A comparative study on shock compression of nanocrystalline Al and Cu: Shock profiles and microscopic views of plasticity

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Shock compressions of nanocrystalline (nc) metals Al and Cu with the same grain size and texture are studied by using molecular dynamics simulations. Results have revealed that the shock front of both Al and Cu can be divided into three stages: elastic, grain-boundary-mediated, and dislocation-mediated plastic deformation. The transition planes among these three stages are proven to be non-planar by two-dimensional shock response analysis, including local stress, shear, temperature, and atom configuration. The difference between shocked Al and Cu is that the rise rate of the elastic stage of Cu is slightly higher than that of Al, and that the shock-front width of Al is wider than Cu at the same loading conditions. For the plastic stage, the dislocation density of shocked Al is lower than Cu, and the contribution of grain-boundary-mediated plasticity to shock front and strain for nc Al is more pronounced than for nc Cu. These results are explained through intrinsic material properties and atomistic analysis of the plastic process. In the case of the shocked Al sample, partial dislocations, perfect dislocations, and twins are observed, but few evidence of perfect dislocations and twins are observed in the shocked Cu. © 2013 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4826624]

I. INTRODUCTION

Nanocrystalline (nc) metals, i.e., polycrystalline metals with grain sizes of typically smaller than ~100 nm,1 are being actively investigated due to their superior and unique mechanical properties compared with coarse-grained (cg) counterparts, such as high strength and high ductility.2–4 Since grain boundary (GB) plays an important role on the mechanical properties of nc metals, it has been widely studied experimentally as well as by molecular dynamic (MD) simulations in recent years.5–13 Vo et al.14 have tried to quantitatively decided the contribution of GBs to total strain by using the total strain minus the strain contributed by dislocations. However, it is difficult to determine the contribution of GB-related plasticity on the total plastic response to mechanical loading directly. One reason is that the structure of GBs and how they deform are unclear. Another reason may be that the influences of GB structures, grain orientations, intrinsic properties of materials, and loading conditions on the plastic processes are highly incorporated.15,16 Therefore, it is necessary to consider the dissociated effects mentioned above on mechanical behavior of nc metals. In this work, we build nc Al and Cu samples with the same GB structures and grain orientations (namely textures) to study the independent effects of intrinsic material properties on the phenomena of shock compression of nc metals. In this way, the complex effects of textures on the plastic process can be dissociated from material properties.

The shock profile is one of the most important macroscopic representation in shock wave physics. It is important to understand the response of different materials to the shock wave in detail for many applications. Especially, understanding of the physical processes in the shock front can help one to know the viscosity and the energy dissipation used in the constitutive relations. The structure of the shock front in the plastic stage and its evolution are determined by microstructural processes.17 However, due to the equipment resolution, one cannot get the detailed shock-front structure in experiments.18–20 MD simulations can rightly provide atomistic level insight on the deformation processes involved in the shock front. The time and length scales of shock-wave processes in nc metals, caused by laser-shock compression experiments, are ideal for investigation via MD simulations.21–23 MD simulations of shock phenomena in nc face-centered cubic (FCC) metals, which mostly used the realistic embedded atom method (EAM) many-body potentials for Cu24 and Ni,25 have been carried out in the last decade, but few concern was on the shock front. The previous studies showed that the partial dislocations emission, propagation, and grain boundaries gliding dominate the plastic mechanisms of nc Cu and Ni under shock compression, but few evidence of full dislocations and deformation twinning were found.24,25 Recently, our MD simulations36 of nc Al under shock loading show that the contributions to shock-front structure from the GB-related plasticity cannot be neglected, which contradict the conclusion by Bringa et al.27 that the effect of GB-related plasticity on the shock-front width can be ignored. Besides, the full dislocations and twins are also observed in the shocked nc Al. The absence of full dislocations and twins in nc Cu and Ni at very small grain size compared with nc Al could be interpreted by the theory of generalized planar fault energy (GPFE) developed by Van

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II. METHODOLOGY

The scheme of MD simulation used herein can be found elsewhere.29,30 The nc Al sample with total atom of 7 834 571, which has been used to study the shock-front structure of nc Al under shock compression,26 is generated by the Voronoi construction method developed by Chen.31 Then, all the grain centers and orientations of nc Al are recorded and used as input for the generation of nc Cu sample (10 384 104 atoms). Therefore, the initial crystallographic orientations and grain boundary structures of these two samples are the same. Both the Al and Cu samples have average grain sizes of 8 nm, 256 grains and sizes of 128 × 32 × 32nm³ (noted as X, Y, and Z directions for easy description). These two samples are then quenched to 0 K for 10 ps to local minimum energy state with periodic boundary conditions in all directions, and followed by an annealing at ambient condition for ~60 ps to obtain global minimum energy state and to reduce the high internal stresses introduced by GBs using MD within the Parrinello-Rahman approach.32 The residual stress of these samples is about 100 MPa, which is similar to the near-equilibrium nc metals synthesized by inert gas condensation and lower than by severe plastic deformation.33 Finally, the samples are relaxed for 10 ps with the boundary conditions along the X direction set as free to attain the free surface for shock loading. The final densities of the Al and Cu samples are about 97% of the perfect crystal value. Prior to compression, the temperatures of samples are set as 1 K to reduce the effect of random oscillation of atoms, and shock compression with piston velocity \( U_p \) (also refer to as particle velocity) is generated by the momentum mirror method.34 The samples hold free surfaces along the shock wave direction and periodic boundary conditions are used in the transverse directions. The atomic interaction is modeled by the EAM potential for Al and Cu parameterized by Mishin et al.35,36 These potentials are fitted to provide stacking-fault energy (SFE) of 145 mJ/m² for Al and 45 mJ/m² for Cu, respectively. The atomic configurations are analyzed by the pair analysis technique.37

### A. Comparison of shock wave profiles

Fig. 1 shows the profiles of shock stress \( \sigma_{xx} \) and von Mises flow stress \( \sigma_{VM} \) of AL0 after 14 ps shock compression, as well as CU1 and CU2 after 20 ps shock compression, where the von Mises flow stress is identified as

\[
\sigma_{VM} = \sqrt{\frac{(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{xx} - \sigma_{zz})^2 + (\sigma_{yy} - \sigma_{zz})^2}{2}}.
\]  

The start of the shock-induced plasticity of AL0 has been found above a critical stress (Hugoniot elastic limit, HEL) of about 7.6 GPa, which is marked in Fig. 1, whereas the HEL of CU1 and CU2 is about 13.5 GPa and 7.7 GPa, respectively. All of HEL simulated here are much higher than the experimental value of cg counterparts.40 One reason may be that the simulated samples are almost defect-free except for the GBs, and another reason is that the HEL is strongly strain-rate related. The second reason can be illustrated distinctly for that the HEL of CU1 is higher than CU2 since the strain rate of CU1 is higher (Table I). The third reason may be that the HEL or the elastic stress is a function of sample thickness and shock wave propagating time, since several laser-generated shock experiments show ultrahigh elastic stress about a few GPa even 12 GPa for thin samples.41,42 Because the final \( \sigma_{xx} \) depends only on the intrinsic properties of materials and the loading intensity, the final \( \sigma_{xx} \) is Virial stress in slices of two lattice constant thick, perpendicular to the shock direction.39

### III. RESULTS AND DISCUSSION

In order to give a comparative investigation of the shock profiles and its corresponding mechanisms of nc Al and Cu, we have simulated the shock response of the Al and Cu samples with the same states of stress or strain. The 8 nm grain-sized Al is subjected to a piston velocity of 1 km/s, and the nc Cu sample is shocked under \( U_p = 0.754 \) km/s and \( U_p = 0.443 \) km/s, as shown in Table I. We call these three simulations at various shock compression conditions AL0, CU1, and CU2, respectively. The simulations AL0 and CU2 have the same shocked states of stress,40 and the simulations AL0 and CU1 have the same state of strain or so-called shock strength which is defined as \( U_p/c_0 \) by Holian and Lomdahl.34

<table>
<thead>
<tr>
<th>Simul.</th>
<th>( U_p ) (km/s)</th>
<th>( \sigma_{xx} ) (GPa)</th>
<th>( U_p/c_0 )</th>
<th>( \varepsilon )</th>
<th>t (ps)</th>
<th>( \Delta r ) (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL0</td>
<td>1.0</td>
<td>17.9</td>
<td>0.19</td>
<td>15.1%</td>
<td>10</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>14</td>
<td>35</td>
</tr>
<tr>
<td>CU1</td>
<td>0.754</td>
<td>33.3</td>
<td>0.19</td>
<td>15.1%</td>
<td>15</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>20</td>
<td>22</td>
</tr>
<tr>
<td>CU2</td>
<td>0.443</td>
<td>17.9</td>
<td>0.11</td>
<td>9.8%</td>
<td>14</td>
<td>26</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>20</td>
<td>30</td>
</tr>
</tbody>
</table>
of Al and Cu showed in Fig. 1 is close to the experimental values. 

Fig. 2 shows $U_p$ versus shock distance at different times for AL0, CU1, and CU2, where the shock front and the elastic wave amplitude (or the HEL amplitude) are marked for clarity. We define the shock front as the profile between the edge of the front ($\sigma_{xx} = 0$ or $U_p = 0$) and the point where the velocity (or stress) is 95%, which are also indicated by A0-A2 in Fig. 1. Henceforth, only the shock-front region of the profiles will be compared for Al and Cu in this paper.

We can clearly see the well-known split-elastic-plastic structured shock wave in Figs. 1 and 2. Although the shock wave profiles shown in Figs. 1 and 2 are calculated on short distances not above 100 nm due to the constrict of computing capability, the regular pattern for shock waves propagating over longer distance can be analogized. Indeed, we have already simulated shock compression of nc Al whose length is close to 200 nm along longitudinal direction. Although the simulations AL0 and CU1 correspond to a strong shock wave in traditional shock theories, and the simulation CU2 correspond to a weak shock wave, the shock profiles are broadened with the increase of propagation distance since the velocity of the plastic wave in these simulations is slower than the elastic precursor wave, as shown in Fig. 2 and Table I. The reason would be that the Hugoniot state of all the simulations AL0, CU1, and CU2 in our work lies under the intersection point of the extension line of the start point (original state) and the cusp at HEL and the curve of pressure-volume relation in the shock Hugoniot diagram due to the ultrahigh HEL for MD simulation. Even when the shock intensity exceeds this intersection (strong shock wave), the plastic wave still cannot overrun the elastic precursor in MD simulations. The elastic wave amplitude at previous steps shown in Fig. 2 is slightly higher than the final step, this phenomenon is called the elastic precursor decay or the attenuation of the HEL amplitude for weak shocks. The elastic precursor decay or the attenuation of HEL amplitude implies a time- and space-dependent shock response. The elastic precursor decay and broadened shock-front width are typical characteristics of short shock compression of thin films and are also observed in the shocked cg Al experiment. It should be note that the shear stress relaxation during the attenuation of the HEL amplitude is still unclear and would be useful to explain the physical mechanisms of shock response.

Fig. 3 displays the three-dimensional (3D) view of deformation structures of (a) AL0, (b) CU1, and (c) CU2 at the final step. Considering Figs. 1 and 2 with Fig. 3, we can see that the shock front can be divided into three stages in which the dominated deformation mechanisms are elastic,
GB-mediated plastic and dislocation-mediated plastic, like the shock-front structure of another nc Al sample studied before.\textsuperscript{26} The points B0, B1, and B2 in Fig. 1 roughly mark the transitions between GB- and dislocation-mediated plastic process, at which the slopes of the shock profiles varied. This is a common characteristic of shock fronts of nc Al and Cu, although the transition between GB- and dislocation-mediated plastic stage for nc Al is more pronounced than for nc Cu. The differences between the shock-front structures of nc Al and nc Cu can be found with further detection at full length. First, as shown in Figs. 1 and 2 and Table I, the shock-front width ($D_S$) of the AL0 at the final step is wider than the CU1 and CU2. We also try to simulate these two samples subjected to shock compression at similar $U_P$, and find that the $D_S$ of nc Al is greatly wider than of nc Cu because the $D_S$ decrease with the increase of $r_{xx}$.\textsuperscript{49} Second, the internal structures of the shock front for these two nc metals are slightly different. For the elastic stage of the shock fronts, since the lattice constant of Al is slightly larger than Cu, leading to a more extended deformation range before softening,\textsuperscript{50} it will need more time to compress the Al atom than Cu. Thus, the rise rate of Cu in the elastic stage of shock front is slightly higher than Al. The factors affecting the rise rate of the plastic stage would be complex, and the comparison between the rise rate of this stage should be treated more carefully. We introduce the time history of $\sigma_{xx}$ and shear stresses $2\tau$ for the transition points A0-A2 and B0-B2 (in slices of 2 nm thick along X) to investigate the stress rise procedure of GB- and dislocation-mediated plasticity, as displayed in Fig. 4, where the shear stress $2\tau$ is defined as

\[ 2\tau = \sigma_{xx} - \frac{\sigma_{yy} + \sigma_{zz}}{2}. \]  

Figs. 4(a)–4(c) clearly show that the rise rates of $\sigma_{xx}$ for B0-B2 are very similar to the first part of A0-A2, after which the slope of curves of A0-A2 is changed. Like the 1D spatial distributions of $\sigma_{xx}$, the time evolution of $\sigma_{xx}$ also can be divided into two stages according to the slope of curves. The rise time of A0-A2 which represent the rise time of shock front measurable in experiments is about several picoseconds, as shown in Figs. 4(a)–4(c). It is in good agreement with the experimental rise time of shock wave in Al film.\textsuperscript{20} The corresponding $2\tau$ time history in Figs. 4(d)–4(f) illustrates the deformation procedures of points A0-A2 and B0-B2. Initially, when the shock wave traveled to these points, $2\tau$ increases rapidly from 0 until it exceed the shear stress needed for plastic deformation (GB gliding). Then, $2\tau$ rises a little more slowly due to the release of shear by GB-mediated plasticity. This is because the prevailing increase of $2\tau$ induced by shock compression offsets the decrease of $2\tau$ by GB-related plastic deformation. Finally, $2\tau$ decreases once dislocations nucleate or emit, and we find that the decreasing rate of $2\tau$ depends on the scale of dislocation-dominated plastic deformation (i.e., dislocation density). The short stage of slowly rising of $2\tau$ of CU1 in Fig. 4(e) means that the effective time of GB-mediated plastic process in CU1 is very short. Comparing to CU1 and CU2 in Figs. 4(d)–4(f), the influence of GB-mediated plastic deformation in AL0 is stronger since $2\tau$ decreases slightly at 11 ps before the dislocation emission. However, because the strain rate of AL0, CU1 and CU2 are different, we cannot use the rise rate of $\sigma_{xx}$ to do a direct comparison of shock-front structures between nc Al and Cu.

Fig. 3 clearly shows that the defect configurations of nc Al and nc Cu, after shock compression, are mainly partial dislocations, which leaves stacking faults behind after its emissions and propagations in the grains. GBs often act as sources and sinks of partial dislocations in the deformed nc metals. Like the defect configurations observed in nc Al, Cu, and Ni by other MD simulations,\textsuperscript{7,8,24,25} full dislocations and deformation twins can be observed in shocked Al (Fig. 3(a)),
but cannot be observed in shocked Cu (Figs. 3(b) and 3(c)). In the GPFE theory, whether the trailing partial dislocation could be emitted in the time scale of MD simulations depends on the ratio between the stable SFE and the unstable SFE. If this ratio is close to unity, full dislocations or twins can be observed. This is the case for Al, but not the case for Cu. Asaro and Suresh predicted that full dislocations can be found in Cu with grain size larger than 40 nm, but only 10 nm in Al. The samples of Al and Cu studied here satisfied these conditions rightly, so we can only find full dislocations and twins in shocked nc Al.

Comparing Fig. 3(a) with Figs. 3(b) and 3(c), we can see that the partial dislocations shown at the surface of the shocked Al are less than in the shocked Cu even at the same shock stress or strain. Since the plasticity of monocrystalline (mc) metals (without GBs) are all mediated by dislocations, the method to calculate the maximums of dislocation density $\rho_d$ for mc metals suggested by Bringa et al. is not suitable for nc metals. We introduce a specific number of HCP atoms to the total number of atoms to represent $\rho_d$. Although some atoms at GB are mistaken as HCP by the pair analysis technique (see Fig. 7, for example, or just see these HCP atoms as GB dislocations), the $\rho_d$ at 0 ps can be neglected compared to the final $\rho_d$. Table II together with Fig. 3 shows that the $\rho_d$ of AL0 is lower apparently than CU1 and CU2 at the final step. A possible reason is that the full dislocations generated in shocked Al are sunk at the opposite GBs, leaving no stacking faults. However, we find full dislocation is limited in nc Al. We believe the main reason is that there are more partial dislocations emitted in shocked nc Al than in nc Cu at the same loading conditions. Asaro and Suresh have proven that the critical resolved shear stress (CRSS) needed to emit a leading partial dislocation from a preexisting GB dislocation or from stress-induced dislocation nucleation at GB for nc Al, whose grain size and grain orientation are the same as with nc Cu, is much larger because of a higher SFE and other intrinsic properties (e.g., lattice constant and shear modulus). In the case of the nc Al and Cu studied in this

### Table II. The fractions of different structures and dislocation density $\rho_d$ before and after shock compression.

<table>
<thead>
<tr>
<th>Simul.</th>
<th>t (ps)</th>
<th>FCC (%)</th>
<th>HCP (%)</th>
<th>GB (%)</th>
<th>$\rho_d$ (cm$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL0</td>
<td>0</td>
<td>79.4</td>
<td>0.1</td>
<td>20.2</td>
<td>$0.02 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>70.0</td>
<td>3.9</td>
<td>26.1</td>
<td>$1.4 \times 10^{-12}$</td>
</tr>
<tr>
<td>CU1</td>
<td>0</td>
<td>79.5</td>
<td>0.1</td>
<td>19.7</td>
<td>$0.01 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>56.3</td>
<td>14.9</td>
<td>28.8</td>
<td>$5.9 \times 10^{-12}$</td>
</tr>
<tr>
<td>CU2</td>
<td>0</td>
<td>79.5</td>
<td>0.1</td>
<td>19.7</td>
<td>$0.01 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>69.5</td>
<td>8.0</td>
<td>22.5</td>
<td>$3.0 \times 10^{-12}$</td>
</tr>
</tbody>
</table>

FIG. 5. 2D distribution of local stress $\sigma_{xx}$ (a)–(c), shear stress $\tau$ (d)–(f), and kinetic temperature $T$ (g)–(i) profiles, for AL0 at 14 ps, CU1 and CU2 at 20 ps. The averaging thickness along Z is 0.4 nm.
paper, as mentioned in Sec. II, the grain size and initial textures are the same. Though GB structures may change some after annealing and relaxation (see the circled GB of Fig. 6 for example), the changes of grain orientations are supposed to be omitted because no pronounced grain rotation is found during the relaxation process. We believe that the intrinsic properties such as high SFE of Al are the cause for a lower $q_d$ compared to nc Cu under similar shock conditions.

On account of that deformation twins can be treated as partial dislocations emitted at adjacent planes, all the strain of nc metals induced by shock compression are contributed by dislocation- and GB-mediated plastic process. Therefore, the strain contribution from GB-mediated plasticity in AL0 is larger than in CU1 and CU2, since the $q_d$ of AL0 is lower than CU1 and CU2, although the shocked strain of AL0 is larger than CU1 and equal to CU2 but with lower dislocation density. That is to say, the GB-mediated plastic process is more active in nc Al than in nc Cu, and dislocation-mediated plasticity contributes more in nc Cu than in nc Al under the same loading conditions. Similarly, because all of the strains induced by elastic and plastic deformation are completed in the shock-front region, we think that the contribution of GB-mediated plasticity to the shock-front width for nc Al is higher than nc Cu. This is a possible reason for Bringa et al.\textsuperscript{27} to conclude that the effect of GB-mediated plasticity on shock-front width can be ignored.

**B. Atomistic views of plasticity**

In the shock profiles presented above, we omit the structure variation normal to the shock direction by spatially averaging the stress and $U_p$ across 16 grains situated in the YZ plane. Despite that, there exists strong elastic and plastic anisotropy along the different orientations.\textsuperscript{53,54} Neglecting the transverse spatial variations may cover the microstructural effect on the shock response and lead to incorrect conclusion. Thus, two-dimensional (2D) or 3D interpretation of the shock front is necessary to gain the microscopic view of plasticity and other mechanisms that occur in response to shock compression. We obtain the 2D interpolation of $r_{xx}$, $T$, and kinetic temperatures (T) by averaging the corresponding atomistic terms for them in boxes with a width of two lattice constants for shocked AL0, CU1, and CU2, as presented in Fig. 5. The atomistic views of unshocked samples, as shown in Figs. 6(a)–6(e), are obtained by tracing all the atoms in Figs. 6(b)–6(f) at 0 ps.

The 2D profiles give spatial resolutions of the cross-sections along the shock direction X. The longitudinal (along Y direction) distribution in $\sigma_{xx}$, $T$, and $\tau$ that have been shown in Fig. 5 are severely inhomogeneous and far from negligible when compared to Figs. 1 and 2, even behind the shock-front regions ($X < \sim 90\,\text{nm}$ for CU1, and not shown for AL0 and CU2). This will lead to a nonuniform distribution of shear strength in the post-shock region, and the unsteadiness of $\sigma_{VM}$ at $\sim 40\,\text{nm} < X < \sim 75\,\text{nm}$ in Fig. 1 rightly specifies this nonuniform shear strength. The transverse (along X) distribution of $\sigma_{xx}$ in Figs. 5(a)–5(c) roughly presents the three-stage shock fronts in 1D profiles (Figs. 1 and 2). Initially, the low $\sigma_{xx}$ narrow band implies the elastic stage, then it grows in amplitude, forming GB- and dislocation-mediated plastic stage. We can see that each
transition line between these three stages is not straight. The interface between unshocked and shocked materials can simply be explained with an anisotropy of the elastic wave. The roughing of elastic-plastic transition may also be influenced by an anisotropy of the plastic wave; however, it is mainly affected by the different starting point of plasticity for grains located along YZ plane. That is to say, while a point in one grain along Y (or Z) has launched plastic deformation, but an other point with the same X coordinate might still in the elastic stage. The transition between GB- and dislocation-mediated plasticity should also be influenced by this reason, i.e., dislocation emission happening in one grain but not in others with the closed X coordinate. For these reasons, we can also infer that these transition planes from 3D views are not planar. Thus, the 1D profiles got by shock experiments may be not accurate enough for some special applications.

An evident difference presented in Figs. 5(a)–5(c) between Al and Cu is that the GB-mediated stage for Al is wider than for Cu, which reasons have been explained in the last section. Since the elevated free energy of GBs and the existence of free volume at GBs reduce the energy barrier to plasticity nucleation, the release of shear stress at GBs in Figs. 5(d)–5(f) indicates that GB sliding happens prior to dislocation nucleation and emission after the elastic stage is complete. This release of $\tau$ due to GB sliding makes $\tau$ at internal grains smaller than at GBs (comparing Fig. 5(d) with Fig. 6(b) for AL0 for clarity), and further delays dislocation nucleation. The contrast of $\tau$ release between GBs and internal grains is more obvious in the shocked columnar nc Cu.\footnote{Compared to the release of $\tau$ by dislocation shown at the later stage of Figs. 5(e) and 5(f), the contributions to the shear release of CU1 and CU2 from GB-mediated plasticity are relatively smaller than those of AL0. Both dislocation-mediated shear deformation and GB sliding induce local heating, as shown in Figs. 5(g)–5(i). Since the atoms in shock-front regions are of in a state of severe non-equilibrium, we use the kinetic energy of Y (or Z) direction to denote the temperature. This is a kind of energy dissipation mode driven by the shear stress. The 2D distribution of $T$ also represents the process of plastic deformation, namely, a higher elevation of $T$ corresponding to higher local stress. However, the transitions among three-stage shock fronts can not be observed easily. Because the $\sigma_{xx}$ of CU1 is higher than AL0 and CU2, the shock-induced elevation of $T$ for CU1 is higher than AL0 and CU2. On the other hand, due to a higher heat capacity for Cu, the elevation of $T$ in CU2 is lower than for AL0 at the same $r_{xx}$. The elevations of temperature for AL0, CU1, and CU2 in general are confined in the region of 200 K due to a very low initial temperature setting and a weak shock intensity.}

The contrast between Figs. 6(a) and 6(c) shows that the atom configuration of the Al sample is nearly identical with the Cu sample before shock compression, except for the white circled position. Because the atom interaction of Al and Cu is totally different, some low angle GB may change, or even vanish to reduce energy and internal stress after annealing and relaxation. However, when we compare the orientation of each corresponding grains carefully and find that they are almost identical. From the comparison between
the unshocked atom configurations to the shocked ones as shown in Fig. 6 of AL0, CU1, and CU2, the dislocations emission and propagation can be identified clearly. Similarly, the GBs thickening (see enlarged views in the circles of Fig. 7 for example) and transformations of some GB structures can be found, which are representations of GB sliding and are marked by arrows in Fig. 6 for clarity. The GBs thickening is also reflected by the increase of GB fraction values in Table I. At the same time, the arrows in Fig. 6 display the difference of the GB-related plastic processes of Al and Cu under the same loading conditions. A GB of AL0 marked by a white arrow in Fig. 6(b) bends while the similar GB of CU1 in Fig. 6(d) emits two dislocations to the neighboring grains. The grain marked by an arrow and a circle in Fig. 6(b) emits several dislocations simultaneously at different places which are pinned inside the grain, whereas countable dislocations are emitted and propagated to the opposite GB in the counterpart grain of CU2 in Fig. 6(f). To sum up, the microscopic plastic deformations in the shock front of nc Al and Cu are so different that GB- and dislocation-mediated plastic procedures vary, and finally lead to different shock fronts.

One scenario for GB thickening induced by GB sliding may be that the upper (or left) part of a GB sliding relative to the lower (or right) part makes one direction of the GB to become shorter because of shock-induced hydrostatic compression, and atoms at GB must move towards the grain inside along another direction since the atoms cannot be so close to each other. Fig. 7(a) gives a sketch model of this scenario, and MD simulated atom configuration evidences for nc Al and Cu are circled in Figs. 7(d)–7(f). Another possible scenario may be that some normal FCC atoms in grain are compressed so close to GB atoms that Honeycutt-Andersen analysis identifies them as GB atoms. As a result of the GB thickening, the distance between each atom near GB is compressed to make internal stress accumulate; then dislocations may be nucleated and emitted once the internal shear stress overcomes the CRSS needed with further compression. The white circled GB in Fig. 7(d) is an example. The GB thickening is a product of hydrostatic pressure with the assistance of shear stress, so pure shear stress like tensile loading cannot make GB become thicker. That may be a possible reason for the tension and compression strength asymmetry of nc metals, because the GB thickening will make the compressed GB to be able to resist greater shear stress. Another sketch shown in Fig. 7(b) gives a rare deformation mode, what we call it GB bending, found in shocked nc Al that have not been reported in our sight. This type of GB-mediated deformation process, indicated by an arrow in Fig. 7(d), is situated almost along the compression direction. When shear stress is not great enough to emit dislocation or generate other crystal plasticity in the adjacent grains to release shear stress, the accumulated normal and shear stress bends this GB, as shown in Fig. 7(d). Whether the GB bending can occur or not mainly depends on the GB structures, the magnitude of stress and the CRSS of the material. We cannot observe this type of GB deformation mechanism in nc Cu, as indicated by the arrow in Fig. 7(f). For CU1, it emits two dislocations due to the high shear stress and low CRSS instead of bending. Both the GB thickening and bending play a less important role in the plastic deformation studied in this paper. We guess that the GB thickening is a ubiquitous deformation mode in nc metals, since it is a precursor of dislocation emission; and that the GB bending is a rare deformation mode which needs cooperation of the orientation of GB, the loading direction, and other critical conditions. However, because both of these can strengthen the GB, which is considered to be the weakness in strengthening nc materials, correctly designed GB structures that could enable these mechanisms would be a powerful method for strengthening nc materials. Additional investigation should be done in order to take further advantage of GB thickening and bending.

IV. CONCLUSIONS

In this paper, we have studied the comparative behaviors of nc Al and Cu under shock compression from two different aspects. First, the macroscopic responses of nc Al and Cu are compared through the shock-front structures and dislocation densities. Second, the microscopic plastic processes of nc Al and Cu are described in depth by comparing the atom configurations before and after shock compression. The results show that the shock-front width of nc Al is wider than nc Cu at whatever the same shocked stress, shocked strain, and particle velocity. We also find that the high SFE of Al leads to a higher CRSS for nc Al to emit dislocations, and finally results in a lower dislocation density compared with the nc Cu having the same grain size and texture. Although the plastic stage of nc Cu can be roughly divided into GB-mediated and dislocation-mediated procedures just like nc Al, the effect of the GB-mediated plastic stage of nc Cu is relatively small when comparing it to nc Al. Inversely, the contribution to strain from GB-mediated plasticity for nc Al is larger than it is for nc Cu. These results are also supported by the 2D shock front and atom configuration analysis. We believe that the essential reason for these differences between nc Al and Cu with same grain size and texture at the same shock conditions is the different intrinsic properties, such as SFE, lattice constant and shear modulus and so on. Further studies should be done in order to obtain a quantitatively relationship between intrinsic properties and shock response. Comparative microscopic analysis of the unshocked and shocked atom configurations finds that GBs thickening in nc Al is more pronounced than in nc Cu before dislocation emission during the plastic deformation process. Another GB-related deformation that we call GB bending is observed in shocked nc Al. We think that it is the cooperation of hydrostatic pressure and shear stress induced by shock compression that causes the occurrence of GB thickening and bending, which cannot be observed under tensile loading. Designing GB structures to enable GB thickening would be a possible method for strengthening nc metals under compression, and it should be studied further.

The short-time/high-strain-rate restrictions inherent to MD simulations make it difficult to quantitatively determine the viscosity coefficient or energy dissipation process or even the strength of shocked materials needed in the
constitutive plasticity. However, some variation rules depending on the intrinsic properties, applied loading conditions, grain sizes, and so on can be obtained. Therefore, the comparative response of nc Al and Cu to shock compression studied in this paper will help to comprehend the atomistic deformation process and improve the understanding of shock fronts for different metals. Additional studies of the quantitative effects of material properties on shock front will be considered further.

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