Computational Materials Science 154 (2018) 393–404

Contents lists available at ScienceDirect

Computational Materials Science

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

Molecular dynamics investigation of void evolution dynamics in single crystal iron at extreme strain rates

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ARTICLE INFO

Keywords:
Void nucleation and growth
Single crystals
High strain rates
Molecular dynamics
Iron

ABSTRACT

High strain rate deformation and fracture of materials is of interest for high velocity impact and penetration problems. In this work, we perform triaxial deformation of single crystal BCC iron at $(1.5\times10^{8}$–$1.5\times10^{10})\,s^{-1}$ volumetric strain rates with 300 K temperature and find that at very high volumetric strain rates, relaxation of tensile stress takes place first through the structural changes (phase transformation) and then via nucleation and growth of voids. While at lower volumetric strain rates, the nucleation and growth of voids is the only route to release the built up stress. High void nucleation events occur at volumetric strain rate of $1.5\times10^{10}\,s^{-1}$ while average void growth rate is high at $1.5\times10^{8}\,s^{-1}$ volumetric strain rate. This suggests that the nucleation of voids is more preferred at $1.5\times10^{10}\,s^{-1}$ volumetric strain rate while void growth is more preferred at $1.5\times10^{8}\,s^{-1}$ volumetric strain rate to accommodate the applied strain. The evolution of individual void volume fraction takes place through the discrete jumps indicating coalescence events. All the nucleated voids do not grow with equal rates and hence do not make significant contribution to the overall void volume fraction. Size distribution of voids follows exponential distribution in the region where nucleation and growth processes of the voids contribute most to the overall void volume fraction while power law function describes the void size distribution in the coalescence dominated regime of the overall void volume fraction. A framework to compute overall void volume fraction in terms of the individual voids is presented. The results can be useful to develop the fracture models at high strain rates to describe the damage evolution at continuum length scales.

1. Introduction

Solid fracture at high strain rate is of interest for high velocity impact and penetration problems. It is also very relevant to the inertial confinement fusion facilities (e.g. National Ignition Facility, USA) where fragmentation of the metal targets subjected to the high intensity laser irradiation leads to the damage of the equipments [1]. Therefore, a basic understanding of the fracture and overall behaviour of materials under the extreme conditions of temperature, pressure and large deformation is required.

The fracture at high strain rates takes place through the nucleation, growth and coalescence of voids [2] due to the tension resulting from the interaction of release waves from the free surfaces of the flyer and target in the high velocity impact experiments [3]. At these strain rates, slow processes such as diffusion of vacancies for the nucleation and growth of voids [4] do not occur [5] and the lattice instabilities [6] lead to the nucleation of voids. The length and time scales involved at these strain rates for the nucleation, growth and coalescence of voids are comparable with those accessible by molecular dynamics (MD) simulations.

To study the strength and fracture properties of the materials, there are various controlled methods to produce high strain rates in the material. The most commonly used methods for different level of strain rates are Split Hopkinson Pressure Bar (10^{2}–$10^{4}\ s^{-1}$) [7–9], Gas Gun (10^{5}–$10^{6}\ s^{-1}$) [10,11] and Laser (10^{7}–$10^{10}\ s^{-1}$) [1,3,12–17].

The real materials are polycrystallines which contain grain boundaries, impurities and different kinds of defects. All of these play a great role in the plastic deformation and fracture of the polycrystalline materials. Therefore, a systematic study is needed to understand the effect of individual defect (grain boundaries, impurities etc.) on the plastic deformation of the materials. Single crystals are free of coarse defects, such as grain boundaries. This is why various experiments [3,18–27] have been performed on single crystals to understand the microscopic deformation mechanisms of the materials subjected to high strain-rate loading. For example, to study the shock induced fracture properties (e.g. spall strength), various workers have performed experiments on single crystals of copper [19–21,28], aluminum [29], molybdenum [3,28,30], niobium [28,30], iron [18,31,32] etc. In addition to the

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https://doi.org/10.1016/j.commatsci.2018.08.010
Received 13 April 2018; Received in revised form 1 August 2018; Accepted 4 August 2018
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experimental studies on dynamic fracture, molecular dynamics (MD) simulations have been performed to study the nucleation and growth of voids in FCC [33–36] and BCC [37,38] materials under triaxial as well as uniaxial loading conditions at extreme strain rates.

Spall fracture is a multi-scale problem where nucleation, growth and coalescence of voids at nano-scale lead to fracture at macro-scale. In this regard, from continuum point of view, one would be interested to know: How the overall void volume fraction distributes among the voids? Do the voids follow any size distribution? How strain rate affects the microstructural evolution, overall void volume, number of voids and their growth rates? What is the role of nucleation, growth and coalescence processes of the voids on the evolution of overall number of voids? Do all the nucleated voids make significant contribution to the overall void volume? Does overall void volume fraction evolve due to the evolution of few voids or many voids? How does the individual void volume evolve? These and allied questions may help in understanding the void evolution dynamics at extreme strain rates and provide a basis to develop a fracture model in terms of the evolution of individual voids at extreme strain rates.

Mechanical properties of Fe-Cr based Ferritic/Martensitic (FM) steels under dynamic loading conditions are of interest for future fusion reactors and experiments have been carried out at strain rates up to $10^3\,s^{-1}$ to study the dynamic properties of these materials [39]. Plate impact experiments have also been performed to study the effect of helium bubbles on the spall strength of the materials [40], although those studies do not involve FM steels as a target material.

The objective of the present work is to investigate the effect of applied strain rate on the microstructural evolution and void evolution dynamics in single crystal iron triaxially deformed at extreme strain rates at room temperature. Here we consider triaxial deformation which represents an ideal case of loading condition to investigate the void evolution dynamics in shock-loaded targets. This type of loading condition is commonly utilized to investigate the nucleation and growth of voids in metallic systems using MD simulations (e.g. [33,35,36,41]). To our knowledge, there is no work on the void evolution dynamics (i.e. the number of voids, void size distribution, evolution of individual voids and void coalescence) in single crystal iron under triaxial loading conditions.

2. Computational method

We simulate the triaxial expansion of single crystal iron at extreme strain rates using the open source molecular dynamics code, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [42]. The computation domain contains 2×10^6 atoms corresponding to $100\times100\times100$ unit cells. The X-, Y- and Z-directions of the simulation domain correspond to $\langle1\,0\,0\rangle$, $\langle0\,1\,0\rangle$ and $\langle0\,0\,1\rangle$, respectively. We use concentration dependent embedded atom method (CD-EAM) potential [43] with parameters obtained by Ackland et al. [44] for Fe-Fe interaction. To integrate the equations of motion using velocity-Verlet algorithm, we use time-step of 1 femto-second. We use periodic boundary conditions in all three directions to remove any finite size effect. To get the temperature of the system at 300 K, we assign the initial velocities of the atoms at 300 K using Gaussian distribution and equilibrate the system at 300 K and 0 bar pressure. To control the temperature and pressure of the system, we use Nose-Hoover thermostat and barostat [45,46]. After the equilibration of the system at 300 K and 0 bar, we turn off the barostat and triaxially expand the system at $(1.5\times10^8$–$1.5\times10^{10})\,s^{-1}$ volumetric engineering strain rates with 300 K temperature. Note that we apply an equal engineering strain rate to X-, Y- and Z-axes of the simulation domain (i.e. $\dot{\varepsilon}_{xx} = \dot{\varepsilon}_{yy} = \dot{\varepsilon}_{zz}$) for triaxial deformation of single crystal iron at a given volumetric engineering strain rate. We use Ovito [47] for visualization of MD results. We have performed the comparison with two other interatomic potentials [48,49] and established the correspondence between our results and that obtained with two other interatomic potentials [48,49].

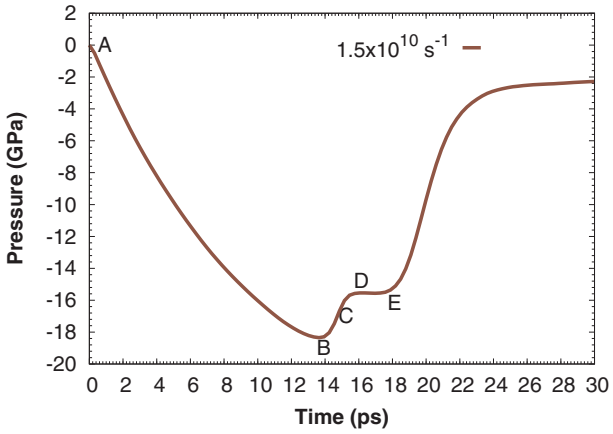

Fig. 1. Internal pressure as a function of time for single crystal iron triaxially deformed at $1.5\times10^{10}\,s^{-1}$ volumetric strain rate with 300 K.

3. Results and discussion

In this section, we discuss the response of single crystal iron deformed at $1.5\times10^{10}\,s^{-1}$ volumetric strain rate. We describe the results in terms of the pressure-time profile and microstructural evolution. In addition to this, we also discuss the effect of applied strain rate on the results (pressure-time profile, microstructural evolution and void evolution dynamics).

3.1. Deformation at $1.5\times10^{10}\,s^{-1}$ volumetric strain rate

In order to understand the response of single crystal iron at volumetric strain rate of $1.5\times10^{10}\,s^{-1}$, we compute tensile pressure as a function of time. The pressure-time profile gives an idea about the overall response of single crystal iron. Fig. 1 shows the internal pressure as a function of time for single crystal iron triaxially deformed at $1.5\times10^{10}\,s^{-1}$ volumetric strain rate with 300 K.

As observed from Fig. 1 that the tensile pressure in the system increases continuously up to a certain time point due to a decrease in the density of the system and at 13.8 ps, it reaches a maximum value of 18.3 GPa and then decreases indicating yielding of the material. At 16 ps, the tensile pressure stops decreasing and then a slight increase in tensile pressure (~0.03 GPa) occurs up to 17 ps. After that, a rapid drop in pressure takes place due to the nucleation and growth of voids. In this regard, it should be noted that in our previous work on single crystal copper (FCC system) triaxially deformed at $1.5\times10^{10}\,s^{-1}$ volumetric strain rate [36], we found only a single dip in the pressure-time profile resulting from the nucleation and growth of voids for temperatures below 1250 K. In those studies [36], a double-dip in the pressure-time profile was observed at 1250 K (near melting point of copper) where first dip in the pressure-time profile occurred due to the structural changes and second dip was due to the nucleation and growth of voids. Note that for single crystal iron (a BCC system), the double-dip in the pressure-time profile (point B and point E in Fig. 1) occurs at 300 K. This indicates that the microstructural evolution of single crystal iron (BCC system) under triaxial deformation is different from that of the single crystal copper (FCC system). Mayer [38] also reported a double-dip in the pressure-time profile in his MD simulations for uniaxial tensile deformation of single crystal iron at $5\times10^9\,s^{-1}$ strain rate at 300 K. He reported that the double-dip in the pressure-time profile was due to the onset of plastic deformation followed by creation of voids [38].

To understand whether the double-dip in the pressure-time profile (point B and point E in Fig. 1) occurs due to the same reasons (i.e. structural changes followed by creation of voids) as observed for single crystal copper triaxially deformed at $1.5\times10^{10}\,s^{-1}$ volumetric strain

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