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Shock induced deformation response of single crystal copper: Effect of crystallographic orientation

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ABSTRACT

We have carried out multimillion atom non-equilibrium molecular dynamics simulations for investigating the effect of crystallographic orientation over the evolution of deformation pathway of single crystal copper under shock compression. Based on symmetry, three different crystallographic directions, $\langle 100\rangle$, $\langle 110\rangle$ and $\langle 111\rangle$ are selected and taken as shock directions. Shock Hugoniot points has been calculated and compared among these different directions up to ~450 GPa of shock pressure i.e. piston velocity of 3.0 km/s. Orientational anisotropy has been observed for the bulk Cu single crystals shock loaded along these three different directions. Even though this feature may not show up explicitly in experimental investigations which typically measures shock-velocity and density Hugoniot curve, it is apparent from large scale atomistic simulations which measures the temperature Hugoniot curve quite accurately. Differences are observed in the von-Mises strain and stress plot distributions for shock loading of different intensities along the three directions. Large directional dependency is also evident in the evolution mechanism of deformation. Temperature profiles at different piston velocities for the shock front and the shock equilibrated regions shows significantly different and interesting patterns along the three orientations. Maxwell-Boltzmann distribution is observed in the atomic velocities (thereby the temperature profiles also) for both the shock front region as well as the shock equilibrated region for shock loading along all the three directions.

1. Introduction

Application of mechanical load to a crystal structure results in accumulation of strains and also global deformation of the material. After a certain specified value of strain for the material, microstructural deformations in the crystal structure originate and thereby results in formation of dislocations and/or twins which globally is manifested as development of plasticity in the material. If more load is applied then there are possibilities of structural or conventional phase transition in the material. The characteristics of deformation microstructure depends on crystal structure, orientation, stacking fault energy along with the type, intensity and duration of the load. Deformation mechanism of metals have been studied for many decades and is of considerable interest to scientific community through out the globe due to it's application in various fields, such as auto-mobile, defence & security, aero-industry and nuclear power plant. The manuscript deals with microstructural deformation mechanisms of bulk face-centered cubic (FCC) metal single crystal Cu under very high strain rate loading situations which are of importance in different situations such as inertial confinement fusion (ICF) chamber, defence aircraft and spacecraft. Typically these high strain situations in which the metal is subjected to very high temperature and pressure within a very short span of time can be experimentally attained through shock-tube and/or laser-ablation studies whereas numerically can be attained through atomistic simulation studies. Large scale molecular dynamic studies has been carried out in this manuscript to develop a comprehensive understanding of the effect of crystallographic orientation for single crystal Cu subjected to different shock load intensities.

The sensitivity of crystal orientation over the dislocation micro structures of a recovered specimen, shocked under laser ablated ultra fast pulses has been reported [1–5] and threshold shock pressure at which deformation mechanism changes from glide to twining has also been reported [4–6]. Enhancement of dislocation density with shock pressure has been reported [4,7,8] in the existing literature. Observance of dislocation cells, microbands, deformation twin [4,9,10] have also been reported in the shock

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experiment recovered samples. The above mentioned researches are primarily experimental in nature and thereby do not necessarily describe the associated residual strains and their evolution leading to the formation of different microstructural defects in the shocked recovered samples, which this manuscript aims to achieve. Moreover, being experimental in nature, these works also do not comment on the effect of lattice orientations over the shock induced temperature rise when single crystal Cu is subjected to shock load along different crystallographic directions at different level of shock intensities.

Multimillion atom molecular dynamics (MD) simulation [11] has been done to investigate plasticity of high symmetry ⟨100⟩ single crystal FCC metal; however the work is limited to shock pressure of ∼48 GPa (i.e. piston velocity of 1 km/s). They also pointed out the need of studying the lower symmetry directions (like, ⟨110⟩ and ⟨111⟩) to reveal the orientational sensitivity of shock induced plasticity of FCC perfect crystal. Appearance of elastic precursor wave structure which separates out the shock front from the plastic region in case of low symmetry (e.g. ⟨110⟩ and ⟨111⟩) directions has been reportedly identified through multimillion molecular dynamics study using different potentials - Lennard-Jones (LJ) [?,12] and embedded atom method (EAM) [13]. Cao et al. [14] carried out atomistic simulation studies to demonstrate orientational anisotropy in shock loaded Cu for [221] orientation primarily looking into the difference of the wave velocities for the plastic wave and its elastic predecessor. Apart from identification of different velocities for the plastic waves and the elastic waves, there are no studies in existing literature which demonstrates the evolution of strains and stresses along with temperature in the samples which this manuscript highlights. It should be noted that the scope of this manuscript is only limited to global spatially averaged variables without taking deeper looks into the type of dislocation interactions along different directions [15].

In this comprehensive numerical study, different crystal orientations of FCC-Cu have been considered which is subjected to range of shock intensities to identify the different microstructural deformations along with its relation to von-Mises strain, stress and also temperature evolution in the samples. Details elucidation of the deformation path-way from a global mechanistic perspective is the primary objective of this work.

2. Simulation methodologies

A series of multi-million atom non-equilibrium molecular dynamics (NEMD) simulations has been performed utilizing a quantum-mechanical many-body potential, embedded atom-method (EAM) potential for FCC single crystal copper (parameterized by Mishin et al. [16]) with different crystal orientations of [100]. The interatomic interactions of copper has been described through the well studied Mishin-EAM [16] potential which is capable to reproduce the thermodynamic and mechanical properties at ambient condition [17,18] and at high pressure situation [19] as well. In addition, this Mishin-EAM [16] potential has been used to predict the equation of state (EoS) up to 300 GPa [20] with noticeable accuracy. In this current work, we have produced the shock Hugoniots up to 450 GPa which shows reasonable agreement with available experimental shock data [21].

However, for simulating shock wave propagation through the target samples of single crystal copper two different types of methodology, direct-shock method i.e. NEMD and multiscale shock technique (MSST) [22] has also been utilized in this current work. Direct-shock or NEMD simulations are used to explore the femtosecond time resolved evolution of plasticity behind the shock front. Whereas, MSST algorithm has been employed for large timescale simulations (for this work, up to 10 ns) for investigating shock equilibrated (after post-shock relaxation) thermodynamical state variables at a significant distance (∼100s of microns) behind the leading shock front. MSST is a simulation technique based on the NavierStokes equations for compressible flow and follows a Lagrangian point through the shock wave which is accomplished by time evolving equations of motion for the atoms, as well as volume of the computational cell to constrain the stress in the shock propagation direction to the Rayleigh line and the energy of the system to the Hugoniot energy condition. This method has been tested for simulating a unidirectional planar shock propagation for various class of materials [23–25] with sufficient accuracy. While performing the MSST simulations, special care has been taken to ensure that there is no significant drift in energy at any time instance with the chosen values of 'q' and 'tscale' (parameters required in MSST simulation as implemented in LAMMPS [26] framework) for a particular shock intensity. Although, it should be noted here that any choice of 'q' (chosen as 1 for current simu-

Table 1
Necessary details of the initial configurations of the NEMD-samples with desired orientations. The mass density of all the samples are 8.806 g/cm^3 at ambient temperature and pressure.

Sample No.	No. of crystal lattice units	Orientation			Size (nm)			No. of atoms
		X	Y	Z	Shock dirn. X	Y	Z	
1.	$500 \times 100 \times 100$	⟨100⟩	⟨010⟩	⟨001⟩	180.75	36.15	36.15	$20,000 \times 10^3$
2.	$350 \times 80 \times 70$	⟨110⟩	⟨001⟩	$\langle 1\bar{1}0\rangle$	178.93	28.92	35.79	$15,680 \times 10^3$
3.	$280 \times 60 \times 60$	⟨111⟩	$\langle 1\bar{1}0\rangle$	$\langle 11\bar{2}\rangle$	175.32	30.67	35.42	$16,128 \times 10^3$

Table 2
Necessary details of the initial configurations of the MSST-samples with desired orientations. The mass density of all the samples are 8.806 g/cm^3 at ambient temperature and pressure.

Sample No.	No. of crystal lattice units	Orientation			Size (nm)			No. of atoms
		X	Y	Z	Shock dirn. X	Y	Z	
1.	$20 \times 20 \times 20$	⟨100⟩	⟨010⟩	⟨001⟩	7.23	7.23	7.23	32×10^3
2.	$15 \times 20 \times 15$	⟨110⟩	⟨001⟩	$\langle 1\bar{1}0\rangle$	7.7708	7.3023	7.77082	36×10^3
3.	$12 \times 15 \times 12$	⟨111⟩	$\langle 1\bar{1}0\rangle$	$\langle 11\bar{2}\rangle$	7.6389	7.7708	7.2012	34.56×10^3