Acta Materialia 144 (2018) 68–79

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Dislocation interactions at reduced strain rates in atomistic simulations of nanocrystalline Al

Maxime Dupraz [a, *], Zhen Sun [a, b], C. Brandl [c], Helena Van Swygenhoven [a, b]

[a] Swiss Light Source (SLS), Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland
[b] NXMM Laboratory, IMX, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
[c] Institute for Applied Materials (IAM-WBM), Karlsruhe Institute of Technology, D-76344, Eggenstein-Leopoldshafen, Germany

ARTICLE INFO

Article history:
Received 20 June 2017
Received in revised form
23 September 2017
Accepted 19 October 2017
Available online 25 October 2017

Keywords:
Nanocrystalline materials
Molecular dynamics
Reduced strain rate
Interaction dislocations/grain boundaries

ABSTRACT

Molecular dynamics simulations of transient stress drops have been carried out in different regimes on a nanocrystalline Aluminum sample with average grain size of 12 nm. Besides confirming the interpretation of experimental results obtained during *in situ* X-ray diffraction, the creep simulations performed at 2 or 3 orders of magnitude lower strain rates than usual reveal deformation mechanisms that have not been observed previously. First of all, it is evidenced that the misfit dislocations available at the GB assist the propagation of a lattice dislocation on a plane with low resolved shear stress. Furthermore, it is shown that the interaction of two dislocations gliding on parallel slip planes can result in the emission of a vacancy in the grain interior. Finally, the importance of the Schmid factor in the activation of slip in nanocrystalline structures is discussed.

1. Introduction

It is well established that plastic deformation in nanocrystalline (NC) metals results from the interplay between dislocation and grain boundary (GB) based deformation mechanisms [1–4]. Molecular Dynamics (MD) simulations suggested that GBs act as both source and sink for dislocations [5–13]. A dislocation that is emitted from the GB or triple junction (TJ), travels through the entire grain and can be eventually absorbed in the neighbouring and opposite GBs. As a consequence, dislocation debris are rarely observed in the grain interiors upon unloading (or post-mortem analysis), which is also consistent with the observed suppression of a dislocation network during deformation [14]. Of course, dislocation emission and absorption require also GB accommodation mechanisms and so it is difficult, if not impossible, to separate both type of deformation mechanisms. Atomistic simulations performed for Al and Cu showed a shift from dislocation-mediated plasticity to GB sliding corresponding to a maximum flow strength [8,10,15]. Experimentally, measurements of strain rate sensitivity and flow stress activation volumes confirmed that grain boundary activity is enhanced but not yet dominant in 10 nm grain sized Cu [16] and in 20 nm grain sized Ni-20%Fe alloy [17]. Transmission electron microscopy (TEM) observations in 10 nm grain sized Ni led to the same conclusions [18]. On the other hand, simulations have also suggested that when the grain size is small enough (of the order of 5 nm), plastic deformation could be solely obtained by GB accommodation mechanisms [11,19,20]. Finally, subsequent MD simulations [21] and experimental observations [22] have evidenced that the relative contribution of dislocation glide and GB sliding depend on the amount of plastic strain.

The inherent high strain rates of MD simulations make it however very challenging to determine the rate limiting deformation mechanisms occurring at the much lower strain rates used in experiments. It has been shown that the application of higher strain rates results in higher flow stresses [23,24]: decreasing the strain rate from 5×10^8/s to 5×10^7/s results already in a 15% reduction in the flow stress of NC copper [23]. With these high flow stress, GB accommodation mechanisms are mainly stress driven [24] and dislocations are enabled to propagate athermally through the stress intensities present in GBs. The latter is suggested by the reduced number of cross-slip events at higher strain rates [25,26].

Experimental transient stress-drop tests allow identifying relevant strength contributions of those deformation mechanisms that are not rate-limiting at flow stress levels, but still contribute to the overall strength of the material [22,27,28]. The combination of *in situ* X-ray diffraction and transient stress-drop experiments allow

* Corresponding author.
E-mail address: maxime.dupraz@psi.ch (M. Dupraz).

https://doi.org/10.1016/j.actamat.2017.10.043

to link the kinetic signatures of the deformation mechanisms to their structural footprints. In the diffraction peak analysis, dislocation slip is associated with an increase of the full width at half maximum (FWHM) of the diffraction peak, whereas GB accommodation mechanism are expected to decrease the FWHM [29]. Such experiments have been performed on NC Ni with average grain size of 65 and 35 nm [28]. It was shown that at small stress drops, where the stress dependence of strain rate is high, the FWHM continues to increase due to dislocation-based mechanisms. At large stress drops, recovery mechanisms that reduce the FWHM are dominating and defect recovery mechanisms play an important role in the generation of plastic strain. Interestingly, at intermediate stress drops, the FWHM first decreases and then starts increasing again, suggesting an accommodation of the GBs followed by a re-activation of slip mechanisms.

Inspired by the transient testing experiments we carried out molecular dynamics simulations of stress drops in the regimes similar to those experimentally performed, with the aim to explore the mechanisms responsible for GB accommodation and to verify whether dislocations are still emitted when strain rates after the stress drops are up to 2 or 3 orders of magnitude lower than those usually applied in atomistic deformation simulations. Although still orders of magnitude higher than the experimental strain rates, the contribution of thermally activated processes to the deformation mechanisms [26] and in particular to the GB accommodation mechanisms is indeed expected to be higher at these lower strain rates of 10^6/s.

Our approach confirms the enhancement of the GB accommodation processes at a strain rate of 10^6/s, as well as the slip of dislocations on planes experiencing relatively low resolved shear stress. Additionally, a new GB-dislocation interaction mechanism is evidenced, where the misfit regions available at the GB assist the propagation of a lattice dislocation on a plane with low resolved shear stress. Furthermore, it is shown that the interaction of two dislocations gliding on parallel slip planes can result in the emission of a vacancy in the grain interior. For similar strains obtained with a strain rate of 10^8/s strain rate as usually applied in MD, both mechanisms are not observed and dislocations slip preferentially on high Schmid factor planes.

2. Technical details of the simulation

MD simulation of stress reductions were performed with the open-source Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [30] on a NC Al sample that contains 15 randomly orientated grains with an average grain size of approximately 12 nm (~ 10^6 atoms) in an orthonormal simulation box of the initial size 27.5 × 27.5 × 27.5 nm^3. The initial sample was geometrically constructed using the Voronoi procedure [31] under full 3D periodic boundary conditions, which are maintained during all simulations. It was then relaxed athermally and equilibrated for 100 ps at 300 K and zero stress MD using the Nose-Hoover thermostat and Parrinello-Rahman barostat [32]. The interatomic interaction was modelled using the Al embedded atom method (EAM) potential of Mishin et al. [33].

The sample was uniaxially loaded with constant strain rate (10^8/s) parallel to the z direction, with lateral zero stress conditions imposed by the Parrinello-Rahman method [34] up to 5.2% total strain. The stress drops were imposed by instantaneous switching to stress boundary condition in the tensile direction.

The structural analysis is performed at instantaneously quenched configurations by viscous damped dynamics for 250 fs at constant simulation box to filter thermal fluctuations. The local crystalline structure is analysed by the common neighbour analysis (CNA) [35], where face centred cubic (FCC) atoms, hexagonal close-packed (HCP) atoms and other coordinated atoms are coloured in grey, red, and blue, respectively. The presence of an intrinsic stacking fault is identified by two consecutive {1 1 1} planes of HCP atoms and a twin fault by only one single {1 1 1} HCP plane. The atomic displacements are corrected by subtracting the simulation box changes to map only the internal, microscopic displacements of atoms. In past work [25,36,37], it has been shown that the local hydrostatic pressure concentrations are sensitive indicator for GB structural changes once dislocation activity occurs, e.g. dislocation emission, pinning, and absorption. In the present work, the local hydrostatic pressure variations within the NC sample are also analysed. This is achieved by calculating the stress tensor of a volume element of radius of 4 Å (as it was done in previous work [25,37]) centred around each atom using the momentum conserving approach derived by Cormier et al. [38]. The open-source software 'Open Visualization Tool' (OVITO) [39] is used to visualize the atomic configurations. The local displacement gradient tensor for each particle within an angstrom cut-off radius corresponding to the distance between the first and second neighbours is used to estimate the local von Mises invariant shear strain. Finally, the dislocation analysis (DXA) [40] as implemented in OVITO and the slip vector analysis method [41] are used in combination to identify and determine the Burgers vector of the dislocations. The line representation of the dislocation defects used in some figures of this manuscript is also computed using the DXA.

3. Results

3.1. Overview of the stress reduction series

Fig. 1 a provides a schematic representation of the stress reduction test. Each specimen is first strained to a pre-defined stress σ_0, and fast unloaded by a certain amount of stress. At the reduced stress σ_r, the specimen is allowed to creep some period of time. The ratio between both stress levels is denoted by the relative reduced stress $R = \sigma_r/\sigma_0$. Fig. 1 b displays the MD simulated stress-strain curve deformed at room temperature at a constant strain rate of 10^8/s. Stress reduction tests series are performed when the sample is strained to an engineering strain of 5.2%, where the flow stress reaches $\sigma_0 = 1.52$ GPa. A wide range of R values was covered from 0.92 to 0.33 similar to the experiments performed in Ref. [28]. After each stress reduction, the specimen was simulated for 1700 ps under constant stress conditions at σ_r. Fig. 1 c displays the corresponding creep strain-time curves. Notably, these curves are found to be stress dependent, and exhibit similar trends as those found in the *in situ* experiments: *i.e.* when the stress drop is mild, there is a continuous forward strain with creep time [28]; when the stress drop becomes larger, an initial anelastic black flow dominates, after which forward strain continues; for the largest stress drop no forward straining is observed within simulated creep time. Fig. 1 d evaluates the number of mobile dislocations propagating during the creep periods for each relative reduced stress R. Dislocation activities including nucleation and propagation are largely suppressed with decreasing R. At moderate stress drops freshly nucleated dislocations can propagate after a certain incubation period. For large stress drops such as $R = 0.53$ and 0.33, nucleated dislocations do not propagate anymore within the time scale of the simulation.

3.2. A medium stress drop with longer creep

The creep strain for the stress reduction with $R = 0.86$ is followed during a longer period of 2290 ps as shown in Fig. 2. In this curve, each pronounced strain burst reflects the propagation of a dislocation across a grain. As expected from a NC material the