Fatigue Deformation of Polycrystalline Cu Using Molecular Dynamics Simulations

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Abstract

Molecular dynamics (MD) simulations have been performed to investigate the fatigue deformation behaviour of polycrystalline Cu with grain size of 5.4 nm. The samples were prepared using Voronoi algorithm with random grain orientations. Fatigue simulations were carried out by employing fully reversed, total strain controlled cyclic loading at strain amplitude of ±4% for 10 cycles. The MD simulation results indicated that the deformation behaviour under cyclic loading is dominated by the slip of partial dislocations enclosing the stacking faults. At higher number of cycles, the grain boundary migration leading to coarsening of larger grains at the expense of the smaller grains has been observed. The cyclic stress-strain behaviour, the deformation mechanisms and the variation of dislocation density as a function of cyclic deformation have been discussed.

Keywords: Molecular dynamics simulations, Polycrystalline Cu, Fatigue, Partial dislocations and grain growth.

1 Introduction

Fatigue deformation in polycrystalline materials is a multi-scale problem involving the crack nucleation at the atomic scale to the final failure at the engineering scale [1]. Therefore, understanding the fatigue deformation at multiple length scales becomes important in order to design the optimum microstructure against the fatigue failure. Due to difficulties in performing experiments at the atomic scale, most of the studies in the past have concentrated on the damage at the micro and/or macro scales. With the rapid advancement of computational capability and the availability of reliable inter-atomic potentials, molecular dynamics (MD) simulations have become a major tool to examine the mechanical behaviour of materials at the atomic scale. However, the grain sizes accessible by the MD simulations are in the order of nanometers (nm). Therefore, the nanocrystalline materials with a grain size in the order of few tens of nm can only be studied using MD simulations.

Several MD simulation studies on the deformation of nanowires/nanocrystalline materials under monotonic loading conditions have been performed [2, 3, 4]. Only few studies exist in the literature pertaining to the MD
simulations on cyclic deformation of metals [5, 6, 7]. Further, due to time and length scale limitations involved in MD simulations, the cyclic deformation studies have been carried out only for few cycles. Rupert and Schuh [5] performed MD simulations to understand the cyclic deformation behaviour of polycrystalline Ni with grain sizes of 3, 4, 5, and 10 nm. The observed strengthening during cyclic deformation in Ni has been attributed to the grain boundary relaxation and the formation of low energy boundaries [5]. Recently, Panzarino et al. [6] characterized the grain structure evolution during the cyclic deformation of polycrystalline Al having grain size of 5 nm for 10 cycles. The cyclic strengthening was associated with the grain rotation, grain growth and the formation of many twin boundaries [6]. Like polycrystalline Al and Ni, MD simulations on the polycrystalline Cu with 5.5 nm grain size revealed the occurrence of grain coarsening during the cyclic deformation [7]. However, it is not clear whether cyclic deformation leads to softening or, hardening in Cu [7]. In order to understand the effect of cyclic loading on the strength and deformation behaviour of polycrystalline Cu, MD simulations have been performed on Cu with a grain size of 5.4 nm for 10 cycles. The cyclic stress-strain behaviour along with the observed deformation mechanisms with respect to number of cycles has been presented.

2 Simulation Details

MD simulations have been carried out in large scale atomic/molecular massively parallel simulator (LAMMPS) package [8]. MD simulations require an appropriate interatomic potential capable of modeling the plastic deformation. In view of this, embedded atom method potential for Cu given by Mishin et al. [9] has been used to describe the inter-atomic forces between the Cu atoms. This potential is widely used in the literature for studying the plastic deformation in Cu [4]. The polycrystalline Cu samples were prepared using Voronoi algorithm with random grain orientations [10, 11]. The overall size of the sample was about $10.8 \times 10.8 \times 21.6$ nm (aspect ratio of 2:1) consisting of 204,000 atoms (Fig. 1a). The sample contains 32 grains with an average grain diameter of 5.4 nm. In order to examine the size effect, MD simulations were also performed for grain sizes 7.2 and 9.4 nm. Since the surfaces play an important role under cyclic loading, periodic boundary conditions were used only along the length direction and the remaining two directions were kept free to mimic the free surfaces. In order to relax the internal stresses, the model system was equilibrated by heating to 500 K and then cooling to the required temperature of 10 K, where the actual fatigue simulations were performed. Upon completion of equilibrium process, the fatigue simulations were carried out at strain amplitude of ±4% for 10 cycles under total strain controlled cyclic loading and by employing fully reversed sinusoidal waveform with a time period of 100 ps (Fig. 1b). This provided a constant strain rate of $1.6 \times 10^9$ s$^{-1}$. The average stress is calculated using Virial expression [13]. The visualization of atomic configurations is accomplished in AtomEye [10] with common neighbour analysis (CNA) coloring [12].

3 Results and Discussion

Nanocrystalline materials generally exhibit wide elastic strain limits that vary with grain size, temperature and strain rate [3]. In order to identify the strain range where the plastic deformation initiates, MD simulations were performed on tensile deformation of polycrystalline Cu with grain size of 5.4 nm at 10 K (Fig. 1b). It has been
observed that the polycrystalline Cu undergoes an elastic deformation up to a strain level of 0.03 followed by the irreversible plastic deformation. Based on this, the strain amplitude of ±4% has been chosen for fatigue simulations. Typical stress-strain hysteresis loops corresponding to 1st, 5th and 10th cycles are shown in Fig. 2a. Similar to monotonic loading, the stress increases linearly during elastic deformation followed by yielding and plastic deformation up to 4% strain. Upon reversal at 4% strain the stress-strain varies linearly followed by yielding at relatively lower stress and plastic deformation up to -4% strain in compression. A well defined hysteresis loop develops due to irreversible plastic deformation and subsequent cyclic loading resulted in cyclic hardening. Figure 2b shows the variations in peak cyclic stress response (CSR) in tension and compression as a function of number of cycles. Cyclic softening up to 3 cycles followed by continuous hardening till the end of 10th cycle can be seen in Fig. 2b. MD simulation results for the grain size 7.2 and 9.4 nm also exhibited similar cyclic stress response. The observed cyclic stress response is in agreement with those reported for nanocrystalline Ni [5, 14] and Al [6] examined using experiments [14] and MD simulations [5, 6].

Figure 1: (a) A typical polycrystalline Cu sample after the equilibration and (b) fatigue waveform employed in MD simulations are shown. The front surface was removed for clarity in (a). The atoms were colored according to the CNA [12]. The red atoms represents surface and grain boundaries, blue atoms represents perfect FCC atoms and cyan atoms represents HCP atoms. Each 100 ps equivalent to one cycle is shown as one vertical grid in (b).

Figure 2: (a) The monotonic and the cyclic stress-strain behaviour at a strain amplitude of ±4% for polycrystalline Cu. The peak cyclic stress response in tension and compression with number of cycles is shown in (b).
The progressive plastic deformation with number of cycles at 3% total strain in tension for 1st, 5th and
10th cycles is shown in Fig. 3. The plastic deformation is mainly dominated by the glide of 1/6<112> partial
dislocations nucleating from the grain boundaries. The 1/6<112> partial dislocations have been found by
enclosing the stacking faults. It can be seen that, during the first cycle, the plastic deformation is activated only
in few grains (Fig. 3a), and with increase in the number of cycles, more grains participate in the deformation
process (Fig. 3b,c). The partial dislocations nucleating from one grain boundary (Fig. 3h) moves towards the
opposite grain boundary and gets annihilated. This suggests that the grain boundaries acts as a source as well as
sink for dislocations. The nucleation, glide and annihilation of partial dislocations leave a stacking fault ribbons
within the grain. Many such stacking fault ribbons produced by the movement of partials dislocations are shown
with white arrows in Fig. 3. The continuous nucleation of partial dislocations from the incoherent twin boundary
(ICTB) (Fig. 3h) and their reverse motion upon strain reversals converts the ICTB into a coherent twin boundary
(Fig. 3a). The coherent twin boundary formed during first few cycles remains highly stable during further cyclic
deformation (Fig. 3b). Contrary to this, the high angle grain boundaries have been found to be highly unstable
under the cyclic deformation. It has been observed that the heavily deformed grains coarsen at the expense of
undeformed grains associated with grain boundary migration. This grain coarsening results in the appearance
of large but lower number of grains at the end of 10th cycle (Fig. 3c). Our preliminary analysis indicates that
the grain growth is due to continuous impingement of partial dislocations on the grain boundary. The observed
cyclic deformation induced grain growth is in agreement with those reported by Panzarino et al. [6] in Al and
Sciotz [7] in Cu. This is also consistent with the deformation-induced grain growth in nanocrystalline materials.

Figure 3: The atomic snapshots showing plastic deformation in nanocrystalline Cu at a strain level of +3 % for (a) 1st,
(b) 5th and (c) 10th cycles. The front surface was removed for clarity. The atoms were colored according to the CNA [12].
The red atoms represent the grain boundaries, dislocation cores and surface atoms. Blue atoms represent perfect FCC
atoms and cyan atoms represent HCP atoms.

In order to further confirm and quantify the grain coarsening, the number of disordered atoms have been
calculated and presented as a function of cyclic deformation in Fig. 4. The disordered atoms include the atoms
in the surface, partial dislocation core and grain boundaries. By assuming the surface atoms to be constant
and the dislocation core atoms to be low during the deformation, the observed overall decreases in % disordered
atoms indicates that the total grain boundary area decreases with increase in cyclic deformation, thus confirming
the observed grain growth. The fluctuations observed in Fig. 4 are due to fluctuations in dislocation core
atoms during the deformation. The plastic deformation dominated by the glide of $1/6\langle112\rangle$ partial dislocations nucleating from the grain boundaries has been also observed at relatively larger grain sizes of 7.2 and 9.4 nm. Further, similar coarsening of heavily deformed grains at the expense of undeformed grains associated with grain boundary migration has been found for the grain size 7.2 and 9.4 nm. In nanocrystalline materials, it is well known that the grain size and strength are related by the inverse Hall-Petch equation. Based on this, the observed increase in strength from 3rd to 10th cycles can be attributed to the increase in grain size [6]. In order to understand the initial softening followed by hardening, the variations of dislocation density and % stacking fault atoms have been calculated as a function of cyclic deformation (Fig. 5). The dislocation density is calculated by using dislocation extraction algorithm [15]. The average dislocation density exhibited an increase up to 300 ps, i.e., 3 cycles followed by a continuous decrease up to 1000 ps or, 10th cycle (Fig. 5a). The initial increase in dislocation density has been associated with a similar increase in the % stacking fault atoms in the first 3 cycles followed by nearly constant % stacking fault atoms at higher number of cycles (Fig. 5b). Since the deformation in all the grains is not activated in the first cycle, the increase dislocation density and stacking fault atoms up to 3-4 cycles is mainly due to the continuous activation of dislocation sources in the undeformed grains. Contrary to this, the decrease in dislocation density from 4th to 10th cycle arises mainly from the decreases in dislocation sources (grain boundaries) resulting from the grain growth. This decrease in dislocation sources leads to the hardening as observed from 3rd to the end of 10th cycle.
4 Conclusions

Large scale molecular dynamics (MD) simulations have been performed to investigate the fatigue deformation behaviour of polycrystalline copper. The cyclic stress-strain behaviour is characterized by initial softening up to 3rd cycle followed by hardening till the end of 10th cycle. The MD simulation results indicated that the deformation behaviour under cyclic loading is dominated by the glide of partial dislocations enclosing the stacking faults. During the cyclic deformation, the twin boundaries were found to be stable boundaries, while the remaining high angle grain boundaries were highly unstable. As a result, an extensive grain growth is observed during the cyclic deformation. The initial softening followed by hardening has been inversely correlated with the dislocation density.

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