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Microstructural investigation of the hardening mechanism in fcc crystals during high rate deformations

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ABSTRACT

The present paper studies the hardening mechanism in fcc metallic structures during high rate deformations by incorporating the dislocation network properties. The large scale atomistic simulation is used to study the variations of dislocation length distribution and its characteristic lengths as the strain rate changes. First, the dislocation length distributions at different strain rates are studied to qualitatively capture the relation between the material strength and applied strain rate. It is observed that increasing the strain rate decreases the dislocation network lengths. Accordingly, the required stress to activate the dislocation sources increases. Since dislocation movements sustain the imposed plastic flow, higher activation stress leads to material hardening. Furthermore, the results show that the properties of dislocation length distribution at high deformation rates are different from those of lower strain rates due to the activation of cross-slip mechanism at high strain rates. In order to quantitatively describe the relation between the material strength and dislocation network properties as the strain rate varies, the variations of average and maximum dislocation length are investigated in the cases of different applied strain rates. The relation between the material strength and average length of mobile dislocations is captured using an inverse linear equation which shows a good agreement with the atomistic simulation results.

1. Introduction

Up to now, many strengthening mechanisms have been identified in bulk metallic samples including forest hardening mechanism (i.e. interaction of dislocations with each other), Hall-Petch effects (i.e. interaction of dislocation with the grain boundary), solid-solution strengthening, precipitation strengthening, and variation of lattice resistance [1]. When it comes to the high rate deformations, the experimental and theoretical studies have demonstrated intriguing deformation and strengthening mechanisms that are different from those of the slower rates. Several experimental techniques of gas guns, split Hopkinson bars, Z-pinch, and high-energy pulsed lasers have been developed to study the material behavior during high rate deformations [2,3]. The experiments cover a wide range of strain rates up to 10^{10} s^{-1}. Recently, Crowhurst et al. [4] incorporated a laser pulse to accelerate the free surface of tantalum and studied its yielding at strain rates up to 10^{9} s^{-1}. Remington et al. [3] reviewed the application of high-power pulsed to induce the strain rates of $10^{6} - 10^{10}$ s^{-1}. They addressed the fundamental issues at high strain rates including dislocation velocity, the slip-twinning transition, and the transition between thermally-activated and phonon drag regimes [3]. The experimental results showed that the mechanisms governing the strengthening in the high rate deformations are different from those of the slower strain rates. As an example, Park et al. [2] showed that the plastic flow in metallic materials is independent of the grain size at ultrahigh pressures and strain rates and the conventional Hall-Petch effect is not available anymore.

The governing deformation mechanisms in metallic samples depend on the applied strain rate. The Frank-Read source operation, which is a well-stablished deformation mechanism (see, e.g., Hirth and Lothe [5] and Hull and Bacon [6]), is the primary mechanism of deformation for strain rates up to $10^{3} - 10^{6}$ s^{-1} (see, e.g., Gurrutxaga-Lerma et al. [7]). Increasing the strain rates, the cross-slip [7–16] and homogenous dislocation nucleation [7,17–21] become the dominant mechanisms of deformation. The relation between the material strength and strain rate have been captured using various mechanisms. The primary relation between the material strength and strain rate can be developed using the Arrhenius form equation that leads to a linear relation between the strength and the natural logarithm of strain rate. The linear relation is applicable for strain rates up to 10^{4} s^{-1} [22–24]. In this range of strain rates, the thermal-activation mechanism controls

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the variation of strength as the strain rate changes [23,24]. Gurrutxaga-Lerma et al. [7] captured the variation of strength versus the strain rate by relating the activation time and strength of Frank-Read sources to the applied strain rate that is applicable to strain rates up to 10^6 s^{-1}. The relation between the strength and strain rate for strain rates higher than 10^4 s^{-1} can be described using the interaction between the moving dislocations with phonon drag [23,24]. Furthermore, in the cases of strain rates larger than 10^4 s^{-1}, Fan et al. [22] incorporated the non-Arrhenius behavior in their model to capture the relation between the strength and the applied strain rate.

Theoretical models which define the relation between the strain rate and strength of fcc metallic structures have been widely investigated (see, e.g., Hirth and Lothe [5] and Hull and Bacon [6]). The microstructural studies can be incorporated to evaluate and modify the developed models. In the case of fcc metallic structures, the hardening mechanism is controlled by the properties of dislocation network (see, e.g., Hirth and Lothe [5] and Hull and Bacon [6]). In order to study the evolution of dislocation network as the strain rate varies, the incorporated microstructural method should be able to capture dislocations as separate entities. Discrete dislocation dynamics (DDD) has been incorporated to study the hardening mechanisms in metallic materials using the dislocation network properties (see, e.g., El-Awady et al. [25]). In the case of high rate deformations, the cross-slip is one of the major governing deformation mechanisms [7–16]. The cross-slip has been incorporated in DDD using some ad-hoc assumptions (see, e.g., Wang et al. [11] and Hussein et al. [15]), and more investigations should be conducted to evaluate the accuracy of DDD to capture the cross-slip at high strain rates. Furthermore, Gurrutxaga-Lerma et al. [26] showed that a dynamic DDD should be incorporated to capture the hardening mechanism at high strain rates. However, until now, an investigation of the hardening mechanism in bulk fcc materials at high rate deformations that relates the material strength to the dislocation network properties, such as dislocation length distribution, has not been conducted using a DDD which incorporates a well-established cross-slip model and appropriate dynamic framework.

Another method to investigate the microstructural evolution of metallic structures as the strain rate varies and its relation with the hardening mechanism is to model the sample with full atomistic details using molecular dynamics (MD). After defining appropriate atomic interactions, MD is fully capable of capturing all the deformation mechanisms, such as cross-slip, without using any ad-hoc approximation. However, MD, due to its nature, has limitations on the simulation length scale and time scale. Nowadays, by developing efficient parallel algorithms and powerful supercomputers, samples consisting of one billion atoms can be modeled using atomistic simulation [27–30]. In the case of time scale, although the MD cannot capture the quasi-static experiments, it is an appropriate method to model the high rate deformations [31–34]. Unlike the DDD which directly reports the dislocation properties, MD only calculates the atomic trajectories and velocities. Accordingly, the dislocation properties should be obtained from the atomic trajectories using some post-processing methods. Stukowski [35] implemented and compared various methods of defect detection in crystalline materials including energy filtering, centrosymmetry parameter analysis, bond order analysis, Voronoi analysis, adaptive common neighbor analysis, and neighbor distance analysis. Stukowski and his co-workers [35,36] have developed the Crystal Analysis Tool which is able to extract the required dislocation information including the dislocation length, position, and Burgers vector from atomic trajectories. Until now, the dislocation density or the total length of dislocations are the only variables which have been considered to study the hardening mechanisms in fcc bulk metallic samples [16,28,31,37–42]. Accordingly, deeper understanding of dislocation network properties, such as dislocation length distribution, average length of dislocations, and maximum dislocation length should be acquired to fully capture the hardening mechanisms.

One of the most important properties of dislocation network is the dislocation length distribution. In the case of metallic bulk samples and quasi-static strain rates, El-Awady et al. [43] incorporated the experimental results reported by Mughrabi [44] and described the probability density function (PDF) of the dislocation length using a Weibull distribution. In the cases of metallic samples of confined volumes with free surfaces, such as pillars, the PDF of the dislocation length changes due to the interaction of dislocations with free surfaces [43,30]. Accordingly, the size effects in pillars can be captured using the modified dislocation length distribution [43,30]. In the cases of bulk metallic samples and high rate deformations, however, the evolution of dislocation length distribution has not been investigated as the strain rate varies.

In this work, the large scale atomistic simulation is incorporated to investigate the hardening mechanism in fcc bulk materials during high rate deformations using the properties of dislocation length distribution. The variations of dislocation network and its characteristic lengths including the average and maximum dislocation length versus the strain rate are quantitatively studied using large scale atomistic simulation. As the strain rate increases, the dislocation density increases to sustain the imposed plastic flow. Accordingly, increasing the dislocation density leads to the reduction of the characteristic lengths of dislocation network. Some characteristic lengths of the dislocation network including the average and maximum dislocation length are investigated to capture the variation of strength as the strain rate changes. The smaller dislocation characteristic lengths lead to the larger strength. It is due to the fact that larger stresses are required to activate smaller dislocations. Accordingly, increasing the strain rate leads to the material hardening.

2. Simulation details and methodology

Large scale atomistic simulation of a Ni single crystal cube, as an example of fcc material, during uniaxial compression test is incorporated to study the hardening mechanism in the region of high strain rates ($\dot{\varepsilon} \approx 10^8$ s^{-1}). The cube with the dimensions of 1500 Å, 1500 Å, and 1500 Å along $[1\ \bar{1}\ 0]$, $[1\ 1\ \bar{2}]$, and $[1\ 1\ 1]$ directions, respectively, is generated (Fig. 1). The parallel code LAMMPS [45] is incorporated to perform the atomistic simulation. The sample consists of around 310,000,000 atoms. The embedded-atom method (EAM) potential developed by Mishin et al. [46] is used to model the Ni-Ni atomic interaction [47]. The periodic boundary conditions are incorporated for all three directions. Newton's equations of motion are integrated using the velocity Verlet algorithm with a time step of 1.5 fs. The simulations are performed using NPT ensemble. The sample is relaxed for 100 ps with the temperature increasing from 1 K to 300 K and zero pressure in all directions. Next, it is relaxed for another 100 ps at 300 K and zero pressure in all directions. Finally, the uniaxial compression is conducted along $[1\ 1\ 1]$ direction from the sample top and bottom with three constant strain rates of $\dot{\varepsilon}_1 = 2.0e8$ s^{-1}, $\dot{\varepsilon}_2 = 1.0e9$ s^{-1}, and $\dot{\varepsilon}_3 = 5.0e9$ s^{-1} at 300 K and zero pressure on the lateral boundaries (Fig. 1). The Crystal Analysis Tool developed by Stukowski and his co-workers [35,36] is incorporated to extract the dislocation structures from the atomic trajectories, and provide additional information such as dislocation length and Burgers vector. The Crystal Analysis Tool is developed based on the common-neighbor analysis method. The atomic arrangements and structures are initially identified. Next, a pattern matching algorithm