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Grain Boundary Motion under Dynamic Loading: Mechanism and Large-Scale Molecular Dynamics Simulations

Christian Brandl^{a*,†}, Timothy C. Germann^a, Alejandro G. Perez-Bergquist^{b‡}
and Ellen K. Cerreta^b

^aTheoretical Division, Los Alamos National Laboratory, Los Alamos, NM, USA; ^bMaterials Science & Technology Division, Los Alamos National Laboratory, Los Alamos, NM, USA

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Grain boundaries (GBs) are not static structures during shock loading, despite the short timescales. We present a mechanistic explanation for why non-coherent $\Sigma 3$ GBs are particularly mobile, due to their consisting of coherent twin boundaries every third (111) glide plane, separated by incoherent twin boundary segments with three Shockley partial dislocations that can readily glide into either grain. Asymmetric GBs with such structures can thus move in response to the elastic driving force provided by uniaxial compression. We present large-scale molecular dynamic simulations that illustrate this mechanism, which explains the $\Sigma 3$ GB faceting recently observed in shock-recovered copper multi-crystals.

Keywords: Grain Boundary, Shock, Molecular Dynamics

1. Introduction Plastic deformation in metals is normally associated with the formation and motion of line defects (dislocations) within crystalline lattices, and the interaction of these dislocations with different constituent microstructural features, such as grain boundaries (GBs) in polycrystalline metals.[1] In general, accommodate the crystallographic orientation difference of the adjacent crystals.[2] Flat GBs can move when subjected to a thermodynamic driving force resulting from the volumetric free energy difference (pressure) across that interface due to crystal anisotropy (elastic, plastic and/or magnetic).[3] Recently, moreover, stress-driven grain coarsening – and therefore stress-driven GB motion – in nanocrystalline metals is thought to result from the high applied stresses which can be achieved due to the high yield and flow stresses of these nanostructured materials.[4] Under dynamic loading conditions such as shock compression, materials can be subjected to extreme stresses of tens to hundreds of GPa (or greater) for durations of nano- to microseconds.[5–7] As the shock pressure increases, the material behind (or even at) the shock front can be progressively driven through regimes of

dislocation activation [8] and nucleation,[9,10] polymorphic (solid–solid) phase transitions, if any,[11,12] and eventually shock melting.[13] While dislocation-mediated plastic deformation during shock compression and release, including subsequent material failure, has been extensively studied,[5,6,14–16] it has generally been assumed that the short timescales involved limit the role of GBs to mechanically driven GB-mediated deformation processes, and that the GB network itself does not have sufficient time to respond to dynamic loading.

Conventional plasticity models for dynamic loading conditions describe the plastic response in terms of dislocation generation and motion within grains and, when treated at all, the effect that GBs have as dislocation sources or sinks and in hindering dislocation transmission. The structure and possible mobility of GBs, however, have thus far been neglected. Recent examinations of the localization of voids after spall loading signify that the standard geometric descriptors of dislocation-based mechanisms (e.g. Schmid factors) cannot explain the reduced propensity for failure at $\Sigma 3$ disoriented interfaces.[17,18] This statistical analysis indicates the

*Corresponding author. Email: christian.brandl@kit.edu

[†]Present Address: Karlsruhe Institute of Technology, Karlsruhe, Germany.

[‡]Present Address: Oak Ridge National Laboratory, Oak Ridge, TN, USA.

importance that the atomistic GB structure can have upon the resulting macroscopic deformation behavior. The mechanistic origin, however, remains elusive, although the kinetic signatures (critical stress state, energy barrier and its stress/strain dependence) of the deformation mechanism should be intimately linked to the interface structure, which will be special for general $\Sigma 3$ GBs.

Perez-Bergquist et al. [19] have used gas gun experiments with soft (post-shock sample) recovery to examine the response of a large-grain copper multi-crystal sample to shock loading, where the shock front travels along the columnar GB planes. Using transmission electron microscopy to compare the as-prepared and post-shock structures of a non-coherent asymmetric $\Sigma 3$ GB reveals that shock loading induces a faceting of this GB, with steps on the order of 50 – 100 nm. In this letter, we suggest a mechanistic explanation for this faceting, and explain why asymmetric $\Sigma 3$ GBs can in fact be mobile under shock-loading conditions. Atomistic simulation results are presented to demonstrate this mechanism.

2. Method We utilize the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [20] to perform large-scale classical molecular dynamics (MD) simulations to study the structure and shock response dynamics of copper bicrystals containing an asymmetric $\Sigma 3$ GBs with GB normal direction $\mathbf{n} = [1\ 0\ 1]_B \parallel [1\ \bar{1}\ 4]_A$ in the upper grain B and lower grain A . Our sample contains $\approx 1.5 \times 10^8$ atoms in a 189 nm(x) $\times$ 53 nm(y) $\times$ 185 nm(z) geometry, where the GB lies in the xy plane. Periodic boundary conditions are applied in the y direction, but not in the x shock direction

or in the z GB normal direction, to avoid introducing a second (generally higher energy) GB there. Instead, atoms in the resulting $\pm z$ free surface regions are constrained to move according to the forces in the x and y directions, but not in z , in order to maintain uniaxial strain loading.[21] The initial interface structure is generated by an iterative relaxation procedure to minimize the GB energy, by deleting atoms which are too close to each other and by rigidly shifting the grains in directions parallel to the interface plane. After rescaling the resulting 0 K structure to account for thermal expansion to the equilibrium lattice constant at 300 K, the model is equilibrated to 300 K and zero stress by Langevin dynamics. A shock is then introduced by a 2 nm thick piston region which moves at an imposed velocity $u_p = 250$ or 300 m/s, which determines the particle velocity u_p behind the shock front. The stresses are computed from the atomic virial stresses with the equilibrium atomic volume. The defect structures are identified by the common neighbor analysis (CNA),[22] as implemented in LAMMPS where 1, 2, 3 and 4 correspond to local FCC, hexagonal closed packed (HCP), body centered cubic, icosohedral and unknown structures, respectively.

3. Interface Structure Interface dislocations – and therefore interface structure – can be geometrically motivated from the crystallography of the so-called dichromatic pattern (DCP),[23] which visualizes the union of the two disoriented lattices in which each individual lattice has a unique label or color. The $\Sigma 3$ (twin) disorientation grains in FCC crystals in particular can be described by the rotation operation: 60° around a $\langle 1\ 1\ 1 \rangle$ crystal axis, or equivalently via symmetry, $\approx 70^\circ$

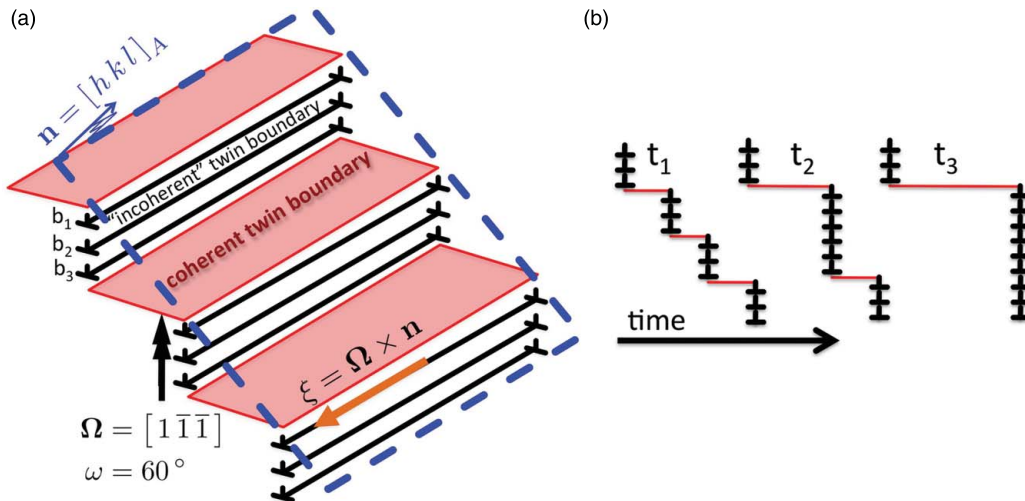


Figure 1. (color online) (a) Structural model of a non-coherent $\Sigma 3$ GB in face centered cubic (FCC) crystals. The dashed blue plane indicates the GB normal. The red area represents the coherent twin planes, which are perpendicular to the rotation axis $\Omega = [1\ 1\ 1]$ (black double-headed arrow) with the rotation angle $\omega = 60^\circ$. Black lines with partial Burgers vectors b_1 , b_2 , and b_3 illustrate the GB dislocations; each array of these partial dislocations an ‘incoherent’ twin boundary. The line direction of the GB dislocation is indicated by the orange arrow ξ . (b) Cross section of the structural model for different times (left to right), when the interface is subjected to shock loading. The directionality of the motion depends on the thermodynamic driving force. (For details, the reader is referred to the text.)

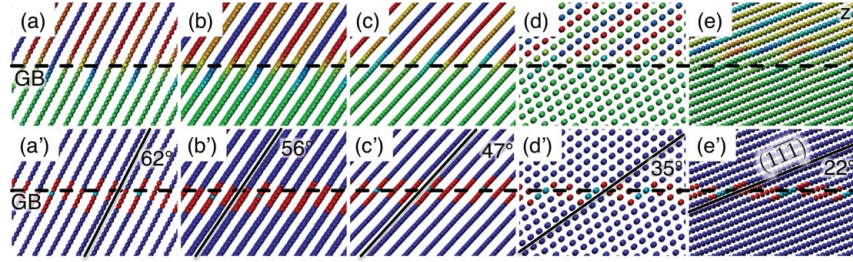


Figure 2. (color online) Atomic models of the $\Sigma 3$ ($\Omega = [1 \bar{1} \bar{1}]$, $\omega = 60^\circ$) GB structure in FCC Cu for different GB normal directions $\mathbf{n} \parallel \mathbf{z}$ in lower grain *A* and upper grain *B* (from left to right): (a) and (a') $[\bar{1} 2 \bar{1}]_B \parallel [\bar{7} 1 \bar{2}]_A$; (b) and (b') $[\bar{3} 5 \bar{2}]_B \parallel [\bar{6} 1 \bar{1}]_A$; (c) and (c') $[\bar{3} 4 \bar{1}]_B \parallel [\bar{5} 1 0]_A$; (d) and (d') $[1 0 \bar{1}]_B \parallel [1 \bar{1} 4]_A$; (e) and (e') $[\bar{3} 1 2]_B \parallel [2 1 3]_A$. From (a) to (e), the inclination of the GB normal direction with respect to the coherent $\Sigma 3$ GB orientation (indicated by the solid black line in (a')–(e')) decreases. In the upper rows (a)–(e), the atoms are colored according to the distance (*z* component & GB normal direction) to the closest atom in an extension of the lower lattice (blue = $-0.5\text{\AA}$, green = $0\text{\AA}$, red = $0.5\text{\AA}$), whereas in the lower rows (a')–(e'), atoms are colored according to the local crystalline structure (cyan = local HCP structure, red = unclassified atoms). The GB plane (indicated by a dashed black line) is aligned horizontally, and the crystals are rotated such that the coherent and $(1 \bar{1} \bar{1})$ planes common to both lattices align (indicated by solid black line in (a')–(e')), which are parallel to the coherent twin fault (i.e. cyan atomic planes in the lower row).

around $\langle 1 1 0 \rangle$ crystal axis. From the $\Sigma 3$ DCP, the GB dislocation Burgers vectors can be deduced to be Shockley partial dislocations, with Burgers vectors parallel to a perfectly coherent $(1 1 1)$ plane. With these ingredients, we motivate the structural model for $\Sigma 3$ GBs (twin boundaries) in FCC metals as illustrated in Figure 1(a) for any GB plane. In general, the GB energies and the detailed structural units depend on the disorientation and the GB plane.[2] The GB normal direction $\mathbf{n}$ in lattice *A* is given by $\mathbf{n} = [h k l]_A$ (indicated by the blue arrow and dashed blue plane). The intersection with the coherent twin plane (indicated by the red planes), which is every third $(1 \bar{1} \bar{1})$ plane (β plane in Thompson notation) along the rotation axis $\Omega = [1 \bar{1} \bar{1}]$ in the DCP, determines the average line directions $\xi = \Omega \times \mathbf{n}$ (orange arrow in Figure 1(a)) of the constituent GB dislocations, which have a Burgers vector equivalent to Shockley partial dislocations of closed-packed $(1 \bar{1} \bar{1})$ planes parallel to the coherent twin plane. Labeled black lines indicate this array of Shockley partial dislocations, which is perpendicular to coherent twin planes to be consistent with the imposed GB plane. Finally, we note that the proposed interface dislocation structure has vanishing long-range stresses for any GB plane, since these partial dislocations ($C\beta$, $D\beta$, $A\beta$ in Thompson notation [1]) have a net zero Burgers vector $\mathbf{b}$ ($\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3 = C\beta + D\beta + A\beta = 0$ for a rotation axis $\Omega = [1 \bar{1} \bar{1}]$).

Using the embedded atom method potential for Cu,[24] MD simulations confirm the proposed structural model for $\Sigma 3$ GBs with different GB normal directions, revealing that the structural units comprise a planar twinning fault on the common $(1 \bar{1} \bar{1})$ plane (coherent twin boundary) interrupted by an array of three partial dislocations on consecutive $(1 \bar{1} \bar{1})$ planes ('incoherent' twin boundary). In all our MD models, the lattices are oriented with $\mathbf{x} = [1 1 1]_B \parallel [1 5 \bar{1}]_A$ for the upper grain *B* and lower grain *A*. The same GB structures – though

differently shaded – are shown in Figure 2(a)–(e) and (a')–(e'), respectively. Measuring the distance between each atom in the upper lattice (grain *B*) with the closest atomic position of a hypothetically extended lower lattice (grain *A*), Figure 2(a)–(e) clearly shows slip traces on the $(1 \bar{1} \bar{1})$ (β) plane in lattice *B*, which terminate at the GB. The relative displacements between slip traces is equivalent to the Burgers vectors of the partial dislocation $C\beta$, $D\beta$, $A\beta$ in both lattices *A* or *B*. Analysis of the GB structure for different GB planes shows that the constituent structural units – dislocation arrays interconnected by planar faults – are unaltered in terms of the coherent planar twinning fault and Burgers vector content (partial dislocations of the $(1 \bar{1} \bar{1})$ (β) plane), although the width of the planar twin boundary, and the line direction of the dislocations are changing. The partition of the GB plane onto the symmetric-equivalent rotation axes from pure tilt towards pure twist GB plane orientation results in a quasi-two-dimensional structure by means of a set of non-intersecting partial dislocations on planes parallel to the coherent twin planes, and lying between the coherent twin regions. Moreover, the closer the GB normal direction is to the normal direction of the coherent twin plane, the longer the coherent twin plane is, which is evident by the larger local HCP structures in the interface model in Figure 2(a')–(e').

The total Burgers vector density of the $\Sigma 3$ GBs is zero, and therefore, the motion of the GB with velocity $v_\perp$ is not geometrically coupled to a shear deformation across the GB with a relative velocity $v_\parallel$, which in case of coupled GB motion normally implies mechanical shear work being associated with the motion of the GBs.[25] Moreover, the 'dipole' dislocation structure of the $\Sigma 3$ GB also allow for an dissociation of the GB under applied stress, since the shear stresses cause opposite sign Peach–Koehler forces on the partial dislocations, which again sum up to a net zero Peach–Koehler force. The

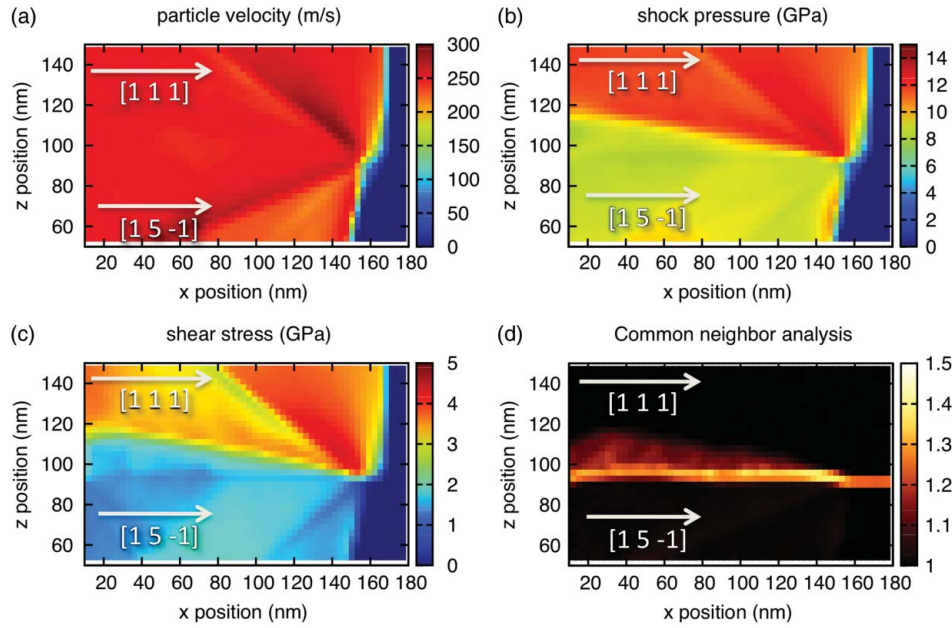


Figure 3. (color online) Snapshot of the through-thickness averaged atomic properties at 30 ps, where the shock front (xy -plane) propagates along the GB (xz -plane). The color scale is given for each property individually. Stresses are estimated from the virial atomic stress tensor and the equilibrium atomic volume, and the shock direction component and maximum shear stress τ ($2\tau = \sigma_{xx} - 1/2(\sigma_{yy} + \sigma_{zz})$) are shown in (b) and (c), respectively. The white arrows in the upper and lower grains indicate the shock directions. The shock front is propagating from the left to the right along the GB.

restoring forces between the partial dislocation (twin and stacking faults, elastic interaction) can reverse the dissociation upon removal of an applied shear stress (see similar discussion in ref. [26]).

Since the partial dislocations of the incoherent part of a general $\Sigma 3$ boundary are essentially glide dislocations of both adjacent crystals, these dislocations can easily move when they are subjected to an external stress. With these structural considerations in mind, Figure 1(b) illustrates a cross section of the GB structure evolution upon loading. In analogy to dislocation–dislocation interactions, the arrays of partial dislocations have a strong anisotropic interaction, which leads to the agglomeration to a larger dislocation array during the process of individual motion of the GB dislocations. This successively activated dislocation motion eventually leads to the formation of larger facets as a consequence of GB motion. Generally, for the proposed $\Sigma 3$ GB dislocation model, the relative position of the adjacent GB dislocations determines whether locally a twin fault configuration, extended intrinsic/extrinsic stacking fault configuration, and/or the 9R structure is observed; this is therefore consistent with published $\Sigma 3$ GB structures in FCC metals.[2,27,28]

4. Shock Response Following the initial loading, a shock wave develops with different velocities in the lower and upper grains due to material anisotropy, in order to maintain the imposed particle velocity behind the shock

front (Figure 3(a)). At the intersection of the shock front with the GB, scattering waves are emitted, resulting in trailing waves in both grains.

Figure 3(b) and 3(c) show the cross section of the spatially averaged ($3 \text{ nm} \times 3 \text{ nm}$) shock pressure and shear stress obtained from the MD simulation. In the upper grain *B*, the shock velocity in the $[1 \ 1 \ 1]$ direction is faster than the $[1 \ 5 \ \bar{1}]$ in the lower grain *A*. However, the rise in the stress state behind the shock front is mainly caused by the predominately planar propagating wave fronts in the respective grains. At the interface itself, the mismatch of the shock front velocities entails an evolving length scale. The mismatch of the shock front velocities is closely linked to the anisotropic elastic properties of the Cu FCC crystal, namely the longitudinal speed of sound. Moreover, the shock pressure in the upper grain is higher than in the lower grain, which is consistent with a uniaxial isostrain loading of the bicrystal setup, since the elastic constant is higher in the $[1 \ 1 \ 1]$ grain than in the lower $[1 \ 5 \ \bar{1}]$ grain. The GB is exposed to $\approx 9 \text{ GPa}$ ($\approx 1.5 \text{ GPa}$) and $\approx 11 \text{ GPa}$ ($\approx 3.5 \text{ GPa}$) shock pressure (shear stress) in the lower and upper grains, respectively (Figure 3(b) and 3(c)), which is also a manifestation of the anisotropic elastic constants and difference of stored elastic energy. Behind the shock front, the discontinuity in the shock pressure and in the shear stress moves into the upper grain away from the GB. Inspection of the averaged CNA (Figure 3(d)) – a measure of defect content – indicates that this is accomplished via dissociation of the GB, in addition to the smaller overall motion of

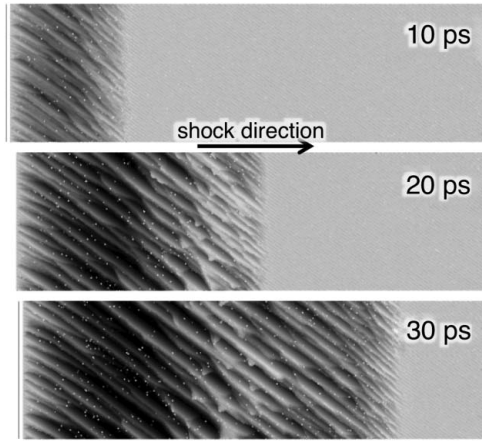


Figure 4. Interface morphology viewed from the lower grain onto the GB. Only non-FCC atoms are shown and colored according to their z position (white = z_0 ; black = $z_0 + 5$ nm).

the interface. Although the GB is moving, no velocity gradient $v_{||}$ is detectable across the moving interface (see Figure 3(a)), which implies no coupled GB motion behind the shock front, which is in agreement with the presented structure model of $\Sigma 3$ GBs.

Figure 4 displays the temporal evolution of the GB position viewed from the lower grain (grain A), and reveals a continuous motion of the interface during shock loading associated with the moving shock front. With increasing time of exposure to the shocked state behind the propagating shock front, the size of the GB facets is increasing, which resembles the facets observed experimentally.[19] The pronounced crystallographic terraces of the GB facets are linked to the motion of the parallel partial dislocations, which are intrinsic to the GB structure. The dislocation motion results in GB dislocation agglomeration into dislocation wall arrays, as indicated in Figure 1.

In addition to the GB motion and faceting, the interface changes by the appearance of a complex structure of parallel extended coherent stacking/twin faults (cyan colored atoms in Figure 5(a) and 5(b)) surrounded by corresponding partial dislocations (red atoms in Figure 5(a) and 5(b)) in the upper grain, where the shock propagation direction is along a $[1\ 1\ 1]$ lattice direction (indicated by black arrow). Inspection of the cross section (Figure 5(b)) demonstrates that the motion of partial dislocations, which are intrinsic to the GB structure (initial line direction ξ indicated by white arrow), results in a collective GB motion into the upper grain. The dissociation of the GB is mediated by the motion of the partial dislocations into the upper grain. Note that the resolved shear stress onto different slip systems would predict only the dissociation without the biased motion towards the upper $[1\ 1\ 1]$ grain (grain B). The interface moves via a collective motion of the constituent partial dislocations, which may result locally in twin faults bounding micro twins (ii in inset of Figure 5(b)), or extended stacking

faults (i in inset of Figure 5(b)). The collective motion of these partial dislocations aligns with the habit plane of the GB dislocations in the structure model, and causes the macroscopic GB motion indicated in Figure 1(b).

Figure 5(c) shows a cross section of the (non-FCC) GB atoms for piston velocity $u_p = 250$ m/s (300 m/s) as black (red) atoms, after 30 ps. We note that the higher driving force ($u_p = 300$ m/s) results in more GB motion, and therefore a higher GB velocity, which is consistent with the customary notion of GB mobility.[3] Inspection of the cross section (Figure 5(b) and 5(c)) also shows that the GB is pinned by the piston region (left end), which is a boundary effect of the simulation setup.

The propagating shock wave has two regimes: the transient loading at the shock front and the approximately constant loading behind the shock front. Due to the crystal anisotropy in the longitudinal (shock propagation) direction, the shock front regime is growing in time as it travels along the GB. The associated shear wave, which departs from the GB region, imposes an additional driving force on the GB dislocations. Figure 6 compares the response of the shock front traveling along the $[1\ 1\ 1] \parallel [1\ 5\ \bar{1}]$ with the inverse shock direction $[\bar{1}\ \bar{1}\ \bar{1}] \parallel [\bar{1}\ \bar{5}\ 1]$ in the upper and lower grains, respectively. By inverting the direction, we only invert the sign of the shear stress resulting from the shear wave at the shock front, but the stress state behind the shock front is unaltered. Inspection of the GB response viewed from the upper grain (grain B) shows that the dissociation of the GB (and the associated GB Shockley partial dislocation) is strongly suppressed upon inversion of the shock direction, suggesting that the GB dissociation is driven by the shear stresses. However, the GB itself is moving behind the shock front, suggesting that the GB motion is mechanically driven by the (approximately constant) elastic anisotropy behind the traveling shock front, whereas the facet morphology and precise dislocation motion are strongly affected by transient dynamics at the shock front.

5. Summary and Discussion With the above considerations – derived from atomistic simulations – we may explain the experimentally observed change of the GB morphology. The emergence of boundary facets can be attributed to the difference in stress state in the adjacent grains, which differ in the region behind the shock front compared to the region at the shock fronts. The evolving shock front imposes a loading heterogeneity, which gradually alters GB morphology with time as the shock wave travels. The different partition of the GB structural building block (height of the incoherent and coherent facets) is equivalent to a rotation of the GB planes without changing the disorientation of the adjacent crystals. GB motion is associated with the growth of the incoherent facets, which can also migrate collectively as a dislocation array.

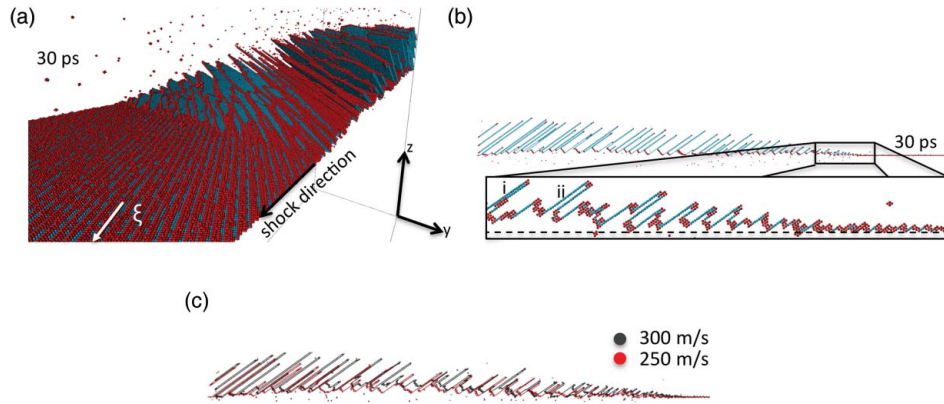


Figure 5. (color online) (A) Perspective view of the GB structure at 30 ps after shock impact. Only non-FCC atoms are shown, and are colored according to their local crystalline class (cyan = local HCP structure, red = unclassified atoms). The black arrow indicates the shock direction. The white arrow indicates the line direction of the GB dislocations (see text and Figure 1(a)). (B) Cross section of the interface (0.5 nm thickness) viewed into the line direction ξ . The shock front travels from left to right. The inset shows an expanded view close to the shock front. The extended HCP atomic planes (cyan colored) correspond either to stacking faults (indicated by i in inset) or twin faults (indicated by ii in inset). The black dashed line indicates the initial GB position.

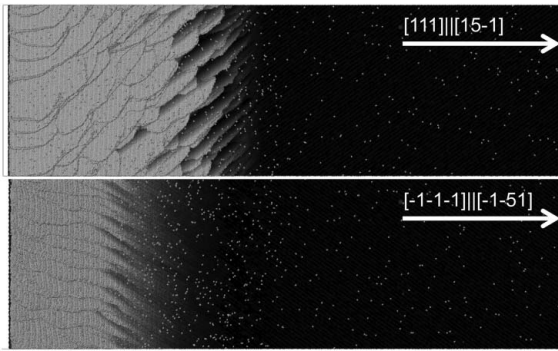


Figure 6. GB morphology viewed from the upper grain at the same time of shock duration, with inverted shock direction in respect to the crystallographic direction. The white arrow indicates the shock direction. Only non-FCC atoms are shown, and are colored according to their z position (black = initial GB position, white higher). In the upper panel, the shock direction is $[111]_B \parallel [15\bar{1}]_A$ in the upper and lower grains, respectively. The lower panel shows the GB motion with the shock direction is $[\bar{1}\bar{1}\bar{1}]_B \parallel [\bar{1}\bar{5}1]_A$ in the upper and lower grains, respectively.

Impurities are assumed to be homogeneously distributed along the interface, and would therefore not contribute the gradient in the facet heights. However, we anticipate impurities as a possible source of pinning strengthening, which will alter the kinetics and therefore also alter time scales and critical stresses for the biased GB motion. Similar to the effect of impurities, lattice dislocations in the adjacent grains serve as pinning points/lines of the GB motion. In addition, a mismatch of the dislocation density in adjacent crystals can also be envisioned as a thermodynamic driving force for GB motion. But we found no experimental evidence that the average spacing of dislocations in the bulk depends on the propagation distance of the shock front; hence, the dislocation–interface interaction is not expected to impose a gradient of the facet spacing in the $\Sigma 3$ GB.

In summary, shock experiments at ≈ 10 GPa peak stress [19] and MD simulations revealed the GB mobility of non-coherent $\Sigma 3$ GBs in Cu to be kinetically and structurally possible under relatively weak shock-loading conditions. The already reported enormous GB mobility [29,30] of non-coherent $\Sigma 3$ GBs can be rationalized by the mobile GB partial dislocations: (1) which have a net zero Burger vector, (2) whose individual Burgers vectors are sessile Shockley partial dislocations in both adjacent bulk lattices, and (c) whose dislocation lines do not intersect in the slip plane.

Since the $\Sigma 3$ GBs have a net zero Burgers vector content, the GB motion does not couple to a shear deformation across the interface region. Additionally, the shear stress on the GB plane are minimized since GB plane is perpendicular to the shock-loading directions (uniaxial straining direction). Therefore, shear deformation as thermodynamic driving force may be precluded for the GB motion observed here. In contrast to the shear deformation in coupled GB motion, the elastic anisotropy, and hence the energy density difference between the adjacent grains, gives rise to a thermodynamic driving force, which enables the biased motion of GB dislocations into the grain with the higher stored energy density (here the $[111]$ grain) without the assistance of diffusion processes. Given that the energy density is proportional to $\epsilon^2 + \mathcal{O}(\epsilon^3)$, the motion should occur into the grain which is elastically harder (i.e. has a higher energy density), irrespective of whether the strain is tensile or compressive. However, anharmonicity [31] and plastic anisotropy [3] – the generation of shock orientation-dependent internal stress states in adjacent grains due to differing dislocation structures [32] – may alter the thermodynamic driving force at high strains. Compared to coupled GB motion, where the driving force is proportional to ϵ , shear deformation across the GB is associated with the

GB motion, which implies non-zero GB Burgers vector dislocation tilt content. This is a rare circumstance, where anisotropic lattice properties result in the mechanical motion of defects on non-diffusive time scales. In particular, shock compression can produce strains large enough that the (usually small) elastic anisotropy mismatch results in strain energies sufficient to produce athermal defect motion at short-time scales.

This work demonstrates that GBs are not static structures under shock-loading conditions. Specifically, non-coherent $\Sigma 3$ GBs have a mobility, which in principle enables the accommodation of heterogeneities resulting from the differing deformation response of the surrounding bulk crystals. This may have implications on the suppression of failure localization (void nucleation), which is associated with the lack of local stress relaxations (plastic zones) to accommodate local heterogeneities, in polycrystalline materials.[17,18]

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