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Mechanistic study of bending creep behaviour of bicrystal nanobeam

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ABSTRACT

In this paper, bending creep deformation mechanism for nickel nanobeam has been investigated using molecular dynamics simulation. Low temperature creep deformation ($T < 0.3\ T_m$) is found to be guided by jog formation and glide motion of grain boundary whereas lattice diffusion, grain boundary migration and sliding are the controlling mechanism for high temperature deformation ($T > 0.5\ T_m$). The occurrence of tertiary creep regime is observed only at high temperature deformation due to creep instability caused by cavity formation. It is revealed through dislocation analysis that intrinsic Frank partial dislocations are the driving factor for cavity generation leading to intergranular fracture.

1. Introduction

One of the factors that determine the life of a component exposed to prolonged loading at extreme conditions is the creep properties of the material. Moreover, if the component is made of nanocrystalline materials, understanding of creep behaviour is far from conclusion as there is a huge deviation in creep properties of nanocrystalline materials compared to its bulk counterpart due to increased volume fraction of inter grain regions (e.g. grain boundary, triple junctions) [1]. For instance, the creep rate of nanocrystalline materials is enhanced fourfold with respect to its coarse-grained structure [2]. Thus, the investigation of underlying mechanism responsible for creep behaviour of nanocrystalline materials is essential as it can contribute towards developing nano structure materials having better creep resisting properties. But conventional tensile and compressive creep tests are difficult to perform because of nano-scaled specimen size and limitation in the threads of conventional creep machine [3]. Consequently bending creep tests are receiving attention as an alternative process since it requires simpler experimental setup to study the creep behaviour of the material [3]. Apart from this, bending creep deformation is also observed in critical parts of gas turbines such as tip shrouds, thus pressing importance to the study of mechanism of creep deformation to determine bending creep properties of metallic systems [4]. Some experimental studies based on bending creep test have been performed to determine the change in viscosity of a porous material [5], and investigating high temperature creep properties of carbon nanotubes [6]. Since bending creep like other creep process is a time dependent phenomenon, it is generally a tedious process and additionally expensive to study at nanoscale. Hence simulation is an alternative way to study the bending creep behaviour. A considerable research has been done at continuum scale to determine the creep properties of materials [7,8], creep damage behaviour [9] through bending creep tests. Although some molecular dynamics (MD) simulation based studies on a simple bending deformation has been performed on metallic nanowires and nanobeams [10–12], neither experimental nor simulation based atomic level study has been performed till date which determines the bending creep deformation mechanism in metallic systems.

2. Simulation methods

A detailed mechanistic study of bending creep deformation for both high temperatures ($T > 0.5\ T_m$) and low temperature ($T < 0.3\ T_m$) have been performed here using molecular dynamics simulation through open source LAMMPS software [13]. Bicrystal nanobeam is chosen for this study to interpret distinctively the effect of grain boundary motion, dislocation and lattice diffusion phenomenon on bending creep behaviour along with the effect of temperatures. We designed a model of nickel bicrystal nanobeam and the grain boundary is formed using the concept of coincidence site lattice with a reciprocal density of coincidence site ($\sum$) equal to 5. The bicrystal have symmetric $\sum 5\ (-3\,1\,0)/(3\,1\,0)$ tilt grain boundary with inclination angle, $\phi = 0^o$ [14]. The nickel bicrystal specimen with $\sum 5$ grain boundary orientation is depicted in Fig. 1. The modelled specimen dimension is (5×5) nm in cross-section and 40 nm in length and contains 87556 atoms. The ends of the specimen are fixed and a load of 0.006 eV/Å (i.e. 9.6 pN) is applied

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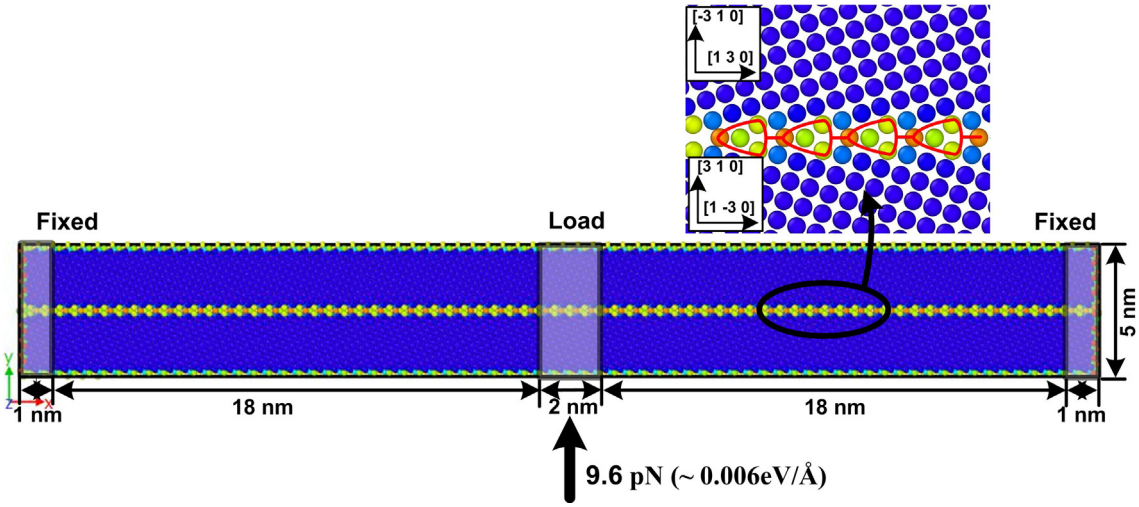

Fig. 1. An illustration of nickel nanobeam specimen with specified dimensions. Fixed and loading regions are depicted with a shaded region in the nanobeam. The inset shows the ∑5 grain boundary and the orientation of two nickel single crystals.

along the Y- direction i.e. [0 1 0] direction as also shown in Fig. 1. Non-periodic and shrink-wrapped boundary conditions have been used to simulate the bending creep deformation process. The simulation has been carried out using Embedded Atom Method (EAM) along with Finnis-Sinclair (FS) potentials at constant volume. Energy minimization or relaxation of the specimen has been performed by using conjugate gradient method, which is robust and effective [13]. The bending creep deformation is performed at constant temperatures taking NVT ensemble and the temperature is controlled by using Nosé-Hoover thermostat [15]. The deformation process is studied for a time period of 8 ns with a time step of 0.002 ps and is visualized using OVITO software [16]. Common Neighbour Analysis (CNA) [17] and Centro-Symmetry parameter (CSP) [18] analysis has been performed to determine the local atomic structure and lattice disorder respectively. Dislocation analysis (DXA) [19] aids in identifying all the dislocation formation in the specimen during the deformation process.

Throughout the creep deformation process, creep strain rate is calculated to plot the creep curves at different temperatures. To calculate the strain, our simulation method first identifies the deflection in the beam and then calculates the change in length of the central plane (ΔL) of the beam according to the following mathematical formula [20]:

$$\Delta L = \frac{12}{5}\frac{\delta^2}{L} \tag{1}$$

where, δ is the deflection of the beam identified through the simulation method and L is the length of the nanobeam. After identifying the deflection in the nanobeam, we have calculated the creep strain using the following equation:

$$\varepsilon = \frac{\Delta L}{L} = \frac{12}{5}\frac{\delta^2}{L^2} \tag{2}$$

where, ε is the creep strain during the bending deformation of the nanobeam.

3. Results and discussion

In this paper, underlying mechanism during bending creep deformation process at low temperature and high temperatures has been investigated and discussed in detail. Fig. 2(a) shows the creep curve for specimens deformed at low temperature (500 K) and high temperatures (900 K, 1100 K and 1300 K). During bending creep deformation at 500 K temperature, primary creep and steady state creep is observed. Whereas bending creep deformation at 900 K and 1100 K temperatures shows primary, steady state as well as tertiary creep. Creep curve during deformation at 1300 K shows increasing trend without distinguished primary or steady state creep until fracture. The occurrence of tertiary creep observed in our study can be attributed to the creep instability which is taken place due to the formation of cavities in the specimen. It has been observed that fracture does not occur in the specimen deformed at 500 K temperature whereas the occurrence of fracture at high temperature deformation is observed at tertiary creep regime [21]. The specimen is found to be fractured after 6.9 ns, 2.3 ns and 1.7 ns during creep deformation occurring at 900 K, 1100 K and 1300 K temperatures respectively. It is observed in the bending creep stain rate plot that failure at higher temperature occurs more rapidly which can be attributed to enhanced rate of grain boundary cavitation [22]. However with increase in creep temperature, specimens have exhibited higher plasticity before fracture mainly due to accelerated grain boundary motion and lattice diffusion, which is at par with the findings reported in literature [23]. Fig. 2(a) indicates that specimens deformed at low temperature attained a maximum strain of 11.3% at 500 K whereas specimens deformed at high temperatures attained a maximum failure strain of 28.7%, 30.9%, 53.8% at 900 K, 1100 K and 1300 K respectively.

The dislocation density variations with respect to time during creep deformation occurring at different temperatures are presented in Fig. 2(b). The dislocation density plot shows an overall higher density at low temperature indicating dislocation creep being the prevailing mechanism at that temperature. In the process of low temperature creep deformation, sudden high peaks are also observed in the dislocation density plot. These peaks correspond to the generation of grain boundary dislocation due to the jog formation [24–26]. At low temperatures, jogs are formed by the intersection of edge dislocations located along the grain boundary. Fig. 3 illustrates the jogs along the grain boundary during low temperature creep deformation at 1.2 ns. The inset in Fig. 3 shows the burger vector of the edge dislocations along with the dislocation direction. The edge character of the dislocation is proved by the fact that the dislocation direction and burger vectors are perpendicular to each other. It is evident from the direction of burger vector these jogs help in the movement of grain boundary through