

Atomistic study of $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twin boundary migration in hexagonal close packed ZrLu Jiang^{1,*}, Mark Asta^{2,3}, and Daryl C. Chrzan^{2,3}¹Department of Materials Science and Engineering, City University of Hong Kong (Dongguan), Dongguan 523808, China²Department of Materials Science and Engineering, University of California–Berkeley, Berkeley, California 94720, USA³Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

(Received 19 August 2025; revised 14 November 2025; accepted 15 December 2025; published 6 January 2026)

Molecular dynamics techniques are used to investigate $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twin thickening processes through spontaneous formation of twinning disconnections (TD) under applied shear deformation with a constant strain rate, based on an embedded atom method potential model of Zr. The observed stress responses and twin boundary structure changes verify that both twins thicken through TD formation. However, the thickening processes of $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins show significant differences. While $\{10\bar{1}2\}$ TD loops were observed to form and expand during the twin thickening process, the $\{11\bar{2}1\}$ twin boundary exhibits a more structurally disordered interface throughout the simulation, and no sharp boundary corresponding to a $\{11\bar{2}1\}$ TD ‘loop’ can be identified. Moreover, the $\{11\bar{2}1\}$ twin requires a much lower critical shear stress for twin thickening, approximately 10% of that for the $\{10\bar{1}2\}$ twin. The low critical shear stress of $\{11\bar{2}1\}$ twin thickening also indicates that these twins should grow easily once nucleated. To the extent that these results apply to hexagonal-close-packed (HCP) materials more generally, promotion of $\{11\bar{2}1\}$ twin nucleation may be an effective way to enhance twinning deformation and twin boundary-related work hardening in HCP materials, with the potential to manipulate the balance between strength and ductility.

DOI: [10.1103/kdll-phvv](https://doi.org/10.1103/kdll-phvv)

I. INTRODUCTION

Deformation twinning plays an essential role in the plastic deformation of hexagonal-close-packed (HCP) metals, where the number of operative dislocation slip systems is limited. Among various twinning modes in HCP metals, $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twinning are two commonly observed tension twins [1]. Specifically, $\{10\bar{1}2\}$ is the most frequently observed twinning system in most HCP metals and even the only operative twinning mode for metals with limited ductility [1]. In contrast, $\{11\bar{2}1\}$ twinning is observed at low temperatures in metals such as Zr and Ti, and may enhance the room temperature ductility [2,3]. For Re, a refractory metal with combined high-temperature strength and room-temperature ductility, $\{11\bar{2}1\}$ twinning is found to be predominant regardless of the loading conditions and temperature [4–6]. The work presented here focuses on a comparative study of the processes underlying the growth (thickening) of these two twins, to contribute to advancing insights into conditions favoring the activation of both twinning modes. In so doing, the intent is to contribute to promoting understanding to guide materials design strategies involving the use of twinning-induced deformation processes to enhance ductility and work hardening.

Twin thickening, i.e., the twin growing normal to the $\mathbf{K}_1$ plane, is a crucial process of twin formation. The kinetics of twin thickening influence the twinning morphology and deformation accommodation capability. It is well established that twin thickening relies on twinning disconnections (TDs) [7], which are line defects located on the twin boundary plane that have both Burgers vector and step height components. The crystallographic character of the $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ TDs, i.e., the Burgers vectors and step heights, was obtained by Serra and Bacon through analyzing the symmetry of the HCP crystal [8]. Moreover, the TDs have been investigated through atomistic simulations using pair potentials and the Zr embedded atom method (EAM) potential [8,9]. The revealed structures and energies derived from these studies [8,9] indicate that each of these two twinning modes has one crystallographically valid and stable TD. The detailed structural parameters reported for the TDs in these studies are listed in Table I.

For twin thickening, different mechanisms for the formation of TDs have been proposed. These include lattice dislocation dissociation, grain boundary (GB) emission, and spontaneous nucleation [10,11]. Previous experimental and theoretical studies have shown that the thickening process of $\{10\bar{1}2\}$ twins in Mg and Zn is independent of slip dislocations [10,12,13], and GB emission is possible only when the twin forms from a GB, leaving spontaneous TD nucleation as a theoretically more plausible nucleation mechanism for many experimental systems. As proposed by Christian and Mahajan in 1995, a closed loop of a TD can form through thermal activation and then spread outward under the influence of the applied stress, resulting in twin thickening [14]. Later research on Mg alloys also proposed the thermal activation and

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TABLE I. Burgers content and step height of $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twinning disconnections (TD). The length of the Burgers vector and the value of the step height were calculated with lattice constants of the Zr EAM potential ($a = 3.234 \text{ \AA}$, $c = 5.168 \text{ \AA}$).

Twinning mode	Burgers vector		Step height	
	Expression ($\Lambda = \sqrt{\frac{2}{3}} \frac{c}{a}$)	Magnitude ($\text{\AA}$)	Expression (# of K_1 lattice planes)	Magnitude ($\text{\AA}$)
$\{11\bar{2}1\} \{11\bar{2}\bar{0}\}$	$\frac{1}{6(6\Lambda^2+1)} [11\bar{2}\bar{0}]$	0.45	1/2	0.772
$\{10\bar{1}2\} \{10\bar{1}\bar{1}\}$	$\frac{2-\Lambda^2}{2+\Lambda^2} [10\bar{1}\bar{1}]$	0.54	2	3.798

expansion of TDs being an important twin thickening mechanism [15]. Nevertheless, an atomistic scale understanding of shear-induced spontaneous disconnection loop nucleation and propagation on the twin boundary has not been fully investigated for the tension twins that form the focus of this work.

In the present study, molecular dynamics (MD) simulations, known to be effective in modeling GB migration kinetics and GB structures (e.g., [16–20]), are used to study the twin thickening process, i.e., TD nucleation and propagation under applied shear deformation. The atomistic structure of stable $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twinning disconnections is investigated, featuring the step character and the elastic field due to the Burgers content. In addition, twin thickening under applied shear deformation is simulated using a classical EAM potential for Zr [21]. We undertake simulations in which disconnection loops are observed to nucleate and expand on twin boundaries that are initially free of disconnections. The critical shear stresses for TD formation at different temperatures are obtained and compared. Moreover, the twin boundary structures of both twins at varying temperatures were studied to explain the critical shear stress difference between the two twinning modes. Furthermore, the overall $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twinning process is discussed based on the twin growth and twin nucleation mechanisms reported in the current work and previous studies. The work provides insights into the mechanisms promoting the growth of both twins.

II. METHODS

Atomistic simulations were conducted with LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [22] using a Zr EAM potential (referred to as #3 in Ref. [21]). To investigate the structure and strain fields associated with the TD line defects (result shown in Sec. III A), a straight TD dipole was built at the twin boundary using the method introduced by MacKain *et al.* [9]. The supercells contain two twin boundaries normal to the z -direction for maintaining periodicity, with one located at the middle of the simulation box, and the other at the periodic boundary. A TD dipole was introduced to the middle twin boundary. The simulation supercells were approximately 50 nm (x) $\times$ 30 nm (z) in size, where the periodic lengths in the y -direction (TD line direction) were the smallest lattice vector length along the TD line direction, in this case, $3.2 \text{ \AA}$ and $5.6 \text{ \AA}$ for the $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins, respectively. The supercells were periodic along all directions. The TDs were positioned to minimize elastic interactions with the other TD or the periodic images. Energy minimization was performed via the conjugate

gradient algorithm to obtain the relaxed structure, with a tolerance for the forces set to $10^{-3} \text{ eV/\AA}$. While the atomic positions were relaxed, the simulation supercell shape and volume were fixed.

For the molecular dynamics simulation of twin thickening under shear deformation (results shown in Secs. III B and III C), a schematic diagram of a simulation supercell is shown in Fig. 1, where a coherent twin boundary is located at the middle of the supercell and is normal to the z -direction. The positions of the atoms in the upper and bottom rigid regions are fixed. The z -direction thickness of each rigid region is twice the Zr EAM potential cutoff. Equations of motion for a canonical ensemble (based on the Bussi-Donadio-Parrinello thermostat [23] with the temperature set at various values indicated below) were integrated in the dynamic region. Periodic boundary conditions were applied along the x - and y -directions, while the z -direction was non-periodic with fixed regions as indicated in Fig. 1. The dimensions of the simulation supercell were approximately 45 nm (x) $\times$ 45 nm (y) $\times$ 12 nm (z) in size and contained approximately 1.0×10^6 atoms. An xz -shear strain was applied through incrementally adding a small displacement to the upper rigid region with a strain rate of approximately $1.1 \times 10^7 \text{ s}^{-1}$. Comparison tests at lower strain rate indicate this strain rate setting provides sufficient accuracy in stress response under applied strain (see Supplemental Material [31]). The thicknesses of the rigid regions in the z -direction are twice the potential cutoff distance. The details related to computing the stress of the system are provided in the Supplemental Material [31].

For the simulation of equilibrium twin boundary structures at different finite temperatures (results presented in Sec. III D), the supercells have the same dimensions as the supercells in the shear simulations (without applied

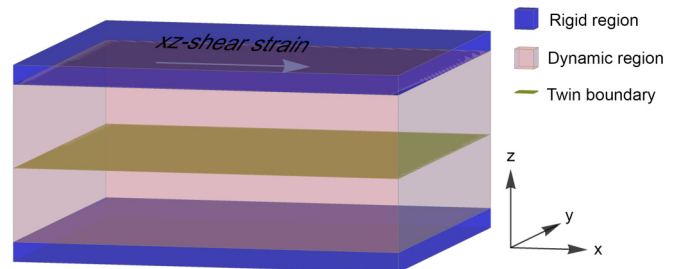


FIG. 1. Schematic diagram of the simulation setup for simulations of twin boundary motion under applied shear. An xz -shear strain was applied to the simulation box through rigidly displacing the upper rigid region as a group.

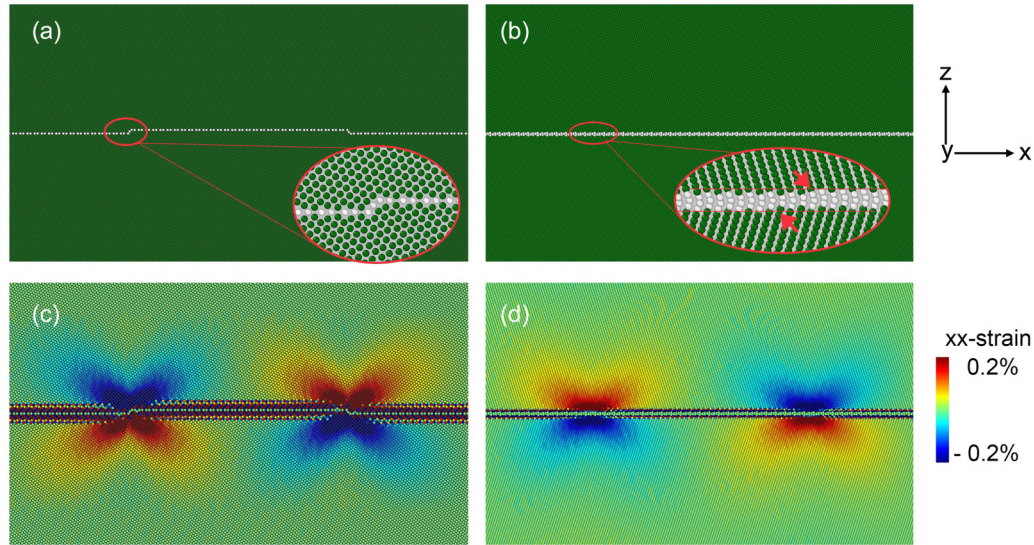


FIG. 2. $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twinning disconnection (TD) structure and strain field. A TD dipole of $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ is shown in (a) and (b), respectively, where atoms that are labeled in green have hexagonal-close-packed coordination, while atoms that are labeled in white are recognized as twin boundary atoms. The coloring in (a) and (b) is based on a common neighbor analysis. The strain field of the same $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ disconnection dipole is visualized in (c) and (d), respectively. (a) and (c) are shown in a $[11\bar{2}0]$ projection; (b) and (d) are shown in a $[1\bar{1}00]$ projection. The coloring by coordination and strain field is made using the OVITO package [28].

deformations), but with periodic boundary conditions applied to all three directions. Equilibrium structures were analyzed in MD simulations conducted at constant energy (i.e., in the microcanonical ensemble).

The $\{11\bar{2}1\}$ twin in all simulations was built according to the relaxed D-configuration as discussed by Minonishi *et al.* [24]. There are multiple metastable $\{11\bar{2}1\}$ twin boundary structures that can be built through varying the corresponding stacking sequences across the twin boundary. The $\{11\bar{2}1\}$ twin boundary structure that was used in this work (the relaxed D-configuration) is the one with the lowest energy and featuring a distorted icosahedron structure on the twin boundary plane [25]. This D-configuration has been used in previous studies of the properties of the $\{11\bar{2}1\}$ twins [25,26]. The detailed discussion of $\{10\bar{1}2\}$ twin boundary structure can be found in previous studies [9,27]. In the following sections, atoms in the twin boundary regions are recognized according to the common neighbor analysis with an adaptive cutoff in the OVITO package [28].

III. RESULTS

A. Disconnection structure

The Burgers vector and step height of $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ TDs that are consistent with crystallographic constraints [8], and found to be energetically stable in previous atomistic studies [8,9], are tabulated in Table I. The $\{11\bar{2}1\}$ TD exhibits a slightly smaller Burgers vector length compared with the $\{10\bar{1}2\}$ TD, as reflected by the relative magnitudes of the elastic strain fields that they induce [Figs. 2(c) and 2(d)]. However, the step height of the $\{11\bar{2}1\}$ TD is significantly smaller than that of the $\{10\bar{1}2\}$ TD. The heights of the $\{11\bar{2}1\}$ and $\{10\bar{1}2\}$ TDs are half of a lattice plane and two lattice planes, respectively. Figure 2(a) exhibits the four-atomic-layer

step feature of a $\{10\bar{1}2\}$ TD, whereas in Fig. 2(b), the step feature of the $\{11\bar{2}1\}$ TD is more subtle.

B. Twin thickening under shear deformation

During shear deformation, the shear stress of the system builds up elastically with the increase of applied strain, until it is accommodated by the nucleation and/or propagation of TDs, which results in twin boundary growth normal to the twin boundary plane (twin thickening). Figure 3 shows an example at 300 K, illustrating how the stress of the system and the average twin boundary position change during the shear simulation, as well as the atomistic structure of the TD that formed spontaneously under shear stress, for both $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins.

At the initial stage of deformation, the stress of the $\{10\bar{1}2\}$ twin increases elastically as the strain increases, which is then followed by a sharp drop in the stress-strain curve when the stress reaches about 450 MPa [Fig. 3(a)]. Correspondingly, the average twin boundary position of the $\{10\bar{1}2\}$ twin stays almost unchanged at the initial stage of the shear simulation, and then a rapid displacement of about 4 Å occurs in the average twin boundary position at the time the stress drops [Fig. 3(a)], which is consistent with the height of a $\{10\bar{1}2\}$ TD (Table I). The inspection of the structure at the stage when the drastic change of stress and average twin boundary position occurs verifies that these changes are due to the nucleation and propagation of the $\{10\bar{1}2\}$ TD loop [Fig. 3(c)]. The TD loop(s) expand quickly under the applied stress, as the stress and average twin boundary position curves are almost vertical in the given time scale at about 0.6% strain in [Fig. 3(a)], until the annihilation with its periodic image due to the finite supercell size. The nucleation and propagation of the disconnection loop lead to the thickening of the twin by two $\{10\bar{1}2\}$ lattice layers. Due to the macroscopic shear associated with

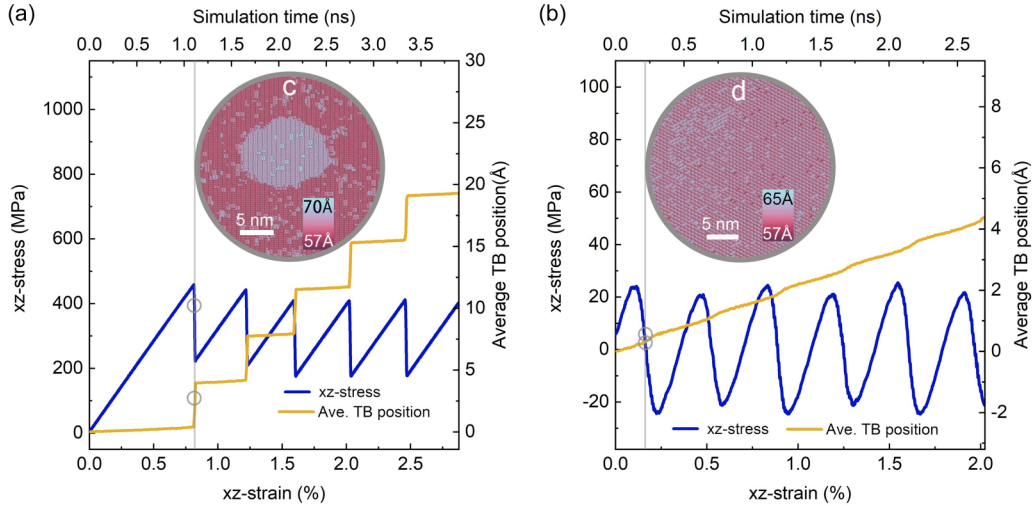


FIG. 3. Stress-strain curves (blue, with values given by the left vertical axis) and twin boundary displacement (yellow, with values given by the right vertical axis) during shear deformation at 300 K, as well as the structure of the TD loop structures viewed looking top-down on the twin boundary plane. (a) $\{10\bar{1}2\}$ twin, (b) $\{11\bar{2}1\}$ twin. (c) Disconnection loop at $\{10\bar{1}2\}$ twin boundary. (d) Disconnection steps at $\{11\bar{2}1\}$ twin boundary. The vertical gray lines and intersection circles indicate when the snapshots of the structures were taken. Twin boundary atoms that are shown in (c) and (d) are colored according to their z -coordinates, with the scale for the color bars shown in the figures. (c) and (d) are projected on the twin boundary plane.

twinning, the applied shear strain is compensated by the newly grown twin layers, so the drop of stress is observed on the stress-strain curve in [Fig. 3(a)].

By comparison to the results for the $\{10\bar{1}2\}$ twin, the $\{11\bar{2}1\}$ twin boundary exhibits different responses under applied shear deformation [Fig. 3(b)]. We consider first the stress-strain curve, where a stress drop occurs at approximately 30 MPa, which is much smaller than the corresponding value of 450 MPa for the $\{10\bar{1}2\}$ twin. In addition, the stress drops relatively smoothly, indicating that the thickening of the $\{11\bar{2}1\}$ twin is a gradual and continuous process beyond the critical stress. Further, the stress reaches a negative value at its lowest point. We interpret the origin of these negative shear stresses as follows. Due to the macroscopic shear nature of the twin (Table S1, Fig. S5), the growth of a new twin layer generates internal shear stress within the simulation box (Fig. S6). The twinning shear that the newly grown layer induces is fixed by its crystallography. Using the magnitude of shear value, the dimensional information, the elastic shear modulus of the system (Fig. S7), the shear stress resulting from twin growth can be calculated (Table S2). The calculated shear stress values are 318 MPa and 62 MPa for the $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins, respectively, which are in close agreement with the stress drop magnitudes observed in simulations (Fig. 3). The deviation is attributed to the stress fluctuations of the system. Due to the periodic boundary conditions and the attractive force between TD segments with opposite signs, the TD tends to rapidly expand across the entire twin boundary once nucleated, causing the stress in the $\{11\bar{2}1\}$ twin system to drop to negative values. Similar behaviors have been observed in the $\{10\bar{1}2\}$ twin at higher temperatures [Fig. 4(a)].

We consider next the average twin boundary position for the $\{11\bar{2}1\}$ twin during the portion of the simulation where a relatively smooth transition is observed. No clear boundary of a $\{11\bar{2}1\}$ TD ‘loop’ can be recognized visually in the atomistic

simulations. Instead, scattered TD steps are observed, consistent with a rough twin boundary interface. The roughness of the twin boundary is maintained not only when the stress drops, but also during the whole simulation process. It is worth noting that the change of the average twin boundary position in one periodic cycle of the stress versus strain plot is consistent with the height of a $\{11\bar{2}1\}$ TD. In addition, at lower temperature (100 K) and with larger twin boundary area [100 nm (x) $\times$ 60 nm (y)], a more recognizable boundary of a $\{11\bar{2}1\}$ TD ‘loop’ is observed (Fig. 6). These results seem to imply that at 300 K, multiple TDs nucleate by the time the maximum shear stress is reached and that these nuclei grow and coalesce to advance the twin boundary plane.

C. Temperature effects on twin thickening

Since the nucleation of the TDs is expected to be a thermally activated process, temperature should have a significant influence on the simulation results [29]. Stress-strain curves and twin boundary displacement curves at varying temperatures for $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins are shown in Fig. 4. It should be noted that the strain rate would also influence the stress responses and TD nucleation behavior. In this section, we present simulations at different temperatures, at the same strain rate of $1.1 \times 10^7 \text{ s}^{-1}$. In addition, a test case with a lower strain rate of $1.1 \times 10^6 \text{ s}^{-1}$ leads to a negligible change in the stress-strain curve for the $\{11\bar{2}1\}$ twin at 300 K (Fig. S2). Therefore, we assume the strain rates that are used in this work are appropriate for the study of temperature effects on the twin thickening behavior.

At lower temperatures, larger shear stresses are required to form the disconnection. At higher temperatures, the twin boundary displacement curves become smoother, and the critical shear stresses required for disconnection loop formation are smaller. Especially, the $\{11\bar{2}1\}$ twin at 600 K and higher

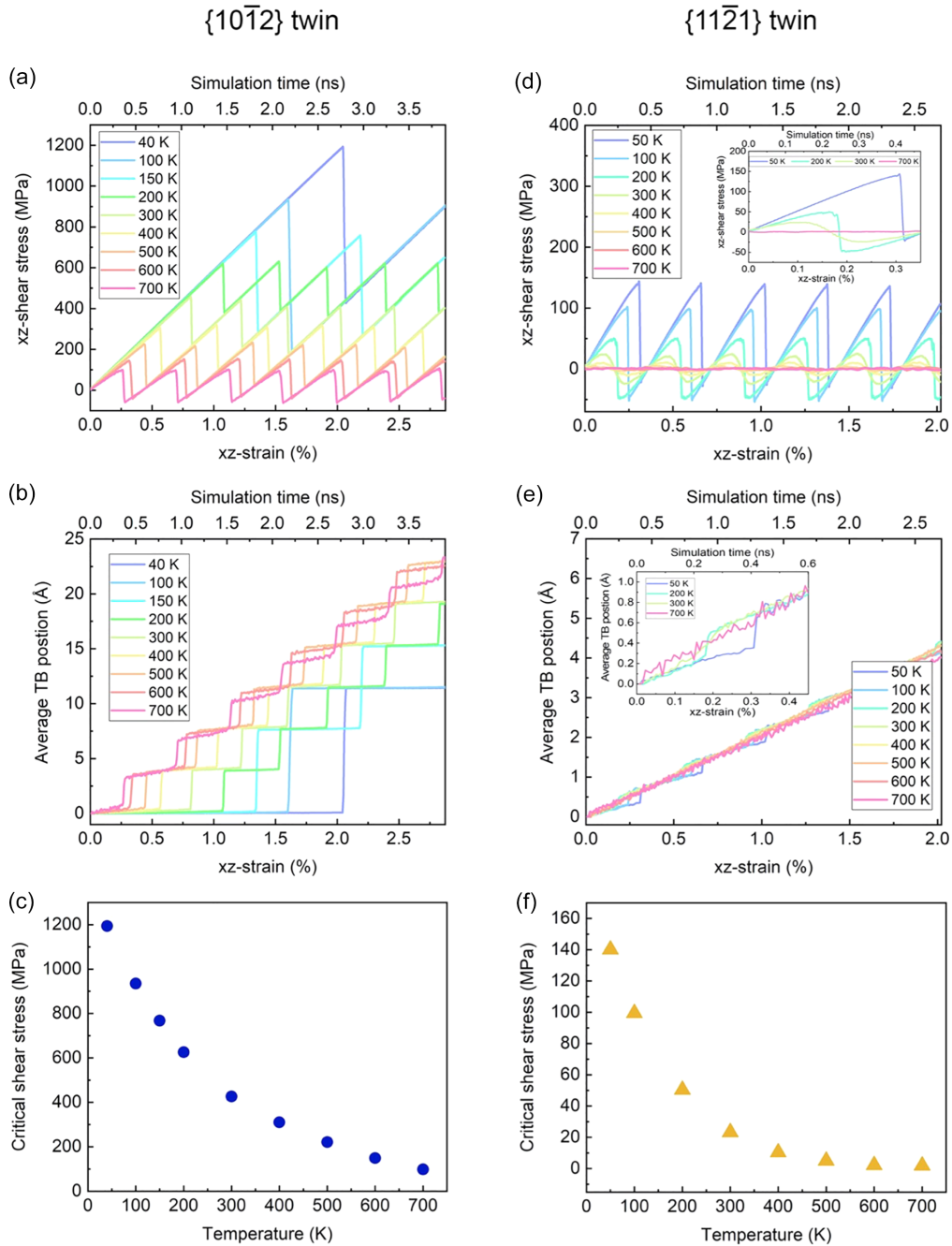


FIG. 4. Stress responses and average twin boundary position changes of $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins under applied shear deformation at different temperatures (a), (b), (d), and (e), as well as the critical shear stress required for twin thickening at different temperatures (c) and (f). The critical stresses in (c) and (f) are the averages of the local maximum stress value(s) before the stress drops that are plotted in (a) and (d), respectively. The standard errors of the critical stresses (when multiple data points are involved) are less than 10 MPa for the $\{10\bar{1}2\}$ twin, and less than 2 MPa for the $\{11\bar{2}1\}$ twin. The left panel and right panel correspond to the $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins, respectively.

temperatures requires a very small critical shear stress for TD nucleation and growth [Fig. 4(d)], and the twin can accommodate applied shear deformation smoothly through twin thickening. This behavior is qualitatively consistent with the behavior of a rough interface where pre-existing fluctuations in twin boundary height can grow under the applied stress (the possibility of twin boundary roughening is discussed in the next section). Generally, the critical shear stresses for twin thickening decrease as temperature increases for both twinning modes, and the $\{11\bar{2}1\}$ twin requires much lower stress

than the $\{10\bar{1}2\}$ twin to activate twin thickening [Figs. 4(c) and 4(f)].

Moreover, when the temperature is less than or equal to 150 K, multiple layers of TDs form sequentially in one stress drop event for the $\{10\bar{1}2\}$ twin, and the twin boundary displacement is correspondingly twice (at 150 K) or three times (at 50 K and 100 K) that of the TD height [Fig. 4(b)]. The structures of multilayer TD loops at 150 K are shown in Fig. 5. At 300 K, even though there is no observation of the formation of multilayer TD structure, multiple TD loops are observed to

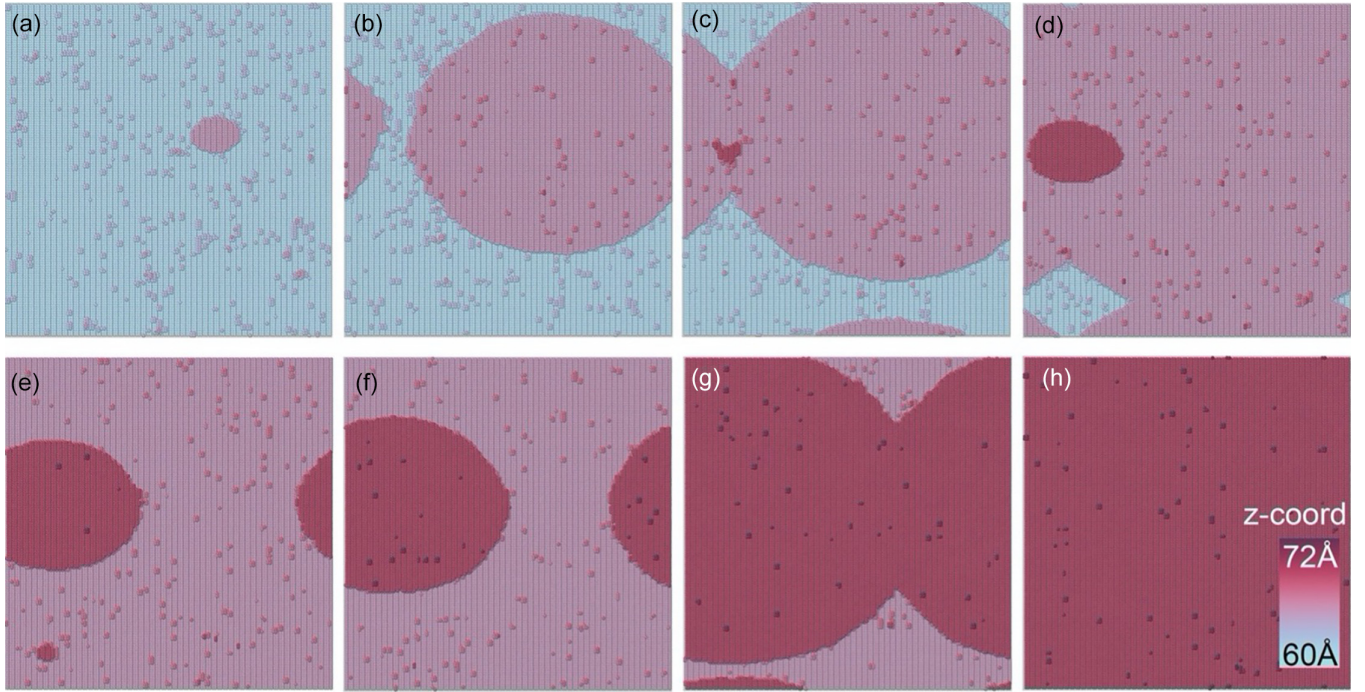


FIG. 5. Sequential snapshots of twin boundary structure showing the formation of two layers of $\{10\bar{1}2\}$ TD loops forming during one stress drop at 150 K. Twin boundary atoms are projected onto the twinning plane and are colored according to their z -coordinates, with the scale bars for the coloring shown in the lower right of panel (h).

form at the same lattice layer (Fig. S1 [31]), which doesn't occur at 400 K or higher temperature. Since the thickening of the twin includes the nucleation and propagation of TD loops, the observation of temperature dependence of the occurrences of multilayer or multiloop TD structure implies that TD propagation velocity varies more rapidly with temperature than the TD loop nucleation rate for the $\{10\bar{1}2\}$ twin.

Although the shapes of the twin boundary displacement curves show differences at different temperatures for both the $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twins [Figs. 4(b) and 4(e)], the amount

of twin boundary displacement in one periodic stress cycle remains almost the same for all temperatures (except for the low-temperature $\{10\bar{1}2\}$ twin cases, where two or three TDs form in one stress drop event), which is consistent with the corresponding TD height. Further, the amount of applied shear strain that the newly grown layer(s) of twins accommodate is consistent with the Burgers content of the corresponding TD. This consistency is the basis for the conclusion that the twin thickening was caused by disconnection nucleation over most of the investigated temperature range and is not the result of twin boundary sliding or nucleation of different types of possible TDs.

D. Twin boundary structures at varying temperatures

The equilibrium twin boundary structures at different temperatures were investigated in order to obtain a better understanding of the TD loop nucleation process due to thermal activation. Atomic shuffling is required in the twin thickening process to restore the atomic arrangement from the parent orientation to the twin orientation. And, the initial shuffling to form the nucleus of the TD loop is assisted by thermal activation. Thus, it is of great importance to study twin boundary structure at varying temperatures.

Here, the relative roughness of the twin boundary interface is defined as the standard deviation of the z -coordinate of twin boundary atoms divided by the height of the corresponding TD. And, the relative roughness of both twinning modes at different temperatures is plotted in Fig. 7(m). The relative roughness of the $\{10\bar{1}2\}$ twin is close to zero when the temperature is near 0 K, because the twin boundary only contains one atomic plane of atoms, and there are

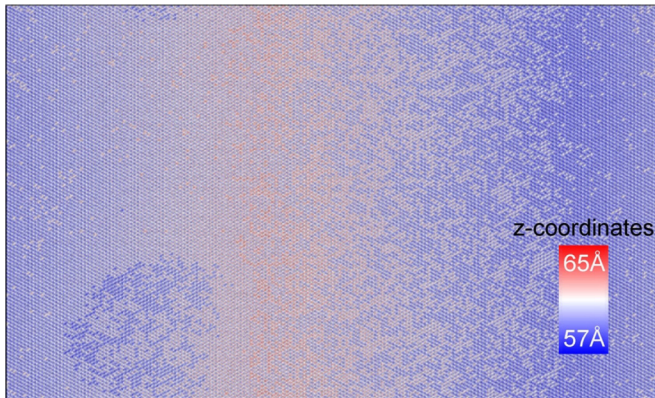


FIG. 6. A snapshot of the $\{11\bar{2}1\}$ twin boundary featuring a disconnection loop at the lower left. The simulation is run at 100 K with the area of the twin boundary being 100 nm (x) $\times$ 60 nm (y). Twin boundary atoms are projected onto the twinning plane and are colored according to their z -coordinates (z axis is normal to the twin boundary plane).

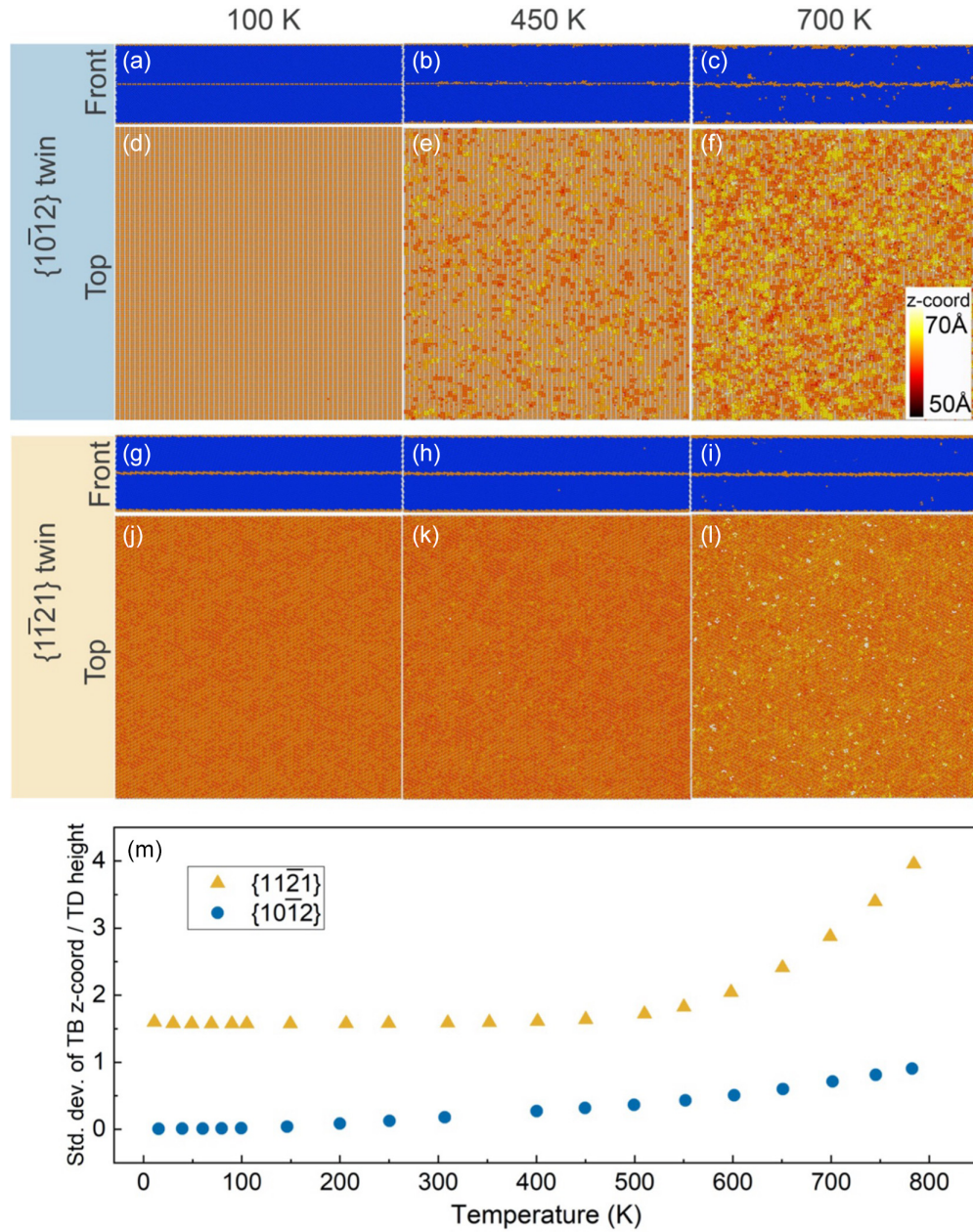


FIG. 7. Twin boundary structures at 100 K, 450 K, and 700 K for $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twin (a)–(l), and relative roughness value of $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twin boundary as a function of temperature (m). Atoms in the front view panels (a)–(c), (g)–(i) are projected parallel to the twin boundary planes and are colored according to coordination through the OVITO package [28], where atoms that are labeled in blue have HCP coordination, while atoms that are labeled in orange are recognized as non-HCP coordination. Twin boundary atoms are projected onto the twinning plane in the top view panels (d)–(f), (j)–(l), and are colored according to their z-coordinates, with the scale bars for the coloring shown in the lower right of image (f). Enlarged front view images of the twin boundary structures (a)–(c), (g)–(i) are provided in the Supplemental Material [31].

minimal thermal fluctuations. As the temperature is increased, the relative roughness steadily increases. The $\{11\bar{2}1\}$ twin boundary exhibits a nonzero relative roughness value near zero temperature, which originates from the special distorted icosahedron structure of the $\{11\bar{2}1\}$ twin boundary [25], such that multiple planes of atoms have non-HCP coordination at the twin boundary. This relative roughness is maintained almost unchanged throughout the range from near 0 K to 500 K, and starts to gradually increase after 500 K for both twin types.

Figures 7(a)–7(l) demonstrate snapshots of the atomic structures of the $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twin boundaries at 100 K, 450 K, and 700 K, respectively. While the twin boundary interface is flat for the $\{10\bar{1}2\}$ twin at 100 K [Fig. 7(d)], there are scattered steps that are one atomic plane higher on the $\{11\bar{2}1\}$ twin boundary, even at this low temperature [Fig. 7(j)]. The multiplane feature and the nonflat surface make the $\{11\bar{2}1\}$ twin boundary intrinsically rougher than the $\{10\bar{1}2\}$ twin boundary at low temperature. At 450 K, fluctuations of atomic positions on the $\{10\bar{1}2\}$ twin boundary are up

to a few atomic planes in height, while for the $\{11\bar{2}1\}$ twin boundary, the relative roughness value at this temperature is still mainly caused by the multiple twin boundary plane feature of the intrinsic twin boundary structure, and the amount of fluctuation in the z -direction is similar to that in 100 K. At 700 K, the fluctuations on the $\{10\bar{1}2\}$ twin boundary are larger than the lower temperature ones, and steps with heights that scale with TD height are observed [Fig. 7(c)], which can be potential sites for TD loop formation and growth. For the $\{11\bar{2}1\}$ twin, while the standard deviation of twin boundary z -coordinates is slightly smaller than that of the $\{10\bar{1}2\}$ twin, the relative roughness of the $\{11\bar{2}1\}$ twin boundary is large, indicating the easy formation of TD.

IV. DISCUSSION

One major difference between the two twinning modes concerning twin thickening under applied shear deformation is that the $\{11\bar{2}1\}$ twin requires much lower critical shear stress for twin thickening. The critical shear stress for $\{11\bar{2}1\}$ twin thickening is approximately 10% of that for the $\{10\bar{1}2\}$ twin at all temperatures investigated in this work. At higher temperatures (larger than 600 K), the critical stress for twin thickening for the $\{11\bar{2}1\}$ twin essentially vanishes, and the twin can accommodate the applied shear strain continuously with a nearly linear stress-velocity relationship consistent with a rough interface.

We propose that the reasons for the critical shear stress differences are twofold. First, the different TD geometrical factors, dictated by the twin boundary crystallography, contribute to the critical shear stress differences. Specifically, the $\{11\bar{2}1\}$ TD exhibits a much smaller step height than the $\{10\bar{1}2\}$ TD. The Burgers contents of these two TDs are similar, which is anticipated to result in similar long-range elastic effects. The difference in atomic shuffling, which involves a different number of atomic layers, is considered the key reason for the energy barrier difference of TD nucleation. Through our analysis of the atomic position changes during TD formation, we found that certain atoms need to shuffle to specific positions to form a $\{10\bar{1}2\}$ TD dipole, whereas the formation of a $\{11\bar{2}1\}$ TD dipole mainly requires a uniform shift between two half-crystals plus a slight adjustment of atomic positions near the twin boundary (see Fig. S4 in Supplemental Material [31]). Therefore, the relatively simple shuffling of $\{11\bar{2}1\}$ TD appears to make its formation lower in energy. Second, the intrinsic roughness of the $\{11\bar{2}1\}$ twin boundary structure is beneficial to the TD formation. The multiplane feature and the nonflat surface of the $\{11\bar{2}1\}$ twin boundary result in easy TD nucleation. For the $\{11\bar{2}1\}$ twin at moderate temperature, the results indicate the presence of existing TDs, consistent with a rough interface, such that the stress to nucleate TDs is diminished.

Our study suggests that $\{11\bar{2}1\}$ twin thickening requires a lower critical shear stress than for the $\{10\bar{1}2\}$ twin. Nevertheless, $\{11\bar{2}1\}$ deformation twinning is less commonly observed in HCP metals relative to the $\{10\bar{1}2\}$ system. A possible explanation is that the $\{11\bar{2}1\}$ twin exhibits a higher energy barrier concerning other parts of the twinning process, such as twin nucleation. Because the $\{11\bar{2}1\}$ twin is distinguished by the large magnitude of shear, we surmise that it will hinder

twin nucleation [14,30] and that this nucleation barrier is an important factor limiting $\{11\bar{2}1\}$ twin development in HCP metals. Our previous work also shows that the predominance of $\{11\bar{2}1\}$ twinning in HCP Re can be possibly explained by the combination of low twin boundary energies and high elastic moduli that enable a $(\mathbf{c} + \mathbf{a})$ dislocation to be a potential $\{11\bar{2}1\}$ twin nucleation source, such that $\{11\bar{2}1\}$ twin nucleation is easier in Re than in other metals [26]. Therefore, promoting $\{11\bar{2}1\}$ twin nucleation through methods such as adding alloying elements to reduce the $\{11\bar{2}1\}$ twin boundary energy may be an effective way to introduce more $\{11\bar{2}1\}$ twins to the materials and influence work hardening behavior toward the control of the strength and ductility combination.

V. CONCLUSIONS

Molecular dynamics techniques were used to investigate $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ twin thickening processes through spontaneous TD loop nucleation under applied shear deformation with a constant strain rate of 10^7 s^{-1} . The stress responses and structures at varying temperatures of both twins were studied. The analysis leads to the following conclusions:

(1) Both twins thicken through TD formation. The $\{10\bar{1}2\}$ TD loops were observed during the twin thickening process. On the contrary, no clear boundary of a $\{11\bar{2}1\}$ TD ‘loop’ can be recognized due to the small step height feature of the $\{11\bar{2}1\}$ TD. The $\{11\bar{2}1\}$ twin boundary exhibits a corrugated interface throughout the simulation. Both twin boundaries become structurally rougher at higher temperatures.

(2) The $\{11\bar{2}1\}$ twin requires much lower critical shear stress for twin thickening (around 10% of that for the $\{10\bar{1}2\}$ twin), which is likely due to the differences in geometrical factors of the TDs and the roughness of the twin boundary structure.

(3) The low critical shear stresses required for twin thickening for $\{11\bar{2}1\}$ twin indicate that $\{11\bar{2}1\}$ twin thickening exhibits a relatively low energy barrier. Especially at high temperatures, very small critical shear stress for TD nucleation and growth is observed. As a result, promoting $\{11\bar{2}1\}$ twin nucleation can be an effective way to introduce more $\{11\bar{2}1\}$ twins to HCP materials.

ACKNOWLEDGMENTS

Portions of this work were initiated during the Ph.D. studies of LJ at the University of California, Berkeley, and were supported by the Office of Naval Research under Grant No. N00014-16-1-3124. This research is supported by computational resources provided through the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by the National Science Foundation Grant No. ACI-1548562, and the Savio computational cluster resource provided by the Berkeley Research Computing program at the University of California, Berkeley.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not

technically feasible, and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of

this research project. The data are available from the authors upon reasonable request.

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- [31] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/kdll-phvv> for details related to computing the stress of the system, observation of multiple TD loops, stress responses of the system at different applied shear strain rates, schematics of atomic shuffling required by $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$ TD formation, shear deformation analysis induced by twin growth, twin boundary energies, additional snapshots of TD nucleation and propagation, etc.