Computational Materials Science 149 (2018) 125–133

Contents lists available at ScienceDirect

Computational Materials Science

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

Shear relaxation behind the shock front in ⟨1 1 0⟩ molybdenum – From the atomic scale to continuous dislocation fields

Roman Kositski[a,*], Dominik Steinberger[b], Stefan Sandfeld[b], Dan Mordehai[a]

[a] Department of Mechanical Engineering, Technion – Israel Institute of Technology, 32000 Haifa, Israel
[b] Chair of Micromechanical Materials Modelling (MiMM), Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, 09599 Freiberg, Germany

ARTICLE INFO

Keywords:
Shock wave
Molecular dynamics
High strain rate deformation
Plasticity

ABSTRACT

In this work we study shock-induced plasticity in Mo single crystals, impacted along the ⟨1 1 0⟩ crystal orientation. In particular, the shear relaxation behind the shock front is quantitatively inspected. Molecular dynamics (MD) simulations are employed to simulate the deformation during shock, followed by post-processing to identify and quantify the dislocation lines nucleated behind the shock front. The information on the dislocation lines is ensemble averaged inside slabs of the simulation box and over different realizations of the MD simulations, from which continuous dislocation fields are extracted using the Discrete-to-Continuous method. The continuous dislocation fields are correlated with the stress and strain fields obtained from the MD simulations. Based on this analysis, we show that the elastic precursor overshoots the shear stress, after which dislocations on a specific group of slip planes are nucleated, slightly lagging behind the elastic front. Consequently, the resolved shear stress is relaxed, but the principal lateral stress increases. The latter leads to an increase in the resolved shear stress on a plane parallel to the shock wave, resulting in an additional retarded front of dislocation nucleation on planes parallel to the shock front. Finally, the two-stage process of plasticity results in an isotropic stress state in the plane parallel to the shock wave. The MD simulation results are employed to calculate the dislocation densities on specific slip planes and the plastic deformation behind the shock, bridging the gap between the information on the atomic scale and the continuum level.

1. Introduction

Shock deformation of metals was studied extensively in the past century as it is fundamental to the understanding of how metals behave at high strain rate. For instance, when a high-velocity projectile impacts a metallic target, pressures of the order of 10 GPa and strain rates of 10^4 s^{-1} can evolve at the impacted site [1]. A micro-meteorite can impact a satellite or a space station at velocities exceeding 10 km s^{-1} resulting in pressures of a few tens of GPa and strain rates of 10^5–10^6 s^{-1} [2]. In explosion welding (or bonding) pressures of 20–30 GPa can be generated with high strain rates and significant plastic deformation at the joined interface [3]. Even in plane and car crashes, high pressures and high strain rates with large plastic deformation can occur [4]. Despite the considerable amount of research, only recently experiments [5–8] and numerical simulations [9–11] were able to shed some light on the microstructural origins of plastic deformation in metals during the initial stage of shock compression.

The most common technique to experimentally study shock-induced plasticity is by generating a planar shock on a surface of the specimen. As the planar shock wave propagates from the surface into the bulk, the material is compressed uniaxially. As a result, the state of strain right behind the shock is uniaxial with a three-dimensional stress state (stress components on the plane non-parallel to the shock plane are not zero). This stress state may result in shear stresses that are sufficiently high to cause plastic flow. During plastic deformation, the shear stresses are reduced and the stress state approaches an isotropic compression. This process of plastic strain evolution and concomitant reduction of shear stresses is known as plastic relaxation or shear relaxation [12].

Several works attempted in recent years to study the underlying microstructural mechanisms during plastic relaxation. Wehrenberg et al. [8] performed laser-driven shock experiments on single crystal Ta samples to pressures of up to 100 GPa. Using Laue X-ray diffraction they measured the strain anisotropy right behind the shock wave and could measure the relaxation time. They found that for pressures of about 50 GPa the relaxation time is of the order of 1 ns. For a shock pressure of 100 GPa, they could not observe the relaxation and concluded that it must occur in less than 0.3 ns, which is the temporal resolution of the experiment. Milathianaki et al. [5] performed similar experiments on single crystal Cu at pressures of about 73 GPa and measured the strain evolution *in-situ*. From their measurements, they concluded that the

* Corresponding author.
E-mail address: kositski@gmail.com (R. Kositski).

https://doi.org/10.1016/j.commatsci.2018.02.058
Received 18 November 2017; Received in revised form 27 February 2018; Accepted 28 February 2018

shear relaxation process takes about 60 ps with plastic strain evolving to about 6.2%.

The experiments suggest that there is a substantial difference in relaxation times between lower and higher shock stresses. In order to rationalize this observation, a number of models for shear stress relaxation have been developed. Rudd et al. [13] proposed a model for calculating the stress at a given strain, based on the evolution of dislocation density and dislocation glide. With this model, they calculated the relaxation time in shock compressed Ta and found that for shock pressures of 10 GPa to 50 GPa the relaxation time is of the order of a few ns. In this pressure range, the dislocation density first needs to sufficiently increase so that the glide of dislocations can reduce the shear stresses. Motivated by the fact that their model does not account for homogeneous dislocation nucleation, they additionally performed molecular dynamics (MD) simulations. From these simulations, they found that for shock pressures above 66 GPa, dislocations homogeneously nucleate and the relaxation time drops by three orders of magnitude to about 1 ps. This significant difference in relaxation times suggests that the above mentioned experimentally relaxation times result from different dislocation mechanisms.

While the model by Rudd et al. captures the relaxation time to some extent, they employ a continuum model with phenomenological rules for the evolution of dislocation. In addition, homogenous nucleation is not taken into account. To study the plastic relaxation with details of the dislocation structure, and also to include homogenous nucleation, Shehadeh and Zbib [14] used a Discrete Dislocation Dynamics (DDD) framework to perform simulations of shock loaded single crystal Cu. Performing simulations above the nucleation threshold with shock compressive stresses ranging from 20 GPa to 100 GPa they found that the plastic relaxation time is decreasing from about 500 ps to about 150 ps as the shock intensity (and subsequently the strain rate) increases. Based on their DDD simulations they were able to correlate the evolution of dislocation densities to strains and stresses. However, despite the level of details in DDD simulations, their analysis relied on effective quantities, which are insufficient to understand the micromechanical mechanisms behind plastic relaxation in single crystals. In addition, reliable rules for homogeneous nucleation in DDD simulations are still lacking, and the role of homogenous nucleation in the stress relaxation is not clear.

MD simulations are more commonly used than DDD simulation and have been employed to study the plastic deformation behind the shock front and in particular the shear relaxation process, since they naturally incorporate dislocation nucleation and the interaction and evolution of dislocations. In recent years, a large amount of work has been carried out on face-centered cubic (FCC) metals [6,9,15,16] while simulations of body-centered cubic (BCC) metals are less common. Most of the work on BCC metals was on Fe due to its relevance to technological applications. These works were focused on the solid-solid phase transformation occurring in Fe at about 13 GPa and thus less focused on dislocation–mediated plasticity [11,17–19]. For instance, in MD simulations by Cuesta-Lopez and Perlado [20] of Ta, W and Fe, solid-solid phase transformations were observed during shock, which prohibited the nucleation of dislocations, although only Fe was expected to deform via phase transformation. Liu et al. [21] performed MD simulations of shock loading of a single crystalline W specimen at different orientations. They obtained detailed stress profiles along the propagation of the shock front and observed the relaxation of the shear stresses due to plasticity behind the plastic shock front. While focusing on the evolution of stresses, they did not study the underlying micromechanical mechanisms causing the shear relaxation, nor performed a quantitative discussion on it. More recently Ravelo et al. [22] developed a new interatomic potential for Ta. They performed shock propagation MD simulations in single crystal Ta and found that at a certain pressure (or particle velocity) threshold, twins nucleate behind the plastic wave front reducing the shear stresses to practically zero. Tramontina et al. [23] used the same potential but added a nanovoid inside the lattice to act as a nucleation site for dislocations. They found that around the nanovoid dislocations nucleate to a dislocation density of about $10^{13}\,cm^{-2}$ at shock pressures of about 50 GPa.

These examples also demonstrate the shortcomings of MD simulations; they hold temporal information on all atoms in the system and if one wants to relate the discreet nature at the atomic level to the continuum level, the information from all atoms should be related quantitatively to continuous fields [24]. For instance, while dislocations are discrete defects in the crystal lattice, their collective motion results in a continuous plastic deformation. On the other hand, dislocation-based continuum models of plasticity are not restricted to the particular details of each dislocation, as they describe dislocations as continuous fields on different slip planes with some physical rules from length scales below the averaging volume size. In most cases, the way the continuum is related to the atomic scale is by transforming individual dislocations from the MD simulations into a total dislocation density field [9,25]. However, such a field variable is insufficient for computing the spatially heterogeneous plastic deformation and the evolution of shear relaxation since different slip systems contribute differently to plastic deformation [26]. Thus, we would like to benefit from the advantages of MD simulations, in naturally describing dislocation mechanisms, and quantitatively relate them to continuous parameters of the plastic deformation.

One strategy would be to employ MD simulations to study shear relaxation behind the shock front and to develop computational frameworks for data mining that could help to bridge between the atomic and continuum scales. For instance, ensemble averaging and statistical data analysis of information on individual dislocation can be related in a sequential multiscale approach to continuous dislocation fields, in order to develop constitutive rules with quantitative information on the dislocation microstructural evolution and its interplay with the loading conditions. The challenges to fulfill this strategy is two-fold: first, it is necessary to extract quantitative information of dislocations from MD simulations. Recently developed tools, such as the Dislocation Extraction Algorithm (DXA) [27]) made it possible to obtain dislocations as geometrical, line-like objects from the atomic scale. Second, a well-defined strategy to obtain continuous dislocation fields from discrete dislocation lines is required for a suitable data analysis. This Discrete To Continuum (D2C) strategy was recently developed and has been applied to and validated by Discrete Dislocation Dynamics (DDD) simulations [28,29] and has been used for studying nano-scratching with MD simulations [30].

In this work, we employ the combined DXA-D2C strategy to study the evolution of continuous dislocation fields during plastic relaxation in shocked single crystal [1 1 0] Mo from MD simulations. In Section 2 we detail the simulation methods and, in particular, the method to transform discrete dislocation lines to continuous fields. In Section 3 we describe the MD simulation results and the outcome of extracting continuous dislocation. Based on these results, the correlation between continuous dislocation fields and stress that develops in the plastic zone behind the shock is discussed in Section 4, and the highlights of this paper are summarized in Section 5.

2. Methods

2.1. Molecular dynamics

We performed nonequilibrium MD simulations using the open-source code LAMMPS [31]. The interactions between the Mo atoms were described using the embedded-atom method (EAM) interatomic potential, with a parameterization proposed by Ackland and Thetford [32]. This potential was previously used in studying dislocation mobility in Mo [33] and dislocation nucleation and multiplication during plastic deformation of nanopillars [34]. While these works support the validity of this potential to describe plastic deformation, we are not aware of any shock simulation performed with the potential. To further