Evolution of dislocation mechanisms in single-crystal Cu under shock loading in different directions

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Evolution of dislocation mechanisms in single-crystal Cu under shock loading in different directions

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Abstract

Even though there are numerous experiments and molecular dynamic simulations of Cu under shock loading, there appears to be no literature on the evolution of different types of dislocation mechanisms and their mutual interactions during the process of shock loading, which this article addresses through molecular dynamic simulations using the Mishin EAM potential for Cu. Three different directions \(\{100\}\), \(\{110\}\), and \(\{111\}\) that have been considered in this article are subjected to shock compression with piston velocities ranging between \(0.3\)–\(3\) \(\text{km s}^{-1}\). The evolution of Hirth locks, Lomer–Cottrell locks, cross-slips, jogs, and dislocation-originated stacking-fault tetrahedra are demonstrated in this article for different direction shock loading of single-crystal Cu.

Keywords: dislocation, crystal orientation, molecular dynamics

(Some figures may appear in colour only in the online journal)

1. Introduction

Single-crystal Cu under different types of loading conditions has been studied by numerous researchers both experimentally as well as numerically through molecular dynamics investigations. In spite of that, the dislocation dynamics of Cu under shock loading beyond the Hugoniot elastic limit (HEL) in different directions with regards to the temporal evolution of...
different dislocation mechanisms and their mutual interactions has not yet been elucidated comprehensively, which this article aims to address.

Experimental observations of different dislocation microstructures in a recovered specimen, which had been shocked using laser-ablation ultrafast pulses/shock guns, have been reported in several literature [1–7] publications. The experimental investigations are able to provide an observation of the final state (dislocation microstructure) of the recovered sample. However, it is unable to provide the evolution mechanism associated with the final-state observations of residual microstructures. Experimental observations also demonstrate an enhancement of dislocation density with shock pressure [8–10] without characterizing the types of dislocations and their interactions. The main objective of this article is to numerically (through molecular dynamics (MD) simulations) demonstrate the evolution of different dislocation mechanisms and their interactions leading to the final residual state experimental observations of dislocation microstructure.

Results obtained from large-scale molecular dynamics simulations of shock-loaded Cu have been reported by researchers at Los Alamos National Labs [11]. It has been reported [12] that shock waves along the ⟨100⟩ direction form stacking faults (SFs) by slippage along the {111} close-packed planes, the mean spacing of which decreases with increasing value of piston velocity. For shock loading along the ⟨111⟩ direction, three slip planes with nonzero resolved shear stress activate, resulting in the formation of a triangular pattern on the ⟨111⟩ surface [12]. Whereas for shock loading along the ⟨110⟩ direction, a complicated pattern of localized slippage along all four ⟨111⟩ planes is observed [12]. Details regarding the formation of different dislocation mechanisms and their interactions have not been demonstrated in the above-mentioned literature. The nucleation mechanism of dislocation loops responsible for plastic flow in the ⟨100⟩ direction has been identified in the literature [13]. The above-mentioned study contains information only with relation to the high-symmetry ⟨100⟩ direction and not with any other low-symmetry directions. Moreover, the above-cited work only identifies the formation of dislocation loops just behind the shock front, but details of the characterization of the post-shock interactions of the shock-induced dislocations and associated temporal evolution have not been addressed in the work [13], which the current article strives to address. Most recently, Sichani et al [14] has studied dislocation density generation and plastic relaxation for the ⟨100⟩, ⟨110⟩, and ⟨111⟩ orientation of single-crystal Cu, and Mackenchery et al [15] has investigated the dislocation evolution of the ⟨100⟩ single-crystal Cu. This present work aims to explore the directional dependency over the dynamic evolution of dislocation reactions more precisely, and the associated generation of shock-induced defects from a mechanistic perspective, which has not been discussed in the above-cited works.

Apart from the studies by the Los Alamos researchers, one study exists [16] using mesoscale-continuum simulations (using finite-element-based discrete dislocation models) in which plasticity mechanisms for high-strain-rate loading along different directions (namely, ⟨100⟩, ⟨110⟩, and ⟨111⟩) have been explained, based upon total dislocation density (which has been matched with an analytical model [5] and experimental data [17]). It should be noted that no effort has been made with regards to identifying the different competing dislocation mechanisms, their dissociations, and reactions involved during the process of shock loading, which this article aims to address. Thereby, this article aims to improve the understanding of the underlying physics behind the uniaxial shock-compression-induced plasticity of fcc single-crystal metal.
2. Simulation methodologies

Non-equilibrium molecular dynamics (NEMD) simulation using embedded atom method (EAM) potential (developed by Mishin et al [18]) has been carried out to investigate the shock response of perfect monocristalline Cu with orientations [100], [110], and [111]. Initial configurations of pure single crystal with desired orientations have been created and equilibrated by applying isothermal isobaric, NPT ensemble integration scheme (for 100 ps with timestep size of 1 fs) along with the Nosé–Hoover thermostat algorithm at ambient temperature and pressure conditions. Periodic boundary conditions are maintained in all three orthogonal directions during the equilibration period. The details of the samples, including crystallographic orientation, the sample dimensions, and total number of atoms, have been given in table 1. The simulation box size has been chosen carefully, based on prior literature [11], for ensuring the elimination of any artifact of transverse periodic boundary over the shock-induced plasticity mechanisms. The simulation domain size for this study is adequate enough to contain the entire shock in transverse directions and also the shocks are steady in nature in each simulation with a rise time of ~0.51–1.1 ps for the range of piston velocities of 3.0–1.0 km s\(^{-1}\), respectively, for all above-mentioned crystal orientations. Even though the shock rise time, as observed in shock experiments (order of nanosecond), are much higher than the rise time observed in a typical NEMD (order of few picosecond) shock simulation [36, 37], the essential generality of the physics behind the shock-induced deformation mechanisms are unaltered and are in good agreement with the experiments [36].

The accuracy of an MD simulation depends upon the force potential. The EAM potential for Cu developed by Mishin et al [18] has been chosen for this study. It should be noted that the EAM-Mishin potential for Cu has been developed based on \textit{ab initio} and tight-binding methods, and is well accepted by the research community as the standard for simulations of Cu both at ambient temperature and pressure conditions and also at high-pressure and temperature conditions. The potential has been used in describing thermodynamic and mechanical properties [19–21], high-pressure conditions [22, 23], and also in the prediction of the equation of state of Cu up to 300 GPa [24]. In addition, the reader is referred to the tabular comparison of the properties of the potentials [20], which establishes the superiority of the EAM-Mishin potential for Cu over other potentials. This potential shows a good match with experimental elastic constants, with experimental phonon dispersion curves thereby demonstrating its reliability. Apart from the calculation of lattice properties, the potential has also been extensively tested for various structural energies and transformation paths.

The momentum mirror technique has been applied to produce shock waves, details of which can be found elsewhere [25, 26]. During shock compaction simulation, the periodic boundary has been applied along the directions normal to the shock, i.e. Y and Z. The boundary condition has been kept fixed along the shock direction, i.e. X. The microcanonical ensemble has been invoked during shock simulation to ensure energy conservation throughout the time integration of the atoms. Careful measures have been taken to subtract the center-of-mass bias (which arises due to compression of the sample) from the velocity components of each atom during the calculation of stress and temperature. All the MD simulations have been accomplished by the popular MD-solver, LAMMPS [27].

To identify the atomic-level defects produced by shock compression, various techniques, like adaptive common neighbor analysis (CNA), centro-symmetry parameter estimation, coordination per atom, etc, have been used in this work. Dislocation extraction algorithm (DXA) [28] (as implemented in program OVITO, developed by Stukowski et al [29]) has also been utilized, which represents the dislocated crystal into a line-based representation of dislocation network. It should be noted here that apart from distinguishing between different
Table 1. Necessary details of the initial configurations of the samples with desired orientations. The mass density of all the samples is $8.806 \text{ g cm}^{-3}$ at ambient temperature and pressure.

<table>
<thead>
<tr>
<th>Sample no.</th>
<th>No. of crystal lattice units</th>
<th>Orientation</th>
<th>Size (nm)</th>
<th>No. of atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>1.</td>
<td>500 × 100 × 100</td>
<td>(100)</td>
<td>(010)</td>
<td>(001)</td>
</tr>
<tr>
<td>2.</td>
<td>350 × 80 × 70</td>
<td>(110)</td>
<td>(001)</td>
<td>(110)</td>
</tr>
<tr>
<td>3.</td>
<td>280 × 60 × 60</td>
<td>(111)</td>
<td>(110)</td>
<td>(112)</td>
</tr>
</tbody>
</table>
dislocation mechanisms, this algorithm has reported capabilities of recognizing the true Burgers vector of each dislocation segment, grain boundary dislocations (e.g. twinning dislocation), and also dislocation junctions. For identifying local crystal environment in the deformed samples, a well-known program, crystal analysis tool (CAT), developed by Stukowski et al [30, 31] has been utilized. The Voronoi tessellation [32] analysis technique is used to calculate the volume fraction of defects, such as SFs, twins, etc.

3. Results and discussion

Validations of shock data points in the Hugoniot planes as measured from this numerical study (using the EAM-Mishin potential [18]), with shock experiments, are not shown in this article, since those observations of agreements and/or correlations have been demonstrated earlier in the literature using the same force potential [20]. The dislocation densities of the shocked samples are calculated by extracting the length of the dislocated segments through computationally expensive, DXA [28] analysis, in which each of the dislocations is classified based on their respective Burgers vector. The calculated Shockley partial (1/6(112)) dislocation densities have been plotted as a function of shock strength (i.e. piston velocity, $U_p$) and compared between the three above-mentioned crystal orientations, [100], [110], and [111] in figure 1(a). Figure 1(b) presents the calculated cumulative dislocation density of sessile partials (Stair-rod (1/6(110)), Hirth (1/3(001)), and Frank-type (1/3(111))) as a function of shock strength (i.e. piston velocity till 3.0 km s$^{-1}$) and comparison has been made between the above-mentioned crystallographic directions of single-crystal fcc Cu. Plastic compression, as evidenced from the measured dislocation density in figure 1(a), for the orientation of [100] and [110], starts at 750 m s$^{-1}$, whereas for the crystal orientation of [111], plastic compression has been identified to occur at an impact velocity of 1.0 km s$^{-1}$. This onset of plastic deformation signifies the directional anisotropy over the HEL. The HEL point for [100]-fcc
Cu has been reported in previous literature as $\sim 0.65$ km s$^{-1}$ [20] and $\sim 0.95$ km s$^{-1}$ for [111] [33]; hence this current study shows significant correlation with the previous MD simulations.

However, irrespective of crystallographic directions, it can be observed that an increase of shock intensity causes an enhancement of plastic activity up to certain applied strain after which a sharp decrease of plastic activity can be observed. We have calculated the atomic-level strain tensor of each atom by using the algorithm based on the methods developed by Shimizu et al [34] and Falk et al [35], implemented in OVITO [29]. The maximum dislocation density for [100] is observed at an impact speed of 1.0 km s$^{-1}$ and the corresponding plastic and volumetric strains are $\sim 16.33\%$ and 5.32\%, respectively. For the other two lower-symmetry directions, (110) and (111), the maximum dislocation density has been observed at 1.5 and 2.0 km s$^{-1}$ and the associated plastic and volumetric strains are $\sim 21.61\%$, $\sim 6.45\%$ and $\sim 24.53\%$, $\sim 7.75\%$, respectively. The differences in the threshold atomic strain after which the relaxation mechanism of plastic deformation changes for the tested crystal orientations with various symmetry, indicates the underlying directional anisotropy might be due to the geometrical environment of the potential slip systems. From figure 1, it can be observed that after the piston velocity of 1.5 km s$^{-1}$, shock-induced plasticity has decreased for the shocks along (100) and (110) and, interestingly, a signature of solid-to-solid phase transformation resulting in body-centered phase of Cu being observed [42]; which needs further evaluation either through experiments and/or ab initio calculations (which is beyond the scope of this article). Significant differences in magnitude of dislocation density (as observed for different crystallographic directions in figure 1) hint at directional anisotropy for shock-induced plasticity in Cu, which is consistent with earlier studies [14, 16]. Figure 1 shows that for the (100) shock-propagation direction, the nucleated dislocation density (for both glissile and sessile partials) is significantly smaller than the other two directions ((110) and (111)) albeit the calculated volume fraction of hcp is largest ($\sim 39.8\%$) for (100) in comparison to $\sim 14.8\%$ and 9.75\% for the (110) and (111) directions (as obtained from adaptive-CNA analysis [29]). The reason for the nucleated dislocation density being smaller in (100) compared to the other two directions is primarily due to the easy-glide situation of available slip planes, where a slip of a full Burgers vector is facile by virtue of simple geometric orientation of the highly dense atomic planes. This easy glide of a full Burgers vector eventually changes the stacking sequence of fcc (..ABCABC..) into ..ABAB..., i.e. hcp, which demonstrates that the volume fraction of hcp in the (100) direction is high, whereas dislocation density is lower in comparison to the other two directions.

It can be observed that for lower impact speeds, such as 750 and 850 m s$^{-1}$ (just above the HEL for {100} and {110} orientation), the difference between the Shockley partial dislocation densities is quite small (refer figure 1(a)), although a noticeable difference can be observed in cumulative sessile dislocation densities (refer to figure 1(b)). This noticeable difference in sessile partials (for [100] and [110] at impact speed of 750 and 850 m s$^{-1}$) indicates that although the successive slip is occurring in each of the two cases (as evidenced from almost equal Shockley partial density), the interaction of Shockley partials follows different mechanisms, which eventually give rise to differences in the observed dislocation density. Hence, despite having equal Schmid factor, 0.408, for all available slip systems of [100] and [110], the geometrical alignment of the slip planes with respect to the loading axis plays a crucial role in the birth of directional anisotropy. As observed from DXA calculations, for the shock propagation along $\langle 100 \rangle$, the number of clusters (a contiguous crystallite consisting of atoms of the same structural type, generated as internal data structure in OVITO [29]) is fewer, even though the average sizes are $\sim 10$–12 nm$^2$, whereas for the comparative lower-symmetry directions, (110) and (111), the number of clusters is significantly high, but the average sizes are noticeably small, $\sim 5$ nm$^2$. This observation (despite having lower
dislocation density in [100], the average size of the dislocation loops is significantly greater than the dislocation loops observed in [110] implies that during the plastic relaxation in [100] the movement of Shockley segments over the {111} planes encounters less resistance (i.e. able to glide easily) by virtue of less complicated geometrical orientation of slip planes (slip planes are parallel in the (100) case) than the (111) case where activated slip planes are oriented in a triangular fashion [12], which creates additional impediment to the glide of the Shockley dislocations, even though the Schmid factor is identical (Schmid factor = 0.408) for all the activated slip systems for the shocks along (100), (110), and (111).

Figure 1 shows that for the [111] direction of shock loading, no sessile or glissile dislocations are observed prior to the HEL point (∼1.0 km s⁻¹), which indicates stiff resistance being provided by the geometrical alignment of the slip planes with respect to the loading axis. However, after initiation of sessile and glissile dislocations, high dislocation density...
density is observed (compared to that of the $\langle 100 \rangle$ direction), which indicates that as the threshold energy for the formation of sessile and glissile dislocations is reached, the rate of nucleation and growth is fast along $\langle 111 \rangle$ compared to the other two directions.

To investigate quantitatively the slip activity under the shocked state, the contribution from each slip system to the originated SFs has been calculated by filtering out the atomic positions corresponding to the particular SF and measuring the volume fraction of those atoms through Voronoi tessellation [32]. As observed, in the case of the $\langle 100 \rangle$-fcc shock-propagation direction at all impact velocities explored in this present study, eight $\{110\}(111)$, $\{011\}(111)$, $\{10\}[(1\bar{1})11]$, $\{10\}[(\bar{1}1)11]$, $\{10\}[(11)11]$, $\{0\}[(\bar{1}1)11]$, and $\{0\}[(\bar{1}1)11]$, and $\{0\}[(\bar{1}1)11]$, out of the twelve available slip systems (in fcc perfect crystal) have been identified to be operative with four possible $\{111\}$ slip planes having identical Schmid factor of 0.4082, which leads to immediate work hardening. In addition, it has been identified that at an impact velocity of 1.0 km s$^{-1}$ (at which $\langle 100 \rangle$ attains maximum dislocation density) almost all the operative slip systems in the orientation of $\langle 100 \rangle$ contribute approximately equally, $\sim$12.5% (please note, the comparatively smaller contribution, $\sim$8.3%, has been identified for $\{10\}[(1\bar{1})11]$, $\{10\}[(\bar{1}1)11]$, and $\{01\}[(11)11]$) to the formation of thick quad-layered SFs. These calculations of volume fractions of the SFs in this MD study (for the shock-wave propagation direction $\langle 100 \rangle$) show good agreement with previous mesoscale dislocation-dynamics (DD) simulation study by Shehadeh et al [16].

3.1. Shock propagation along $\langle 100 \rangle$

Temporal evolution of individual dislocation densities for shock loading along the $\langle 100 \rangle$ direction at different piston velocities is shown in figure 2. The piston velocities (0.85, 1.0, 1.5 km s$^{-1}$), shown in the figure, correspond to points in the pre-peak, peak, and post-peak regime (see figure 1) for shock loading along the $\langle 100 \rangle$ direction. The cumulative dislocation density of the immobile dislocations is observed to be almost 100 times lower than the glissile Shockley partial density, which eventually signifies low strain hardening in the $\langle 100 \rangle$ direction for all piston velocities, as shown in figure 1. It should be noted that the slip planes in the Cu $\langle 100 \rangle$ orientation are arranged as a parallel family of planes from the surface and two conjugate families intersect each other in an orthogonal manner. Thereby, plastic defects like SFs are observed to originate from the transverse surface of the simulation box, in contrast to the observations of plastic defect origination for other shock-loading directions ($\langle 110 \rangle$ and $\langle 111 \rangle$). It should also be mentioned here that this behavior of origination of SFs (plastic defects) from the transverse surface of the simulation is not an artifact of the transverse dimension chosen for simulation but a characteristic of the slip planes in the $\langle 100 \rangle$ direction.

As depicted in figure 2, the rate of nucleation of Shockley partials is quite high in comparison to the rate of nucleation of other types of immobile dislocations as well as perfect dislocations. An avalanche of Shockley partial nucleation is observed as soon as the shock is introduced in the sample, whereas both perfect and immobile dislocations nucleate after some time instance ($\sim$4–5 ps) of the passage of the shock front. This delay in nucleation of the sessile dislocations indicates that Shockley partials interact to form sessile dislocations and/or locks. Interestingly, it can be observed that the density of perfect dislocations is significantly small compared to that of Shockley partials. It has been pointed out [36] that under the dynamic shock-compression situation, the formation of Shockley partial and perfect dislocations are equally probable. In these simulations, the formation of Shockley partials is observed to be predominant compared to the formation of perfect dislocations. It should be noted that the usual mechanism of the splitting of perfect dislocations into Shockley partials is
not observed from these shock simulations. Amongst the sessile dislocations, Hirth-type $(1/3 \langle 001 \rangle)$ partials predominate ($\sim 67.25\%$) over the others—Stair-rod $(1/6 \langle 110 \rangle$, $\sim 7.52\%$) and Frank partials $(1/3 \langle 111 \rangle$, $\sim 3.55\%$) in all shock-intensity regimes. Typically, the dislocation motion in perfect fcc crystals is resisted by dislocation forests, which eventually results in strain hardening. When two mobile dislocations (e.g. Shockley segments) approach each other, they interact and form different locks with various strengths, which eventually offer resistance to the glide of the dislocations. In general, the paucity of Hirth-type sessile lock in fcc single crystal (despite being energetically favorable) is due to the fact that the Burgers vector, $1/3 \langle 001 \rangle$ (Hirth lock), is not a lattice vector, which is why it requires SFs to be formed on either side of the Hirth dislocation. But in the case of the high-strain-rate loading environment in [100] perfect fcc, such highly thickened SFs are quite abundant, which enhances the possibility for the formation of Hirth barrier, as evidenced from the greater
density of Hirth dislocations among the other sessile dislocations, observed (refer figure 2) in the [100]-fcc orientation.

Typically, a Hirth lock is formed when two perfect dislocations with perpendicular Burgers vectors glide and eventually react on the intersecting planes. Figure 3 shows two perfect dislocations with perpendicular Burgers vectors \(\frac{1}{3}[110], \frac{1}{3}[110]\) starts gliding towards each other over mutually orthogonal slip planes and react upon meeting at the intersection of the slip planes, resulting in the formation of Hirth-type locks \(\frac{1}{3}[100]\) (symmetric about the bisectrix plane that contains the intersection line of the forest and the glide planes) along with two trailing Shockley partials \(\frac{1}{3}[211], \frac{1}{3}[211]\). The reactions leading to the formation of Hirth locks is described as follows:

**Figure 4.** Temporal evolution of dislocation density (up to 16 ps) for shock loading along the ⟨110⟩ direction. All classified dislocations, including perfect dislocations \(\frac{1}{2}⟨110⟩\), Shockley partials \(\frac{1}{2}⟨112⟩\), sessile partials, e.g. Hirth \(\frac{1}{3}⟨001⟩\), Frank \(\frac{1}{3}⟨111⟩\), and Stair-rod \(\frac{1}{6}⟨110⟩\) have been plotted for the piston velocity of \(0.85 \text{ km s}^{-1}\) (i.e. shock pressure and temperature of \(\sim 6.74 \text{ GPa and } \sim 335.12 \text{ K}\), respectively), \(1.5 \text{ km s}^{-1}\) (i.e. shock pressure and temperature of \(\sim 15.04 \text{ GPa and } \sim 385.97 \text{ K}\), respectively), and \(2.0 \text{ km s}^{-1}\) (i.e. shock pressure and temperature of \(\sim 125.75 \text{ GPa and } \sim 2415.31 \text{ K}\), respectively). In the inset, the zoomed figure has been represented for visual clarity of the evolution of sessile dislocations. The dislocation density presented in the figure corresponding to a particular time instance has been extracted from the entire shocked section of the target sample (which excludes the pre-shock volume) to envisage precisely the ongoing dislocation interactions behind the shock front.
It should be noted that even though the mechanism of nucleation and evolution of Hirth locks has been shown for the ⟨100⟩ direction at a piston velocity of 1 km s\(^{-1}\), similar types of evolution mechanisms can be observed wherever a Hirth-lock mechanism is detected (for other crystallographic directions and impact velocities). A detailed observation of the temporal evolution for sessile and perfect dislocations (as shown in the inset of figure 2) demonstrates that at pre-peak regime (piston velocity of 0.85 km s\(^{-1}\)), the Hirth-lock density is followed by the Stair-rod density and in fact the density of Stair-rods equals the Hirth-lock density at around 16 ps. This suggests that at a later stage in the pre-peak regime there is a possibility of the formation of stable Lomer–Cottrell locks instead of Hirth locks. On the other hand, perfect dislocation density can be observed in between the Hirth-lock density and the Stair-rod density for both the peak and the post-peak regime (piston velocity of 1 and 1.2 km s\(^{-1}\)). Based on the trend of the curves, Hirth locks can be described to have a higher propensity of formation compared to other types of sessile and perfect dislocations for the case of shock loading in the ⟨100⟩ direction. It should also be noted that for shock loading in this direction, there is a very small possibility of the formation of Frank loops in all regimes (pre-peak, peak, and post-peak). Typically, the reduction of total dislocation elastic energy [38–41] and residual flow stress causes clustering of dislocation fragments into dislocation cells. The dislocation cell formation event has been observed in the region (width of ∼250–350 Å) near to the piston (i.e. far behind the shock front position); complete growth of the cells requires more time to be relaxed, which has been kept as future scope for understanding dislocation cell formation after shock loading.

\[
\frac{1}{2}[\bar{1}10] + \frac{1}{2}[\bar{1}1\bar{0}] \rightarrow \frac{1}{6}[\bar{2}1\bar{1}] + \frac{1}{6}[\bar{2}11] + \frac{1}{3}[\bar{1}00]
\]
3.2. Shock propagation along (110)

Figure 4 shows the temporal evolution of individual dislocation densities for shock loading along the (110) direction at different piston velocities (pre-peak at 0.85 km s\(^{-1}\), peak at 1.5 km s\(^{-1}\), and post-peak at 2.0 km s\(^{-1}\)—refer to figure 1). Similar to that of the (100) direction, Shockley partial density is significantly higher compared to that of the perfect as well as the immobile dislocations. The nucleation of Shockley partials also starts almost immediately with the passage of shock wave, whereas the other immobile dislocations result from reactions of the Shockley partials after a few picoseconds. It should be noted that the maximum shear stress due to shock loading along the (110) direction is \(\sim 17.06\) GPa, which is significantly higher than the maximum shear stress developed for shock compression along the (100) direction, \(\sim 8.72\) GPa at the peak dislocation density position for both orientations.

It is also observed that the rate of relaxation of developed shear stress is significantly lower in the case of the (110) direction than the high-symmetry (100) crystal orientation, which indicates the accumulation of residual shear stress in the low-symmetry direction, (110). During the progression of the shock front, the gliding motion of the glissile dislocation is prevented by the dislocation forests or by the interaction of dislocations. However, the accumulated residual shear stress in the case of (110) helps the dislocations to either climb, resulting in jog formation (refer to figure 5), or form perfect dislocations, which eventually glide in other planes (mechanism known in the literature as Schoeck–Seeger mechanism of interaction of cross-slips [43, 44], the formation of which is demonstrated in figure 6). Apart from residual shear stress, other factors such as high temperature and pressure along with complex alignment of operative slip planes in [110] are responsible for the evolution of both mechanisms of cross-slip and jog formations. Typically, a jog formation is associated with an irreversible climbing motion, eventually resulting in a change in volume of the crystal [45]. The average jog length is observed to increase with the increase of shock intensity, as calculated from the extracted dislocation segments from DXA: at a piston velocity of 1.0 km s\(^{-1}\), the average jog length is \(\sim 21.5\) Å, whereas it is \(\sim 82.05\) Å at a piston velocity of 1.5 km s\(^{-1}\). The cross-slip mechanism as described by Schoeck–Seeger [43, 44] represents Shockley partials in the primary glide plane recombined into a segment of perfect dislocation, which dissociates and bows out into an inclined cross-slip plane, thereby transferring the dislocation to the new cross-slip plane.

Figure 6. Representation of temporal evolution of cross-slip event as observed for the shock-propagation direction of the (110)-fcc. Figures (a) and (b) correspond to time instances of 8 and 12 ps, respectively. In figure (b), the bowing out of one perfect dislocation segment has been shown. Cylindrical, colored wires indicate the dislocation lines, where green, blue, pink, and yellow represent Shockley, perfect, Stair-rod, and Hirth-type dislocations. Red-colored arrow indicates respective Burgers vectors of the associated segments of the dislocations. Dashed-lined triangles are used to show the respective crystallographic planes.
Temporal evolution of immobile dislocations in the pre-peak and peak regime shows that Stair-rod (resulting in the formation of sessile Lomer–Cottrell lock and Hirth-type partials are the two main competing candidates (see figure 4(a)). However, at higher piston velocities in the post-peak regime (2.0 km s\(^{-1}\) piston velocity), Hirth-type dislocations overrule (see figure 4(c)) other immobile dislocations. The mechanism of Hirth locks (see figure 3) has been demonstrated before. The mechanism of the evolution of the Lomer–Cottrell lock is demonstrated in figure 7. It should be noted that Lomer–Cottrell locks appear when two perfect dislocations of the same \{111\} zone occur, gliding on different planes. The two leading partials are attracted to one another and react along the \langle 110 \rangle line of intersection between the two planes to form a pure-edge \(\frac{1}{6} \langle 110 \rangle\) Stair-rod partial dislocation referred to as the Lomer–Cottrell lock. The reactions leading to the formation of Lomer–Cottrell locks is described as follows:

\[
\frac{1}{2} [\bar{1}10] + \frac{1}{2} [101] \rightarrow \frac{1}{2} [011]
\]

These sessile dislocations (e.g. Hirth, Stair-rod, and Frank partials), as observed in this present study, act as pinning points and contribute differently to the strain hardening. Among these sessile locks, the Lomer–Cottrell lock (resulting from Stair-rod partials) offers the highest impediment [46] to the dislocation glide, whereas Hirth locks possess greater strength in comparison with Frank partials [47]. Interestingly, at high shock intensities, e.g. at a piston velocity of 2.0 km s\(^{-1}\), a significant decrease of Stair-rod dislocations has been observed (see figure 4(c)), in comparison to that of the perfect dislocation segments. This disappearance of...
Lomer–Cottrell locks at high piston velocities might be because in order to form a stable and strong sessile Lomer–Cottrell lock by reaction of two perfect dislocation segments, it is necessary to have extrinsic SFs, which are higher in energy compared to intrinsic SFs. Thereby, there may be an increased tendency to form low-energy Hirth locks (through intrinsic SFs) instead of high-energy Lomer–Cottrell locks, as evidenced from the classified dislocation statistics in figure 4(c). The diminishing density of Stair-rod/Lomer–Cottrell locks at higher shock intensity might also be due to the polarity of the dislocation segments, because, to form Stair-rod partials two perfect dislocations (with opposite polarity) should attract each other and then react, but if they are found to have the same polarity no attraction will occur and eventually no Stair-rod partials will be formed.

Quantification of operative slip systems in the ⟨110⟩-fcc shock-loading direction shows that amongst all the slip systems in fcc, six of them (including conjugate slip systems), [⟨110⟩⟨111⟩], [⟨101⟩⟨1 1 1⟩], and [⟨110⟩⟨111⟩] have been observed to have been initiated and
contribute 34.2%, 28.7%, and 26.5%, respectively, to the total slip activity in the crystal, whereas, a small contribution (less than 20%) comes from [110][111], [101][111], and [110][111]. These calculations of the contribution of different slip systems shows good consistency with previous DD study by Shehadeh et al [16].

3.3. Shock propagation along ⟨111⟩

Temporal evolution of individual dislocation densities for shock loading along the ⟨111⟩ direction at different piston velocities (pre-peak at 1.0 km s⁻¹, peak at 2.0 km s⁻¹, and post-peak at 2.5 km s⁻¹—see figure 1) are shown in figure 8. The rate of nucleation of Shockley partial in the case of this direction is smaller than ⟨110⟩, but greater than ⟨100⟩. On the other hand, the rate of nucleation of sessile dislocation has been observed to be the highest (see figure 1(b)) in the ⟨111⟩ direction. The nature of dislocation distribution for the ⟨111⟩ direction is quite similar to ⟨110⟩, but a significant amount of strain concentration can be identified at the junctions or the point of reactions of the dislocations. Strain delocalization phenomenon is also observed in this direction, which indicates a lesser probability of shear banding. The equilibrium separation distance between the Shockley partials in this direction is

Figure 9. Atomistic configuration of evolution mechanism of an SFT has been demonstrated in the above figure. (A) represents the onset of glide in three {111}, which are oriented in a geometrically triangular fashion and aligned with ⟨110⟩, resulting in an SF and associated nucleation of Shockley partial (green-colored ribbon) and Stair-rod type (pink-colored ribbon) partials. (B)–(D) represent the temporal evolution of the dislocations and corresponding SFs, which eventually forms an SFT. Black-colored dashed line indicates the top view of a complete SFT, whereas, the red-colored arrow indicates the direction of the gliding of those participating SFs. Please note, in the above configurations, only hcp atoms (as identified by the DXA algorithm) are presented.
observed to be smaller than in other directions. Although the geometrical complexity of the slip planes is lower in comparison to (110), the mode of deformation, as observed from the atomic trajectories, is quite similar with (110), but the dynamics of dislocation activity differ a lot, because reactions and/or the multiplication of dislocation primarily depend on geometrical orientation of the containing glide planes and also associated energies. For the case of shock propagation along (111) direction, four slip systems, [101](111), [101](111), [011](111), and [011](111), are observed to have been activated in the three different slip planes and contribute almost equally, congruous with earlier DD simulation work [16]. Temporal evolution of the glissile dislocations show that for the pre-peak regime (piston velocity 1.0 km s\(^{-1}\)) Stair-rod dislocations are marginally higher than the Hirth-type dislocations. In fact, this observance is quite different compared to shock loading in the other directions in which Hirth-type dislocations dominate the glissile dislocations. Even though, for higher shock intensities the Hirth-type locks are more frequent compared to the Stair-rod dislocations. Thereby, it can be mentioned that the propensity of the formation of Hirth locks for this direction will be greater in the higher shock intensities compared to that of low-shock intensities; whereas the propensity of the formation of Lomer–Cottrell locks will be greater at low-shock intensities (pre-peak regime).

Interestingly, Frank partials are quite abundant compared to shock loading in other directions. The reason for this can be traced to the collateral orientation of the slip planes, which eventually results in a pattern of triangular-shaped geometry, thereby resulting in the formation of SF tetrahedra (SFT) i.e. Frank partials. The atomistic mechanism of evolution of the deformation-induced SFT [48] for Cu under shock loading is demonstrated in this article and has been presented in figure 9. As is known, Frank partials are sessile, i.e. unable to glide, hence, they dissociate into a Shockley partial and Stair-rod to be unfaulted. In the atomistic configuration (see figures 9(A)–(D)) as extracted through DXA, it can be observed that the originated SFs are bounded by Shockley partials (green-colored wire) and also Stair-rods (pink-colored wire) confirming the unfaulting mechanism of Frank partials, which eventually helps to form an SFT. It should be pointed out that these dislocation-originated SFT are different from conventional SFT formation, which requires a vacancy (typically induced as a result of irradiation and/or quenching). Typically, these dislocation-originated SFT are of an intrinsic type, which originates from dislocation interactions and contributes significantly to strain hardening.

4. Conclusion

Shock loading of Cu in different directions shows orientation anisotropy. Significant differences could be observed in the density of Shockley partials and other immobile dislocations for shock loading along different directions. The Shockley partials, which generate upon shock loading (beyond HEL point) for Cu in different orientations (⟨100⟩, ⟨110⟩, and ⟨111⟩), eventually interact to form different types of sessile locks. Observations of Hirth locks along with their atomistic evolution have been demonstrated for shock loading along the ⟨100⟩ directions. Lomer–Cottrell locks have been observed to evolve for shock loadings in the ⟨110⟩ direction. Apart from that, due to the presence of significant residual stresses, cross-slip mechanisms as well jogs are observed to form in the ⟨110⟩ direction; the atomistic evolution of which has also been demonstrated for shock loading of materials. The formation of dislocation-originated SFT for shock loading along the ⟨111⟩ direction; the evolution of which is also demonstrated.
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