubic sample of *W* is created by Voronoi tessellation method [30] using Atomsk tool [31] with randomly oriented grains of 2.38 nm, 2.86 nm, 3.57 nm, and 4.76 nm size. The dimension of the cubic sample is taken as 14.27 nm × 14.27 nm × 14.27 nm for every grain size totaling to number of atoms ranging from 180,437 to 181,208. Fig. 1 shows the initial sample after preparation. Periodic boundary condition is imposed in all the three directions. All atomistic simulations are performed with Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [32]. In identifying the molecular processes of deformation, interatomic potential chosen plays a vital role. In this work a modified embedded atom (EAM) potential by Zhou et al. [33] is employed. Ma et al. [34] and Saha et al. [5] used this potential successfully for their works. The potential reproduced the cohesive energy of −8.76 eV and lattice constant of 3.17 A^0 [35] for single crystal *W*. Strain is calculated using the following formula in the