



Full length article

Columnar grain-driven plasticity and cracking in nanotwinned FCC metals

Qiongjiali Fang^a, Frederic Sansoz^{a,b,*}^a Department of Mechanical Engineering, The University of Vermont, Burlington, VT 05405, USA^b Materials Science Program, The University of Vermont, Burlington, VT 05405, USA

ARTICLE INFO

Article history:

Received 13 February 2021

Revised 26 March 2021

Accepted 20 April 2021

Available online 24 April 2021

Keywords:

Coherent twin boundary

Grain boundary plasticity

Columnar grain

Nanotwinned metals

Molecular dynamics simulations

ABSTRACT

The mechanisms of strengthening and plasticity in columnar-grained metals with preferentially oriented nano-sized twins have been examined traditionally by considering dislocation processes, but rarely from the perspective of grain boundary (GB) deformation. Here, the effects of GB strain accommodation on plastic deformation in four different columnar-grained nanocrystalline nanotwinned (nt) face-centered-cubic metals (Cu, Ag, Al, and Ni) were studied by large-scale molecular dynamics simulations. It is observed that in tensile deformation parallel to coherent twin boundaries (CTBs), the dislocation mechanisms in each metal are identical and associated with GB emissions of jog and threading dislocations at small and large CTB spacings, respectively. However, CTB strengthening effects are increasingly more pronounced in columnar-grained nt metals as their shear modulus increases, which is rationalized by the dependence of GB stress concentrations on twin size, metal type and strain rate. Also, while flow stresses in nt-Cu, nt-Ag, and nt-Al metals increase linearly with decreasing CTB spacing, a maximum strength limit is reached in nt-Ni below a critical CTB spacing of 6 nm. The strength limit in nt-Ni results from columnar GB cracking induced by prominent GB sliding. For columnar-grained microstructures, GB sliding is equivalent in nt-Ag and nt-Al and slightly lower in nt-Cu but markedly higher in nt-Ni. These findings underscore the importance of new GB deformation mechanisms on plasticity and fracture in columnar-grained nt metals and enrich our understanding of CTB strengthening in fcc metals synthesized in the literature.

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1. Introduction

Nanotwinned (nt) face-centered cubic (fcc) metals with nanoscale coherent twin boundaries (CTBs) inside ultrafine grains have demonstrated an excellent combination of superior strength and ductility, compared to their twin-free polycrystalline counterparts, by tuning two microstructure dimensions, the twin boundary spacing (TBS or λ) and the average grain size (d) [1–8]. For instance, bulk nt-Cu metals with equiaxial grains exhibit a maximum strength (~1 GPa) and uniform tensile elongations (14%) before failure with $d \sim 500$ nm and $\lambda \sim 15$ nm [3]. Recently, sputter-deposited nt-Ag metals have reached hardness values up to 3 GPa for a range of $\lambda < 7$ nm when $d \sim 50$ nm [9], which is well above any previous hardness record in this metal (~2 GPa). In addition, the low excess energy of coherent nanoscale twins is known to maintain excellent electrical and thermal conductivities [1,9–11], and improve corrosion and radiation resistance [12–14].

In nt fcc metals with equiaxial grains, three typical dislocation mechanisms have been associated with different hardening and softening effects [15,16]. In slip mode I, dislocations glide on a slip plane at 70.5 degrees to the CTB plane and directly intersect them. Higher stresses are thus required to overcome the impediment of dislocation propagation by CTBs, leading to significant hardening. In slip mode II, dislocations are also on a slip plane at 70.5 degrees but propagate toward the opposite GB with a slip vector parallel to CTBs. These paperclip-like *threading* dislocations result in moderate hardening from drag [17] but extend fatigue life [18]. In slip mode III, dislocations only glide on the CTB plane or planes adjacent to it. These *twinning* partials lead to detwinning, which is a softening mode. In general, good ductility in nt metals has been attributed to the intrinsic ability of CTBs to serve as dislocation sink and nucleation or to accommodate plastic strain through detwinning and CTB sliding, similar to conventional GB motion under stress [19–24].

However, a microstructure with (111)-textured columnar grains is more commonly synthesized in pure nt fcc metal films, because CTBs tend to align perpendicular to the growth direction during

* Corresponding author.

E-mail address: frederic.sansoz@uvm.edu (F. Sansoz).

direct-current electrodeposition and magnetron sputtering [8,25]. Compared to equiaxial nt fcc metals with random grain boundaries (GBs), significant plastic anisotropy is found with those (111) textured columnar grains [26–28]. Interestingly, a new mode II slip – a jog dislocation with necklace-like shape that expands across all twin layers connected by a stair-rod dislocation at each CTB [17] – gives rise to continuous strengthening and maintain ductility in columnar grained nt-Cu with small TBS < 2.5 nm. By contrast, however, a ductile-to-brittle transition has been observed in uniaxial deformation of single crystalline nt-Cu nanopillars and nt-Au nanowires containing similarly small twins [29,30], suggesting that there may be intrinsic plasticity mechanisms associated with GB deformation in columnar-grained nt metals. In an earlier study, Zhang et al. [31] hypothesized that the reduced tensile ductility of columnar-grained nt-Cu, compared to that of nt-Cu with equiaxial grains, could be ascribed to a difference in stress-assisted GB sliding, which has been a well-known cause for Hall-Petch breakdown induced by large GB volume fractions at small grain sizes in nanocrystalline Cu [32].

GB sliding has proven essential for a broad understanding of polycrystal plasticity from high-temperature creep in coarse-grained materials [33–35] to low-temperature plasticity and cracking in nc fcc metals [32,36–38] and alloys [39,40]. Yet the intrinsic contribution of GB sliding to the plasticity of nt metals has not been thoroughly investigated so far, except for a few atomistic simulation studies aimed at quantifying GB deformation in nt metals. Tucker et al. [41] employed non-local kinematic metrics to separately investigate the amount of strain accommodated by CTB migration, dislocation nucleation, dislocation glide, and GB-mediated plasticity in columnar-grained Cu metals with and without CTBs. They concluded that the introduction of CTBs changed the primary strain accommodation mechanism from dislocation slip to CTB migration, and that GB strain localization alone increased from 10% to 15%. Furthermore, Ke et al. [9,42] analyzed the local atomic shear strain at GBs in equiaxial grained nt-Ag alloys with $d = 50$ nm and found a pronounced increase in GB sliding rate as the CTB spacing λ was decreased, leading to a strength maximum. While direct experimental evidence of GB sliding in plastic deformation of nt metals remains limited, a recent study in textured nt-Cu films [43] has found some noticeable increase in GB strain leading to columnar grain rotation under tensile deformation at room temperature, which could be indicative of specific columnar-grain GB sliding activity.

In this article, large-scale MD simulations were used to examine how twin size and metal type influence both dislocation and GB sliding processes during plastic deformation of four columnar-grained models in pure nt-Ag, nt-Cu, nt-Al and nt-Ni metals. Our simulation results show good qualitative agreement with the reported experimental data across different sputter-deposited nt fcc metals and point to the importance of GB sliding on metal-dependent plasticity and cracking mechanisms in columnar-grained nt fcc metals.

2. Computational methodology

Our MD simulations were performed using the software LAMMPS [44] with the embedded-atom-method (EAM) potentials for Ag-Cu alloys by Williams et al. [45] and Al-Ni alloys by Mishin et al. [46]. Table 1 shows that stacking-fault energies simulated by these potentials [47] were in good agreement with ab-initio data [48–52] in Al and Ni, but were lower for Cu and Ag. The ratio of the stacking-fault energy γ_S and the unstable stacking fault energy γ_{US} , i.e. the energy barrier associated with the formation of a Shockley partial dislocation, is generally considered important for predicting the nucleation of complete vs. partial dislocations [53], and dislocation–twin interaction processes [54–56]. Table 1 shows

that the EAM potentials in this study predicted γ_S / γ_{US} values ranging from 1.2 in Al to 25.5 in Ag, suggesting that this large difference could potentially result in dissimilar dislocation mechanisms between these metals.

Atomistic structures with ten nt columnar grains in fcc Ag were created using a two-dimensional (2D) Voronoi tessellation scheme [57]. The grain centers were randomly placed inside a xy plane and then the grain regions were extruded along the normal direction z. The average in-plane grain size for the Ag models was around 20 nm. Dimensions of the simulation box were 64 nm $\times$ 64 nm $\times$ 28 nm in the x, y, z directions, respectively, with a total of 6.25 million atoms, as shown in Fig. 1(a). The boundary conditions were periodic in all three directions throughout the simulation. The crystallographic orientation of each grain in z direction was ± 5 degrees to [111], and random in x and y directions. Majority of GBs exhibited a high-angle character, with some low-angle exceptions. Each grain contained evenly distributed CTBs, but the CTB were randomly shifted in the z direction from one column to another, to avoid the alignment of two CTBs on the same plane across a single GB, similar to columnar-grained nt microstructures observed experimentally. The TBS simulated were equal to 1.41 nm, 2.12 nm, 3.53 nm, 4.94 nm, 6.99 nm, 9.08 nm, and 14.06 nm. Identical models of nt-Cu, nt-Al and nt-Ni metals were created from those in nt-Ag by proportionally scaling the atom position, TBS and grain size based on the difference in lattice constant (Cu – 3.615 Å, Ag – 4.09 Å, Al– 4.05 Å, Ni – 3.52 Å).

The potential energy of all models was minimized at 0 K by conjugate gradient method, then relaxed by MD at 450 K for 50 ps, and cooled from 450 K to 300 K at a rate of 2×10^{12} K $\cdot$ s $^{-1}$ using an isothermal-isobaric ensemble (NPT) integration with zero pressure enforced in each direction. The models were thermally equilibrated further at 300 K for 50 ps before deformation. For all metals, uniaxial tensile deformation was simulated by stretching the box in the x direction at an engineering strain rate of 2×10^8 s $^{-1}$ at 300 K until 10% strain, under NPT with zero pressure maintained along the y and z directions. The MD timestep used was 5 fs. Also, to examine the strain-rate sensitivity, four different strain rates between 1×10^8 s $^{-1}$ and 1×10^9 s $^{-1}$ were simulated for only nt-Cu and nt-Ni models.

The tensile stress was calculated by adding the corresponding Virial-theorem stress component along the x-axis of all atoms and dividing by the volume of the simulation box. The flow stress was computed by averaging the tensile stresses at strains ranging from 4% – 10%. Common neighbor analysis (CNA) in the software OVITO [58] was used for visualization of GBs, TBs and dislocations in the model. In the following, atoms with fcc, hcp, and other coordination were colored in green, red, and grey, respectively. The atomic von-Mises shear strain was calculated in OVITO, using the fully annealed model before deformation as a reference. The nearest neighbor cutoff used for Cu, Ag, Al, and Ni was 3.086 Å, 3.496 Å, 3.458 Å, and 3.005 Å, respectively. GB atoms were identified by cutting a wall of 1 nm in thickness for nt-Ag (the wall thickness was proportional in nt-Cu, nt-Al and nt-Ni based on the difference in lattice constant) by Voronoi tessellation with the grain center coordinates recorded before annealing, as shown in Fig. 1(b). This wall thickness was chosen as it included all atoms with unknown coordination in the GB and excluded most fcc atoms, CTBs, and dislocations in the grain. With this method, GB atoms accounted for ~10% of atoms in the model. Each GB atom ID was recorded to calculate the GB accommodated strain, as the average of atomic von-Mises shear strains over all GB atoms, and GB free volume, as the average excess free volume (atomic volume subtracted by atomic volume of the single crystalline phase) of the GB atoms. Atomic volumes were calculated using the Voronoi package in LAMMPS. The atomic-level strain at GBs is generally employed to characterize a variety of GB deformation mechanisms numerically [39,41],

Table 1

Properties of some common fcc metals from semi-empirical EAM potentials used in this study [47] and density-functional-theory data in the literature [48–52]. $\mu_{(111)}$, γ_s , and γ_{us} represent the shear modulus on the (111) plane, the stacking-fault energy, and the unstable stacking-fault energy, respectively. The parameter K^{crit} is the critical stress intensity required to nucleate a partial dislocation from a GB stress concentration based on Eq. (1) with a Poisson's ratio of $\nu \approx 1/3$ for all metals. *As an approximation, the shear modulus was considered identical between Cu and Cu-3.7wt.%Al.

Metal	Embedded-atom method			Density-functional theory			$\mu_{(111)}$ (GPa)	K^{crit} (MPa·m ^{1/2})
	γ_s (mj/m ²)	γ_{us} (mj/m ²)	γ_{us}/γ_s	γ_s (mj/m ²)	γ_{us} (mj/m ²)	γ_{us}/γ_s		
Al	144.8	166.7	1.2	130	162	1.2	24.1	0.108
Ni	123.6	365.5	3.0	110	273	2.5	63.6	0.228
Cu	7.6	60	7.9	41	181	4.4	45.2	0.157
Ag	1.5	38.3	25.5	18	133	7.4	23.8	0.097
Cu-3.7wt.%Al	-	-	-	7	169	24.1	45.2*	0.151

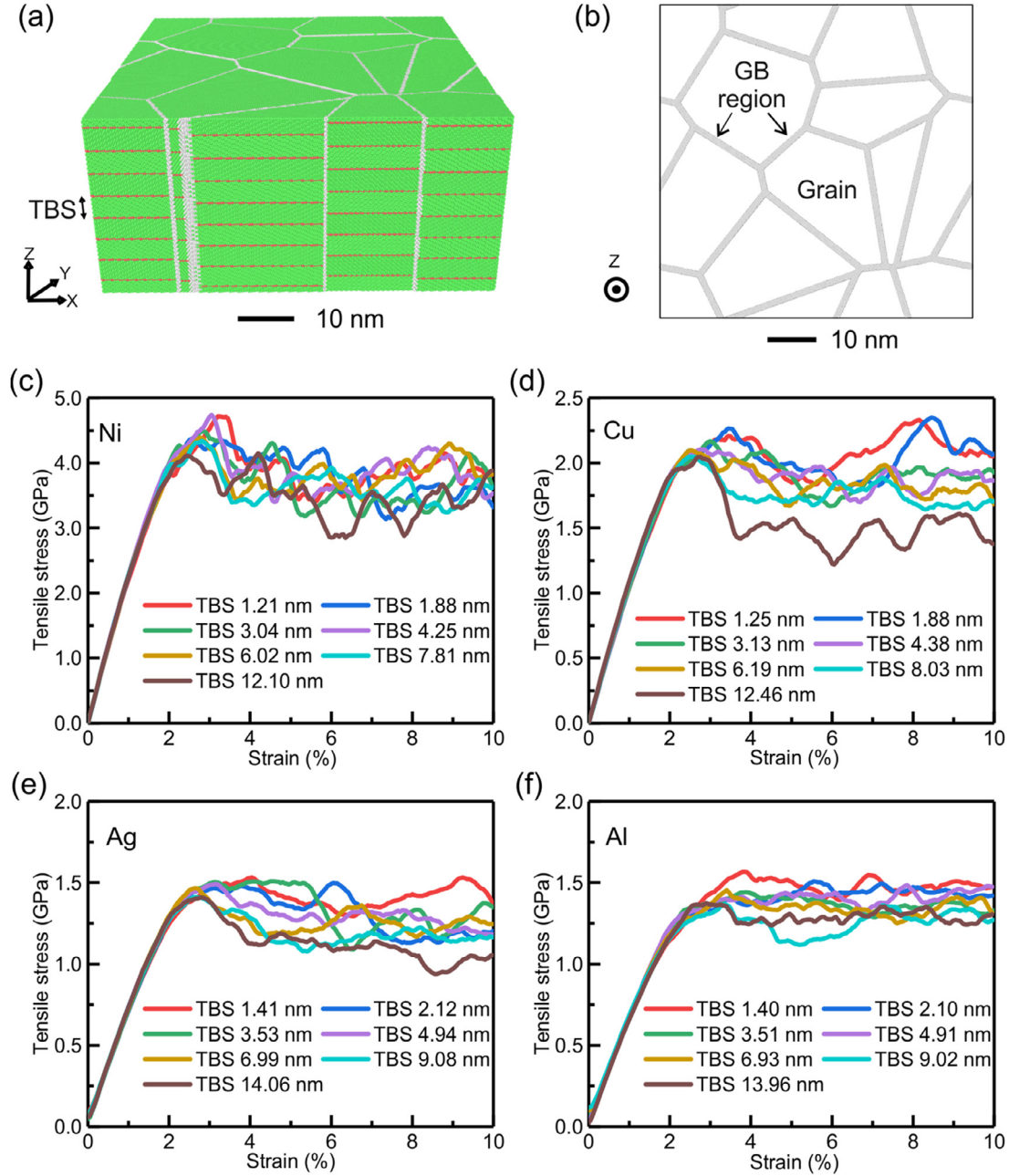


Fig. 1. MD simulation of columnar-grained nt-Ni, nt-Cu, nt-Ag, and nt-Al with different twin boundary spacing (TBS) under tensile deformation at 300 K and strain rate of $2 \times 10^8 \text{ s}^{-1}$. (a) Atomistic model of nt-Cu with TBS = 4.38 nm. Green, red, and grey colors represent hcp, fcc, and other uncoordinated atoms, respectively. (b) Identification of GB atoms using a 1-nm-thick slice along the GB lines. (c–f) Simulated stress – strain curves for tension along x direction as a function of TBS. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

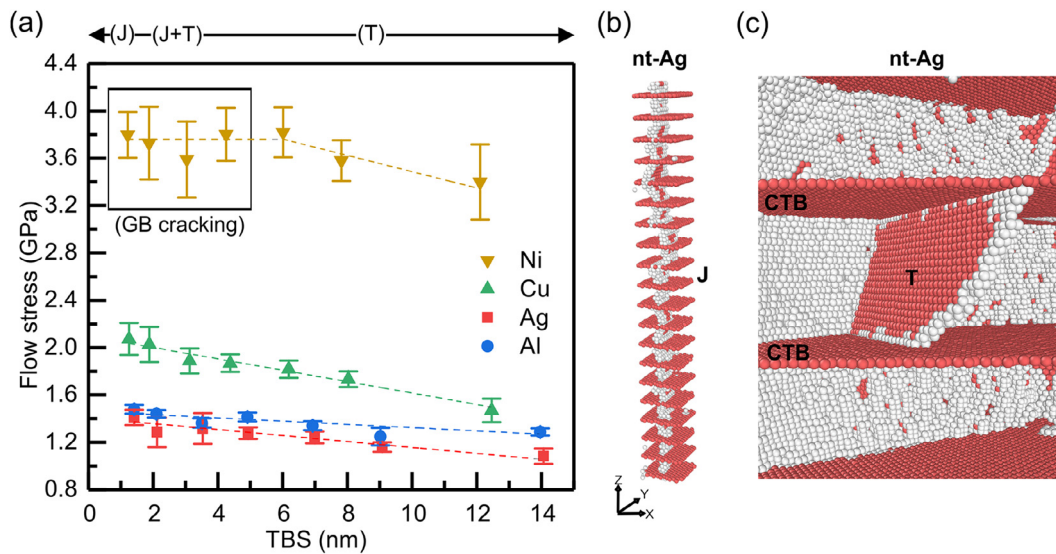


Fig. 2. Flow stress and dislocation mechanisms as functions of twin size and metal type. (a) Flow stress, the average stress in a strain interval from 4% to 10%, for nt-Ni, nt-Cu, nt-Ag and nt-Al. Error bars show the standard deviation of tensile stress over this range of strain. Inset: Cracking is observed in nt-Ni with TBS < 6 nm, when a constant strength plateau becomes visible. (b) Jog (J) dislocation, a dislocation mechanism observed only at smaller TBS. (c) Threading (T) dislocation, the dislocation mechanism observed at larger TBS. Coloring in (b) and (c) is the same as that in Fig. 1(a). Fcc atoms have been omitted for clarity.

such as dislocation activity inside the GB itself [59], atomic shuffling and free volume migration [60]. Furthermore, we calculated the average GB stress concentration by computing the atomic von-Mises virial stress and dividing the averaged 10% highest values found in the GB region by the average von-Mises stress in the grain region, as shown in Fig. 1(b). The simulations were performed on the high-performance supercomputers SuperMIC and Comet in the Extreme Science and Engineering Discovery Environment (XSEDE).

3. Results

3.1. Twin-size dependence of mechanical behavior

Fig. 1(c–f) shows the simulated tensile stress – strain curves obtained for columnar-grained nt-Ni, nt-Cu, nt-Ag and nt-Al with λ varying from 1.2 nm to 14.1 nm. A linear elastic regime up to 2% strain is present in all metals, where the elastic modulus was determined to be 210 GPa, 99 GPa, 66 GPa and 62 GPa in nt-Ni, nt-Cu, nt-Ag and nt-Al, respectively. We observed no variation in the elastic moduli with different λ values.

The dependence of plastic flow stresses on CTB spacing λ is represented in Fig. 2(a). In nt-Cu, nt-Ag, and nt-Al, we find a similar CTB strengthening effect characterized by a linear increase of flow stress as λ decreases. In nt-Ni, the same strengthening effect is only found when $\lambda \geq 6$ nm. For $\lambda < 6$ nm, however, our simulations predict a plateau of constant flow stresses in this metal. The absolute slope value for the increase of strength is 0.069, 0.048, 0.025 and 0.014 GPa per nanometer of twin thickness in nt-Ni, nt-Cu, nt-Ag, and nt-Al, respectively, indicating a higher dependence of flow stresses on λ in nt-Ni and nt-Cu. Apparently, the dependence of strength on twin size in columnar-grained nt metals scales with their elastic modulus, suggesting that it could be linked to dislocation plasticity as discussed in Section 4.1.

3.2. Dislocation-mediated plasticity

We now turn to the effects of twin size on dislocation mechanisms in these metals. The same dislocation mechanisms were observed in all metals: Mode-II jog dislocations expanding through all twin/matrix layers were found when λ is smaller than 2 nm,

Fig. 2(b). By contrast, threading dislocations contained within one layer of the twin/matrix were predicted when λ is larger than 5 nm, Fig. 2(c). For intermediate λ values between 2 nm and 4 nm, both dislocation mechanisms were found to co-exist. The dislocation mechanisms in our study are in good agreement with those predicted by MD simulations in columnar-grained nt-Cu by Zhou et al. [17].

The transition from jog to threading dislocations was further investigated by examining how the number of hexagonal-close packed (hcp) atoms changed with applied strain. Fig. 3 shows that the strains at which the normalized number of hcp atoms starts to increase in all metals is around 2%, i.e. the same strain value at which partial dislocations were first nucleated. However, the number of hcp atoms is found to increase more quickly as λ is increased, because more threading dislocations were nucleated than jog dislocations, which have less extended hcp stacking faults. We attribute the difference in number of hcp atoms at equivalent λ between the four metals (based on lattice constant) to the difference in equilibrium splitting distances between lead and trailing Shockley partials in the threading dislocations, which is proportional to the γ_{US}/γ_S ratio [61]. The trends predicted in Fig. 3 are consistent with the γ_{US}/γ_S ratios calculated from EAM data in Table 1, which is especially evident when comparing the numbers of hcp atoms for nt-Ag and nt-Al metals in Fig. 3(c) and (d), respectively.

3.3. GB cracking

A salient feature of this study is shown in Fig. 4(a) where significant interfacial cracking is manifested along a GB in the top-left corner of the nt-Ni model. In fact, GB cracking was predicted in only nt-Ni models with $\lambda < 6.02$ nm, coinciding with the appearance of a constant strength plateau in Fig. 2(a). Such a unique GB cracking mechanism was not observed in the other three metals up to 10% deformation. Although it is not excluded that cracking could be possible at larger applied strains not studied here, this difference is interesting for two reasons. First, this observation supports the idea that the tensile strength of columnar-grained nt fcc metals could be influenced by GB plasticity mechanisms that have not been carefully studied in the past. Second, GB cracking mechanisms are strongly dependent on the metal type.

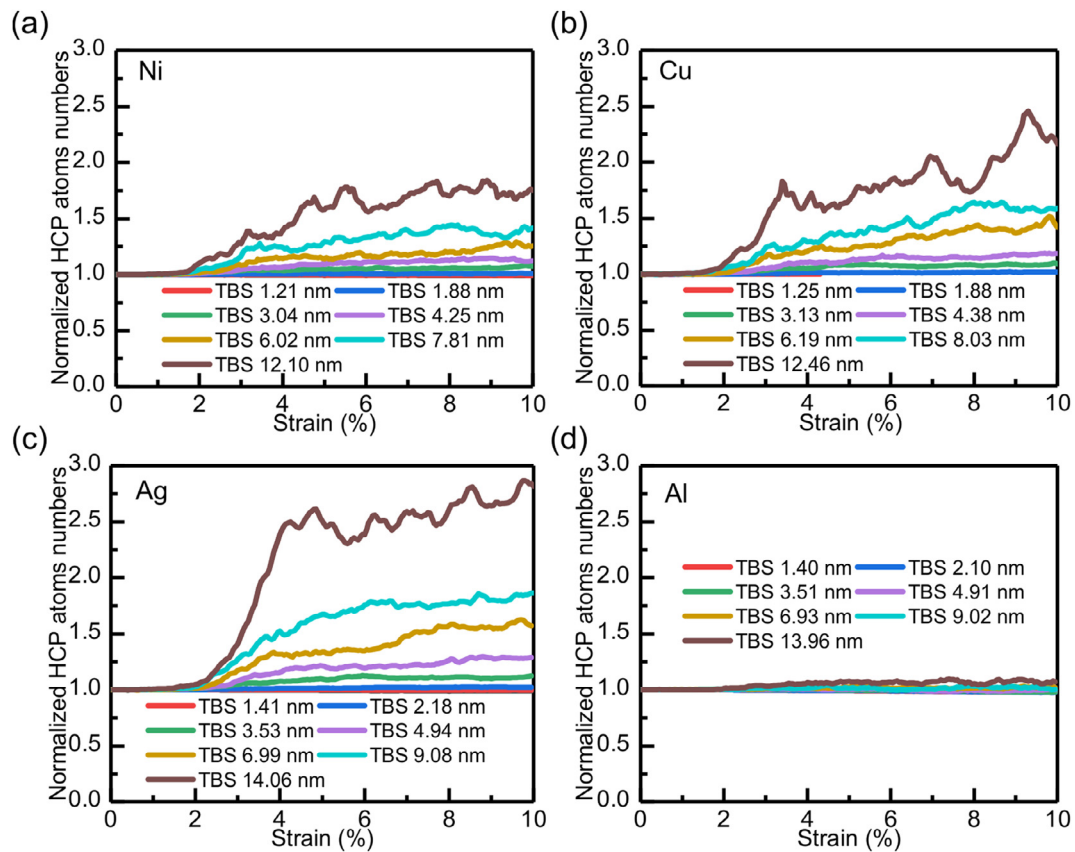


Fig. 3. Number of hcp atoms normalized by the number of hcp atoms in the undeformed models. (a) nt-Ni, (b) nt-Cu, (c) nt-Ag, and (d) nt-Al under tensile deformation at 300 K and strain rate of $2 \times 10^8 \text{ s}^{-1}$.

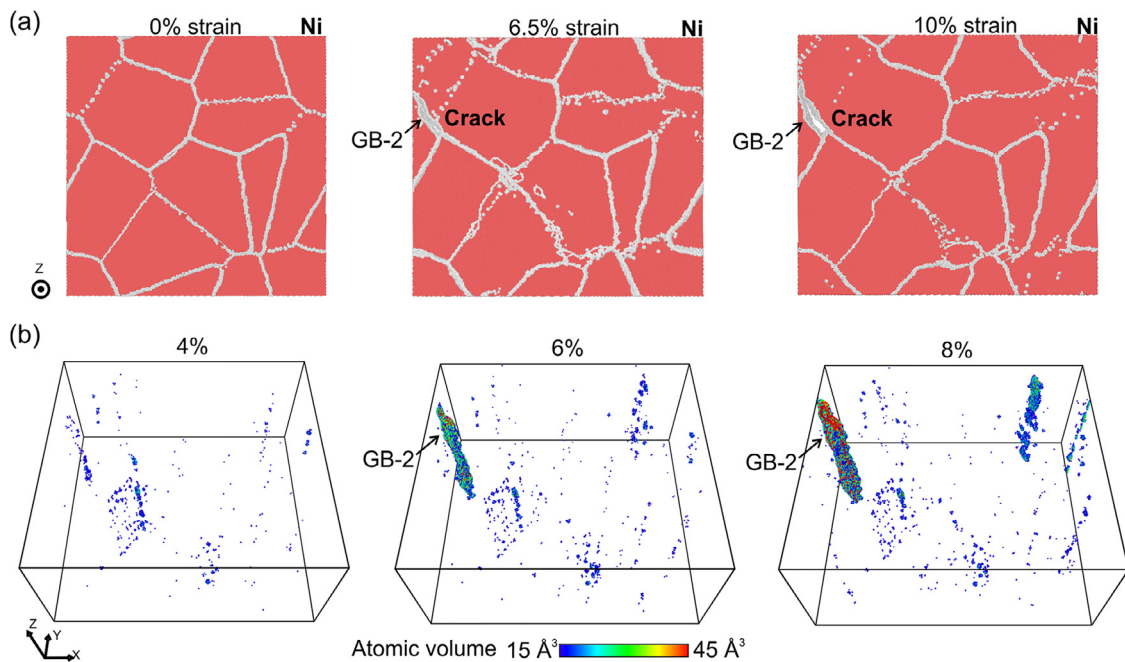


Fig. 4. GB cracking mechanism in columnar-grained nt-Ni with $\lambda = 1.83 \text{ nm}$ as a function of applied strain. (a) Top-view MD snapshots. All fcc atoms are omitted. (b) GB atomic volume distribution. All atoms with atomic volume less than $15 \text{ \AA}^3$ are omitted.

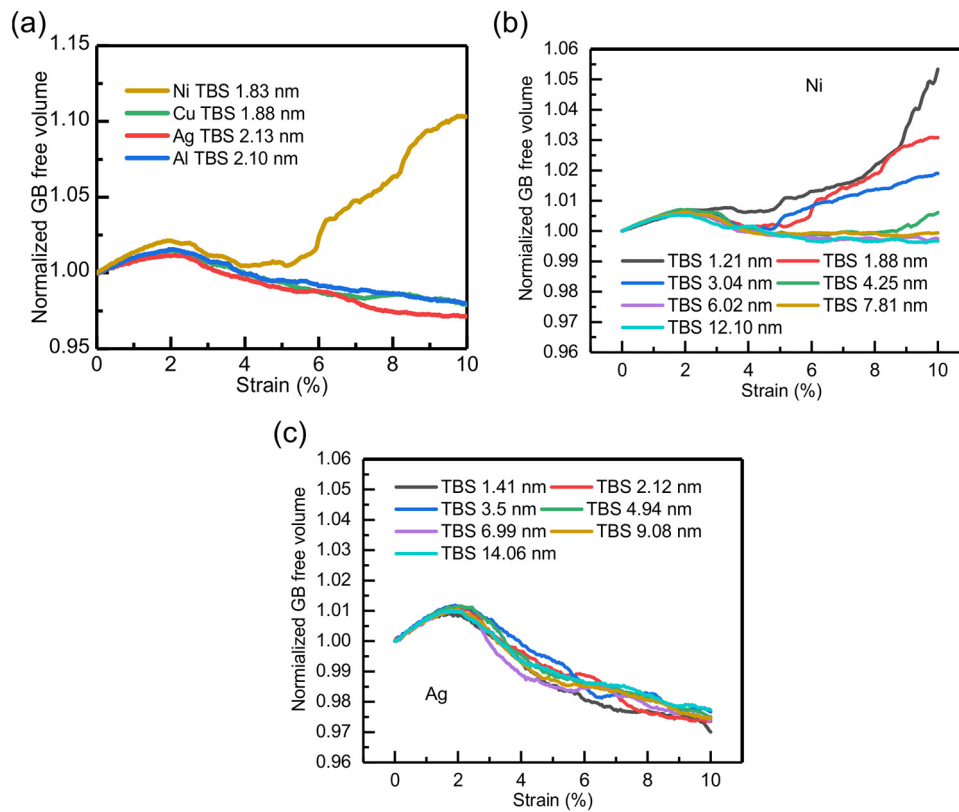


Fig. 5. Normalized GB excess free volume as a function of strain in columnar-grained nt-Ni, nt-Cu, nt-Ag, and nt-Al. (a) Models with same twin size around 2 nm. (b) and (c) Models with different TBS in nt-Ni and nt-Ag, respectively.

The atomic volume was used to study the crack growth process in columnar-grained nt-Ni in Fig. 4(b). For clarity, in this figure, atoms with atomic volume smaller than $15 \text{ \AA}^3$ were deleted (the atomic volume of Ni in its fcc single crystalline phase is $\sim 8 \text{ \AA}^3$). Small voids are seen to form at GBs at 4% strain. At 6% strain, void coalescence results in the formation of a crack throughout the z axis, which continues to grow along GB-2 after 6% strain. Such high GB free volume is only observed in nt-Ni with smaller twin sizes where cracking occurred. Also, some microvoids continue to form in other GB regions of the model, suggesting ductile-like intergranular fracture.

Naturally, the excess volume due to local atom disorder at GBs has been known to result in GB sliding mediated by atom-shuffling and dislocation nucleation mechanisms in nanocrystalline metals [37,60,62,63]. In the present study, Fig. 5(a) shows that the GB free volume increases and then decreases at a transition strain of 2% in all metals, which corresponds to the onset of plasticity discussed above. A similar evolution of GB free volume as a function of strain was observed in $\Sigma 9$ (221), $\Sigma 9$ (114) and $\Sigma 5$ (210) symmetric tilt GBs by Tucker et al. [64], who explained the increased free volume by the slight expansion of structural units prior to dislocation nucleation. Up to 6% strain, Fig. 5(a) shows that the GB free volume is slightly higher in nt-Ni than in the other metals, which could be indicative of higher GB-mediated plasticity, but the trend is relatively similar, i.e. the GB free volume first increases then decreases at 2%. Above 6% strain, however, the average GB free volume increases significantly again in nt-Ni due to GB cracking, whereas it continues to decrease in the other metals without cracking. Fig. 5(b) indicates that the second rise of GB free volume in nt-Ni is increasingly more pronounced as the twin size λ decreases less than 6.02 nm. This observation is consistent with the occurrence of a strength plateau for $\lambda < 6 \text{ nm}$ in this metal,

Fig. 2(a). On the contrary, the GB free volume evolution does not depend on λ in the other columnar-grained nt metals, see for example nt-Ag in Fig. 5(c).

3.4. GB sliding

Fig. 6 presents the distributions of atomic von-Mises shear strain in nt-Ni, nt-Cu, nt-Ag, and nt-Al models with same equivalent λ , i.e. 1.83 nm, 1.88 nm, 2.13 nm, and 2.10 nm, respectively. In-plane MD snapshots in Fig. 6(a) obtained at a post-yielding strain of 3% show that the deformation is more localized on the columnar GBs than in the grain center in all four metals. It is worth noting that at 3% deformation, some dislocation activity already exists, as indicated in Fig. 3, but is not visible in this specific view direction. No significant GB migration is observed, compared to the undeformed models in Fig. 1(a and b). Splitting of a low-angle GB occurs at the top-left corner in Fig. 6(a) as shown by a series of extended stacking faults (red lines) perpendicular to the GB. Three-dimensional snapshots of atomic shear strain distribution at a larger tensile strain of 8% are shown in Fig. 6(b) for each metal. Here, all atoms with shear strains less than 1 were deleted to highlight only GB sliding. We find more pronounced GB deformation along GB-1 in all metals. However, Fig. 6(b) reveals that a crack is formed at GB-2 in nt-Ni, which is a neighbor of GB-1, suggesting that larger GB sliding in this metal could be responsible for GB cracking.

Fig. 6(c) shows the stress – strain curves obtained from the four simulations. From the 0.2% offset limit, it is found that the yield strain is lower by 0.1% in nt-Ni than in the other metals, because GB sliding starts at an earlier stage, as indicated by the average GB shear strain in Fig. 6(d). Overall, we conclude from Fig. 6(d) that the GB sliding behavior is equivalent in nt-Ag and nt-Al and

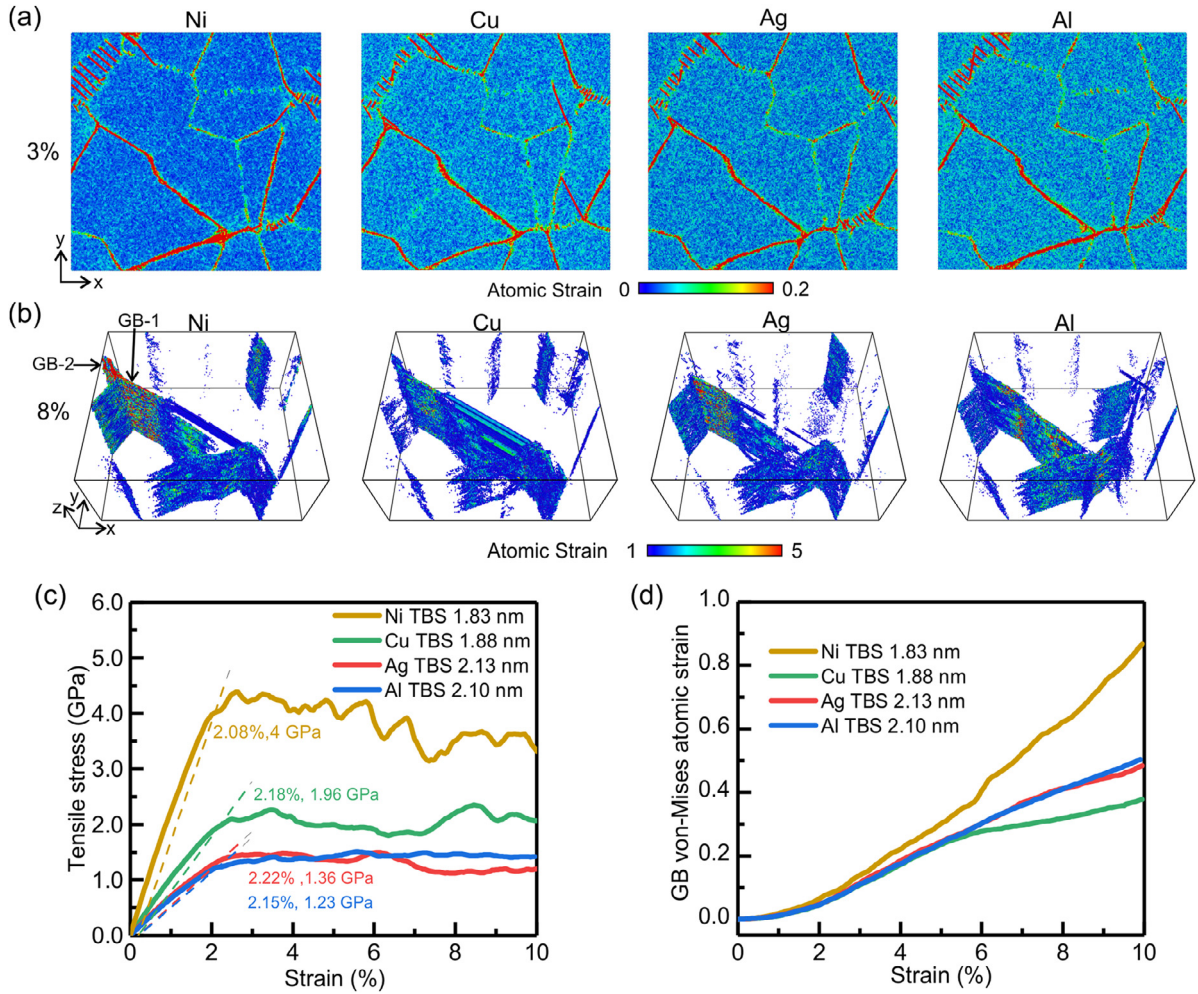


Fig. 6. GB sliding in columnar-grained nt-Ni, nt-Cu, nt-Ag, and nt-Al models with the same number of atoms, same TBS (~ 2 nm), and same initial microstructure. (a) In-plane view of distribution of atomic von-Mises shear strain at 3% deformation. (b) GB atomic strain distribution at 8% deformation with atomic strains inferior to unity omitted for clarity. (c) Simulated tensile stress-strain curves at 300 K and strain rate of $2 \times 10^8 \text{ s}^{-1}$. (d) Average GB von-Mises atomic strain as a function of applied strain.

slightly lower in nt-Cu, but markedly higher in nt-Ni, especially beyond 5% strain. In this study, however, we did not find any significant influence of the twin size on average GB shear strains in columnar-grained nt metals under tension.

Furthermore, since GB diffusivity and sliding are known to enhance strain-rate sensitivity in nanocrystalline fcc metals [65], we studied in Fig. 7 the influence of strain rate on GB atomic strain in columnar-grained nt-Cu and nt-Ni models with same $\lambda = 1.88$ nm and 1.83 nm, respectively. In nt-Cu, Fig. 7(a)–(c) suggests no significant difference in GB sliding over a range of MD-accessible strain rates from $1 \times 10^8 \text{ s}^{-1}$ to $1 \times 10^9 \text{ s}^{-1}$. In nt-Ni, however, Fig. 7(d)–(f) shows that higher GB atomic shear strains were found at the lowest strain rates, especially when GB sliding was more prominent after 5% strain.

3.5. GB stress concentration

It is important to point out that strain-rate effects are not only limited to GB plasticity, but also are important for dislocation mechanisms in nanotwinned fcc metals [19]. For instance, Fig. 8(a) clearly reveals that the yield strength of columnar-grained nt-Cu models exhibited pronounced strain-rate sensitivity, despite a lack of strain-rate effect on GB sliding in Fig. 7(c), and that the strain rate effect was the same for all TBS. This result is attributed to the

strong strain-rate dependence of dislocation nucleation processes in nanocrystalline Cu [66], that are induced by local stress concentrations at CTB-GB intersections in nt-Cu [67]. In fact, Fig. 8(b) shows concrete example of such local stress concentrations in the columnar-grained GBs on our nt-Cu model at 3% deformation and strain rate of $2 \times 10^8 \text{ s}^{-1}$. By calculating the average GB stress concentration obtained at different strain rates, as a function of applied strain, we find that higher strain rates give rise to lower GB stress concentrations after yielding (2%–3%) in Fig. 8(c), and reciprocally higher yield strengths in Fig. 8(a). This result is consistent with past theoretical predictions showing that the stress for partial dislocation nucleation increases with an increase in strain rate [68]. Likewise, in Fig. 8(d), a smaller CTB spacing decreases the average stress concentration at CTB-GB intersections after yielding in nt-Cu, which suggests that CTB strengthening relates to the dependence of GB stress concentrations on twin size in columnar-grained nt metals subjected to tensile deformation.

Furthermore, in Fig. 9, we have computed the effects of materials on the average GB stress concentration with the four metals simulated in Fig. 6(c) and found that the GB stress concentrations are constant and mostly material-independent in columnar nt metals up to 5% strain, which occurs after the onset of GB sliding. However, we also found some noticeable variations in GB stress concentrations at strains larger than 6% due to the onset of GB

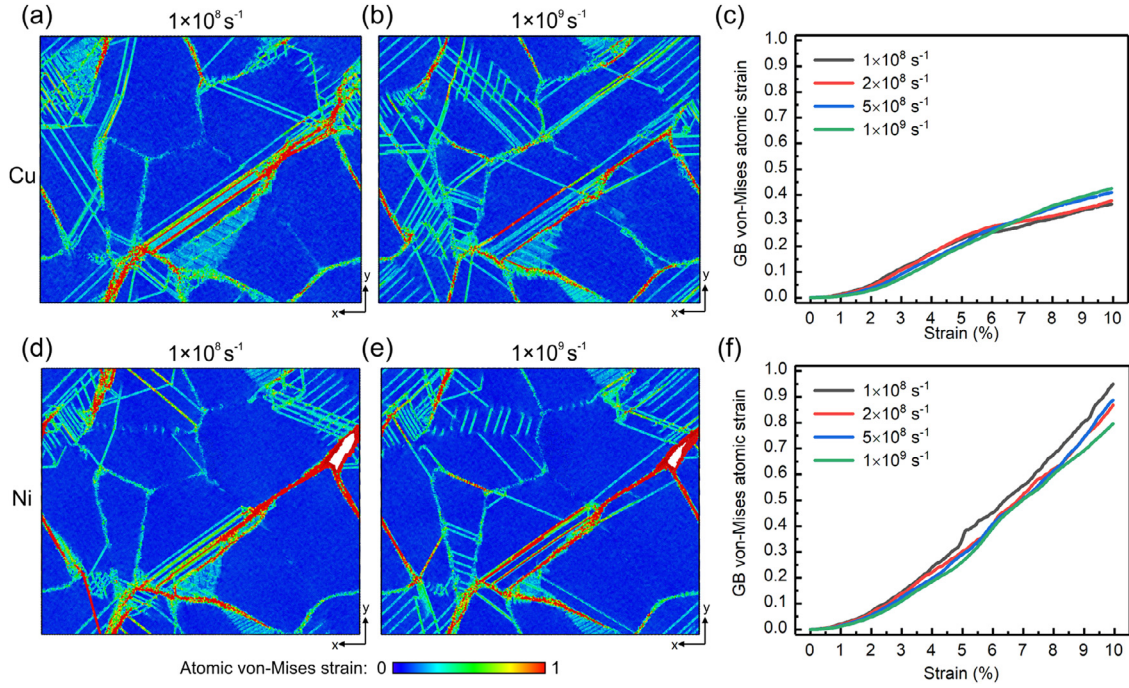


Fig. 7. Strain-rate effect on atomic von-Mises strain. (a)-(c) Nt-Cu with $\lambda = 1.88 \text{ nm}$. (d)-(f) Nt-Ni with $\lambda = 1.83 \text{ nm}$. MD snapshots show in-plane views of the atomic strain distribution at 10% deformation under different strain rates of $1 \times 10^8 \text{ s}^{-1}$ and $1 \times 10^9 \text{ s}^{-1}$.

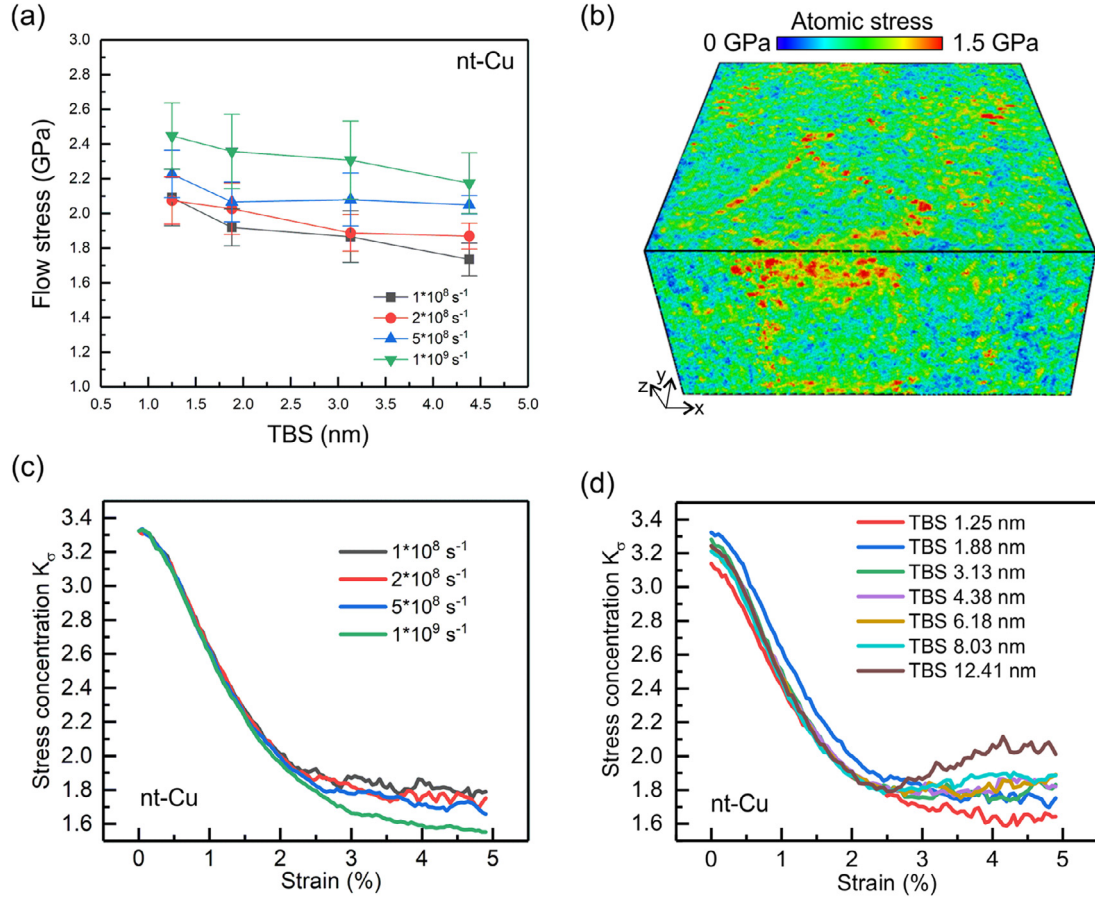


Fig. 8. GB stress concentrations in columnar-grained nt-Cu under tensile deformation at 300 K. (a) Strain rate sensitivity of flow stresses. (b) Distribution of atomic von-Mises stresses at 3% deformation and strain-rate of $2 \times 10^8 \text{ s}^{-1}$ with a twin size $\lambda = 1.88 \text{ nm}$. (c) Strain-rate effect and (d) twin-size effect on the average GB stress concentration K_σ .

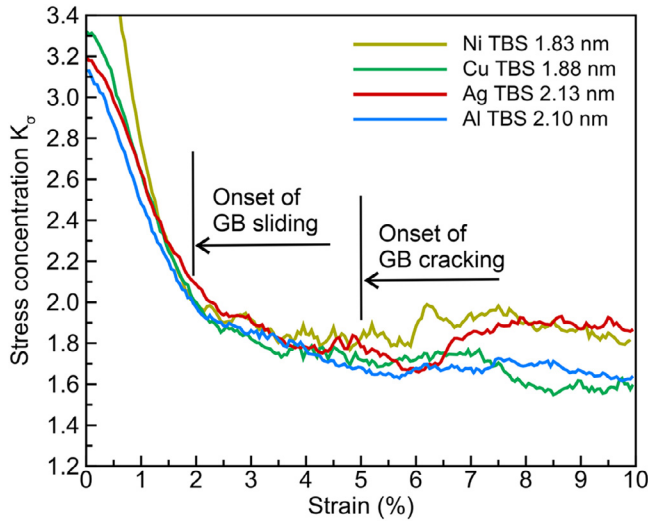


Fig. 9. Materials effect on the average GB stress concentration of the four metals with same TBS of ~ 2 nm simulated in Fig. 6(c).

cracking and void growth mechanisms. In fact, those local variations coincide with net changes in the overall stresses in Fig. 6(c). This conclusion is evidenced by an overall stress decrease in the stress-strain curve of nt-Ni above 6% strain due to a rise of GB stress concentrations in Fig. 9, whereas a net increase in tensile stress in nt-Cu above 7% strain corresponds to a decrease of GB stress concentration for this strain range.

4. Discussion

4.1. CTB strengthening effects compared to past experiments

In direct synthesis using either sputtering or electrochemical depositions, nanoscale CTBs are more frequently formed in fcc metals with low intrinsic γ_s , such as nt-Ag [9,69–72], nt-Cu [31,73–75] and nt-Cu-Al alloys with up to 6 wt.% Al content [76,77]. Recent experimental progress in sputtering techniques, however, has enabled the synthesis of nanotwins in high- γ_s fcc metals, such as Ni superalloys [78,79] and Al-based solid-solution alloys and multilayer films [80–82], which are of special interest and utility over low- γ_s metals for structural applications [53]. Therefore, we include these materials in our survey because pure nt-Ni and nt-Al metals have not yet been synthesized.

Fig. 10 presents a summary of yield stress and hardness data published in the literature on columnar-grained (111)-textured nt-Ag [69–72], nt-Cu [31,73–75], nt-Cu-6wt.%Al [76,77], nt-Ni-14at.%Mo-2.4at.%W [78], and nt-Al(100nm)/Ag(seed) multilayers [80], as functions of twin size normalized by the average grain diameter, λ/d . It should be noted that we have intentionally omitted to show the hardness of nt-Al-Fe alloys [81] and nt-Al-Ni alloys [82] because CTBs present in this type of alloys are characterized by a mix of incoherent twin boundaries and 9R phase that are heterogeneously dispersed between columnar grains, and thus may not be representative of the microstructure discussed in the current study. For completeness, Fig. 10 also displays the flow stresses in columnar-grained nt-Cu with $d = 20$ nm simulated by Zhou et al. [17] using MD. Their yield stress predictions are in excellent agreement with our results for nt-Cu in Fig. 2(a) and matched well with two theoretical strength equations based on interactions of jog and threading dislocations with CTBs, solid and dash lines, respectively. Also, similar dislocation mechanisms were found in all four columnar-grained nt metals simulated in the present study.

The materials comparison in Fig. 10 is interesting in several aspects. First, the dependence of yield stresses on twin size appears to be weaker in experiments than in the MD simulations on nt-Cu. Aside from the high stresses imposed by unrealistically high MD strain rates, it could be possible to attribute this observation to the large difference in grain size, since d changed from $\sim 0.1 \mu\text{m}$ to $19 \mu\text{m}$ in experiments compared to $d = 20$ nm in MD simulation. In columnar-grained microstructures, however, the grain size reduction does not fundamentally change the number of dislocation nucleation sites from CTB-GB stress concentrations, but primarily increases the local stress concentration itself, as this value scales as $\sqrt{\lambda/d}$ in nt metals [83]. From this standpoint, obtaining smaller CTB strengthening effects in experiments with large grain sizes is physically justified. Nevertheless, this study also demonstrates that GB cracking could result in no strengthening at all, especially when this mechanism is more active at smaller λ values, which gives credence that GB plasticity may play an important role in experiments as well.

Second, to better understand the effect of γ_s on yield stresses, Table 1 lists the properties of pure fcc metals in Ag, Cu, Ni and Al, and one Cu-Al alloy obtained from density-functional-theory calculations [48–51]. Asaro and Suresh [84] have proposed to derive the effective stress intensity K^{crit} to nucleate a lead partial dislocation from a GB stress concentration based on the Peierls concept of partial dislocation nucleation from a crack tip [85], using the equation

$$K^{\text{crit}} = \sqrt{\frac{2\mu\gamma_{\text{US}}}{(1-\nu)}} \quad (1)$$

where μ and ν are the shear modulus and Poisson's ratio, respectively. By applying this equation to the five metals in Table 1, we find that nt-Ag and nt-Al have approximately same dislocation nucleation strength K^{crit} , while that of nt-Ni is significantly higher than in the other metals, which is consistent with both MD simulations in Fig. 2(a) and experimental results in Fig. 10. Furthermore, nt-Cu-Al alloys are predicted to have approximately same strength as pure nt-Cu metals, despite a significantly lower γ_s . In Fig. 10, however, yield stresses measured in nt-Cu-Al alloys are up to twice as high as those in nt-Cu. It should be noted that the grain size in nt Cu-6wt.%Al alloys tested was among the smallest from all experimental data, ~ 100 nm [76], but this fact alone does not justify a two-fold stress hike. It can be hypothesized that Al solute segregation in this solid-solution Cu–Al alloy could have strengthened GBs and reduced GB sliding, compared to pure nt-Cu metals, since Al segregation to GBs is theoretically favored in Cu polycrystals [86].

Third, a CTB strengthening effect was observed in all four metals, but a larger TBS dependence of stress was manifested in nt-Cu and nt-Ni with $\lambda > 5$ nm than in nt-Ag and nt-Al metals, Fig. 2(a). CTB strengthening effect in columnar-grained nt-Cu is explained in the literature from the increased stress needed for dislocation propagation as TBS decreases. Jog dislocations are pinned at all TBs by stair rod dislocations [17]. Since the number of pinning points increases as TBS decreases, a larger stress is then required to drag a jog dislocation. Also, threading dislocations are confined within two CTBs. The confined layer slip (CLS) model [87] justifies CTB strengthening by the increased stress needed for propagating threading dislocation loops while maintaining energy balance. The shear modulus of the material influences stresses based on both pinning effect and CLS model [17]. Furthermore, it is possible to interpret the relationship between elastic modulus and twin-size dependence of strength using the Peierls criterion for dislocation nucleation K^{crit} in Eq. (1). Since the strengthening effect is predominantly governed by dislocation nucleation, it can be assumed to the critical strength σ is proportional to $K^{\text{crit}}/K_{\sigma}$ where K_{σ} is the local GB stress concentration at GB-TB triple junctions, which

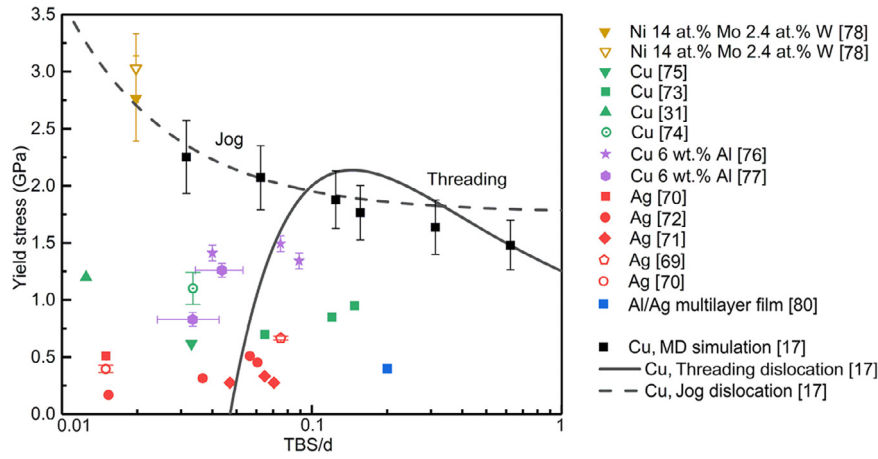


Fig. 10. Literature data on yield stresses measured in columnar-grained nt-Cu, nt-Ag, nt-Ni alloys, and nt-Al (1000nm)/Ag(seed) multilayer films synthesized by sputtering deposition. No data are yet available for pure nt-Ni and pure nt-Al metals. CTB spacing and grain size are denoted as *TBS* and *d*, respectively. Symbols represent either the yield stress or hardness/3. Dashed and solid lines represent theoretical equations for yield stresses in columnar-grained nt-Cu based on propagation of mode II dislocations, either jog or threading, respectively, from Ref. [17].

is also proportional to $(\lambda/d)^{1/2}$. Therefore,

$$\sigma \propto K^{\text{crit}} \sqrt{\frac{d}{\lambda}} \quad (2)$$

From Eq. (2), we conclude that the dependence of strength on twin size (λ) scales with K^{crit} , which is consistent with the K^{crit} parameters estimated in Table 1. Because K^{crit} increases as the shear modulus increases, there is an apparent relationship between elasticity and TB-dependent strengthening effects in columnar-grained nt metals. In fact, we have demonstrated with Figs. 8 and 9 that most of the TB-dependent strengthening effects observed in columnar-grained nt metals can be rationalized through the dependence of average GB stress concentrations on TBS, strain-rate and metal type.

4.2. GB sliding and cracking in columnar-grained nt metals

From the current study, it is demonstrated that sliding of columnar GBs loaded laterally in tension contributed markedly to the overall plastic deformation of nt fcc metals, and that GB sliding was more significant in nt-Ni than in the other columnar-grained nt metals. While flow stresses in nt-Cu, nt-Ag, and nt-Al increase linearly with decreasing TB spacing, our atomistic simulations reveal that a maximum strength limit is reached in nt-Ni below a critical CTB spacing of 6 nm, due to enhanced GB sliding. Because the same initial polycrystals were used, albeit local differences in the atomic GB structures existed for the different metals [63], GB sliding was identical for all metals up to ~2% deformation, Fig. 6(d). For strains between 2%-5%, however, a pronounced rise in GB plasticity and GB free volume occurred in nt-Ni, which was facilitated by GB atom shuffling and λ -dependent GB cracking. GB cracking was only detected in nt-Ni with λ values smaller than 6 nm. The type of cracking observed in this nt metal can be viewed as ductile intergranular fracture, rather than brittle GB decohesion, due to the formation and growth of micro-voids in different areas of the amorphous GB region, Fig. 6(b). In fact, this behavior is reminiscent of micro-cracking in hard and quasi-brittle metallic glasses induced by nanoscale cavitation and excess free volume inside localized amorphous shear bands; see for example Fig. 27 in Ref. [88]. It has been shown in the literature that the nucleation of nanoscale voids occurs preferably at GBs, triple junctions, and GB – CTB intersections in nanocrystalline Ni [89]. At larger TBS, the number of stress concentrations at GB – CTB intersections decreases, which may cause more limited crack initiation sites. At

small TBS, however, cracking along GBs may directly compete with dislocation nucleation mechanisms, which could therefore explain why the plateau of maximum flow stress in nt-Ni appears only for $\lambda < 6$ nm in Fig. 2(a).

Furthermore, because of enhanced GB sliding in nt-Ni, the reduction of GB sliding with increasing strain rate was slightly higher in nt-Ni than in nt-Cu. Therefore, this result suggests that strain rate sensitivity in nanotwinned fcc metals could be larger in columnar-grained nt-Ni than in other metals due to GB sliding. However, Zhang et al. [66] also noted that stress-driven GB plastic deformation mechanisms such as GB sliding and migration, are not as sensitive to strain rate as that expected for the thermally assisted mechanisms such as dislocation nucleation. This hypothesis is consistent with our results in columnar-grained nt-Cu, since this metal exhibited a visible strain-rate sensitivity despite reduced GB sliding, compared to the three other metals.

In addition, the dependence of twin spacing of GB sliding in nt metals remains unclear. This study did not find any significant influence of TBS on GB atomic strain for columnar-grained metals deformed in tension. This result contrasts with the MD simulations of Ke et al. [9] in nt Ag-Cu alloys showing that GB sliding rates increased as TBS was decreased. It should be noted, however, that their polycrystal models contained only equiaxial grains. During tensile deformation, GBs in equiaxial grains are subjected to combined normal and shear loading that could help with the nucleation of additional slip modes impacting with the migration of GB free volume. Also, the lack of TB-dependence on GB sliding in this study was surprising, considering that GB stress concentrations are reduced with decreasing TBS in nt-Cu, as shown in Fig. 8(d), although no direct link between these two properties has been established in the literature. Therefore, understanding the roles of CTBs on intrinsic GB plasticity mechanisms warrants further investigation.

5. Conclusion

MD simulations have been used to study the strength and mechanisms of GB plasticity and GB stress concentrations in four columnar grained nt fcc metals: Cu, Ag, Al, and Ni. A major conclusion is that the dislocation mechanisms, as a function of twin size, are the same for all nt metals with columnar grain morphology, but most of the TB-dependent strengthening effects observed in columnar-grained nt metals can be rationalized through the dependence of average GB stress concentrations on twin-size, strain-

rate and metal type. Also, we found that GB sliding is more significant in nt-Ni than in the other three metals, with higher GB accommodated strain and cracking, which influences the mechanical properties of nt-Ni significantly. An important outcome of this phenomenon is the occurrence of a maximum strength plateau in columnar-grained nt-Ni with $\lambda < 6$ nm due to TB-dependent GB cracking. Therefore, this study emphasizes the necessity to consider and tailor GB properties to further improve the mechanical behavior of columnar-grained nt fcc metals.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

The authors thank Drs. X. Ke and Z. Pan for sharing their respective codes to perform the GB slicing and atomic stress calculations. Support from National Science Foundation grant no. [DMR-1410646](#), U.S. Department of Energy grant no. [DE-SC0020054](#), and the computational resources provided by XSEDE supported by National Science Foundation grant no. [ACI-1548562](#) are gratefully acknowledged.

References

- [1] L. Lu, Y. Shen, X. Chen, L. Qian, K. Lu, Ultrahigh strength and high electrical conductivity in copper, *Science* 304 (5669) (2004) 422–426.
- [2] Y.F. Shen, L. Lu, Q.H. Lu, Z.H. Jin, K. Lu, Tensile properties of copper with nano-scale twins, *Scr. Mater.* 52 (10) (2005) 989–994.
- [3] L. Lu, X. Chen, X. Huang, K. Lu, Revealing the maximum strength in nanotwinned copper, *Science* (2009) 323.
- [4] C. Deng, F. Sansoz, Near-ideal strength in gold nanowires achieved through microstructural design, *ACS Nano* 3 (10) (2009) 3001–3008.
- [5] P. Gu, M. Dao, Y. Zhu, Strengthening at nanoscaled coherent twin boundary in f.c.c. metals, *Philos. Mag.* 94 (11) (2014) 1249–1262.
- [6] Y. Liu, J. Jian, Y. Chen, H. Wang, X. Zhang, Plasticity and ultra-low stress induced twin boundary migration in nanotwinned Cu by in situ nanoindentation studies, *Appl. Phys. Lett.* 104 (23) (2014) 231910.
- [7] X. Li, Y. Wei, L. Lu, K. Lu, H. Gao, Dislocation nucleation governed softening and maximum strength in nano-twinned metals, *Nature* 464 (7290) (2010) 877–880.
- [8] D.C. Bufford, Y.M. Wang, Y. Liu, L. Lu, Synthesis and microstructure of electrodeposited and sputtered nanotwinned face-centered-cubic metals, *MRS Bull.* 41 (4) (2016) 286–291.
- [9] X. Ke, J. Ye, Z. Pan, J. Geng, M.F. Besser, D. Qu, A. Caro, J. Marian, R.T. Ott, Y.M. Wang, F. Sansoz, Ideal maximum strengths and defect-induced softening in nanocrystalline-nanotwinned metals, *Nat. Mater.* 18 (11) (2019) 1207–1214.
- [10] Y. Zhao, T.A. Furnish, M.E. Kassner, A.M. Hodge, Thermal stability of highly nanotwinned copper: the role of grain boundaries and texture, *J. Mater. Res.* 27 (24) (2012) 3049–3057.
- [11] A. Porter, C. Tran, F. Sansoz, Intrinsic nanotwin effect on thermal boundary conductance in bulk and single-nanowire twinning superlattices, *Phys. Rev. B* 93 (19) (2016) 195431.
- [12] K.Y. Yu, D. Bufford, C. Sun, Y. Liu, H. Wang, M.A. Kirk, M. Li, X. Zhang, Removal of stacking-fault tetrahedra by twin boundaries in nanotwinned metals, *Nat. Commun.* 4 (2013) 1377.
- [13] Y. Zhao, I.C. Cheng, M.E. Kassner, A.M. Hodge, The effect of nanotwins on the corrosion behavior of copper, *Acta Mater.* 67 (2014) 181–188.
- [14] Y. Chen, K.Y. Yu, Y. Liu, S. Shao, H. Wang, M.A. Kirk, J. Wang, X. Zhang, Damage-tolerant nanotwinned metals with nanovoids under radiation environments, *Nat. Commun.* 6 (2015) 7036.
- [15] Y. Wei, Anisotropic size effect in strength in coherent nanowires with tilted twins, *Phys. Rev. B* 84 (1) (2011) 014107.
- [16] F. Sansoz, K. Lu, T. Zhu, A. Misra, Strengthening and plasticity in nanotwinned metals, *MRS Bull.* 41 (4) (2016) 292–297.
- [17] H. Zhou, X. Li, S. Qu, W. Yang, H. Gao, A jogged dislocation governed strengthening mechanism in nanotwinned metals, *Nano Lett.* 14 (9) (2014) 5075–5080.
- [18] Q. Pan, H. Zhou, Q. Lu, H. Gao, L. Lu, History-independent cyclic response of nanotwinned metals, *Nature* 551 (7679) (2017) 214–217.
- [19] T. Zhu, J. Li, A. Samanta, H.G. Kim, S. Suresh, Interfacial plasticity governs strain rate sensitivity and ductility in nanostructured metals, *Proc. Natl. Acad. Sci.* 104 (9) (2007) 3031.
- [20] N. Li, J. Wang, A. Misra, X. Zhang, J.Y. Huang, J.P. Hirth, Twinning dislocation multiplication at a coherent twin boundary, *Acta Mater.* 59 (15) (2011) 5989–5996.
- [21] Y.M. Wang, F. Sansoz, T. LaGrange, R.T. Ott, J. Marian, T.W. Barbee, A.V. Hamza, Defective twin boundaries in nanotwinned metals, *Nat. Mater.* 12 (8) (2013) 697–702.
- [22] Q. Fang, F. Sansoz, Influence of intrinsic kink-like defects on screw dislocation – coherent twin boundary interactions in copper, *Acta Mater.* 123 (2017) 383–393.
- [23] Z.-J. Wang, Q.-J. Li, Y. Li, L.-C. Huang, L. Lu, M. Dao, J. Li, E. Ma, S. Suresh, Z.-W. Shan, Sliding of coherent twin boundaries, *Nat. Commun.* 8 (1) (2017) 1108.
- [24] M.K. Kini, G. Dehm, C. Kirchlechner, Size dependent strength, slip transfer and slip compatibility in nanotwinned silver, *Acta Mater.* 184 (2020) 120–131.
- [25] Z.S. You, L. Lu, K. Lu, Tensile behavior of columnar grained Cu with preferentially oriented nanoscale twins, *Acta Mater.* 59 (18) (2011) 6927–6937.
- [26] Z. You, X. Li, L. Gui, Q. Lu, T. Zhu, H. Gao, L. Lu, Plastic anisotropy and associated deformation mechanisms in nanotwinned metals, *Acta Mater.* 61 (1) (2013) 217–227.
- [27] V. Borovikov, M.I. Mendelev, A.H. King, R. LeSar, Effects of Schmid factor and slip nucleation on deformation mechanism in columnar-grained nanotwinned Ag and Cu, *J. Appl. Phys.* 117 (8) (2015) 085302.
- [28] Q. Lu, Z. You, X. Huang, N. Hansen, L. Lu, Dependence of dislocation structure on orientation and slip systems in highly oriented nanotwinned Cu, *Acta Mater.* 127 (2017) 85–97.
- [29] D. Jang, X. Li, H. Gao, J.R. Greer, Deformation mechanisms in nanotwinned metal nanopillars, *Nat. Nanotechnol.* 7 (9) (2012) 594–601.
- [30] J. Wang, F. Sansoz, J. Huang, Y. Liu, S. Sun, Z. Zhang, S.X. Mao, Near-ideal theoretical strength in gold nanowires containing angstrom scale twins, *Nat. Commun.* 4 (1) (2013) 1742.
- [31] X. Zhang, H. Wang, X.H. Chen, L. Lu, K. Lu, R.G. Hoagland, A. Misra, High-strength sputter-deposited Cu foils with preferred orientation of nanoscale growth twins, *Appl. Phys. Lett.* 88 (17) (2006) 173116.
- [32] J. Schiøtz, K.W. Jacobsen, A maximum in the strength of nanocrystalline copper, *Science* 301 (2003) 1357–1359.
- [33] R. Raj, M.F. Ashby, On grain boundary sliding and diffusional creep, *Metall. Trans.* 2 (4) (1971) 1113–1127.
- [34] R.C. Giffkins, Grain-boundary sliding and its accommodation during creep and superplasticity, *Metall. Trans. A* 7 (1976) 1225–1232.
- [35] T.G. Langdon, Grain boundary sliding revisited: Developments in sliding over four decades, *J. Mater. Sci.* 41 (3) (2006) 597–609.
- [36] K.S. Kumar, H. Van Swygenhoven, S. Suresh, Mechanical behavior of nanocrystalline metals and alloys, *Acta Mater.* 51 (19) (2003) 5743–5774.
- [37] H. Van Swygenhoven, P.M. Derlet, Grain-boundary sliding in nanocrystalline fcc metals, *Phys. Rev. B* 64 (22) (2001) 224105.
- [38] Z. Shan, E.A. Stach, J.M.K. Wiezorek, J.A. Knapp, D.M. Follstaedt, S.X. Mao, Grain boundary-mediated plasticity in nanocrystalline nickel, *Science* 305 (5684) (2004) 654–657.
- [39] A. Li, I. Szlufarska, Morphology and mechanical properties of nanocrystalline Cu/Ag alloy, *J. Mater. Sci.* 52 (8) (2017) 4555–4567.
- [40] Z. Pan, F. Sansoz, Heterogeneous solute segregation suppresses strain localization in nanocrystalline Ag-Ni alloys, *Acta Mater.* 200 (2020) 91–100.
- [41] G.J. Tucker, S.M. Foiles, Quantifying the influence of twin boundaries on the deformation of nanocrystalline copper using atomistic simulations, *Int. J. Plast.* 65 (2015) 191–205.
- [42] X. Ke, F. Sansoz, Segregation-affected yielding and stability in nanotwinned silver by microalloying, *Phys. Rev. Mater.* 1 (6) (2017) 063604.
- [43] Y.-J. Li, C.-W. Hsu, Y.-H. Ting, N.-T. Tsou, Y.-C. Lo, W.-W. Wu, K.N. Tu, C. Chen, Deformation induced columnar grain rotation in nanotwinned metals, *Mater. Sci. Eng.* 797 (2020) 140045.
- [44] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, *J. Comput. Phys.* 117 (1) (1995) 1–19.
- [45] P.L. Williams, Y. Mishin, J.C. Hamilton, An embedded-atom potential for the Cu–Ag system, *Model. Simul. Mater. Sci. Eng.* 14 (5) (2006) 817–833.
- [46] Y. Mishin, D. Farkas, M.J. Mehl, D.A. Papaconstantopoulos, Interatomic potentials for monoatomic metals from experimental data and ab initio calculations, *Phys. Rev. B* 59 (5) (1999) 3393.
- [47] C. Deng, F. Sansoz, Fundamental differences in the plasticity of periodically twinned nanowires in Au, Ag, Al, Cu, Pb and Ni, *Acta Mater.* 57 (20) (2009) 6090–6101.
- [48] D. Siegel, Generalized stacking fault energies, ductilities, and twinnabilities of Ni and selected Ni alloys, *Appl. Phys. Lett.* 87 (2005) 121901–121901.
- [49] S. Kibey, J.B. Liu, D.D. Johnson, H. Sehitoglu, Generalized planar fault energies and twinning in Cu–Al alloys, *Appl. Phys. Lett.* 89 (19) (2006) 191911.
- [50] S. Kibey, J.B. Liu, D.D. Johnson, H. Sehitoglu, Predicting twinning stress in fcc metals: linking twin-energy pathways to twin nucleation, *Acta Mater.* 55 (20) (2007) 6843–6851.
- [51] S. Kamran, K. Chen, L. Chen, Ab initio examination of ductility features of fcc metals, *Phys. Rev. B* 79 (2) (2009) 024106.
- [52] M. Muzyk, Z. Pakiel, K.J. Kurzydowski, Generalized stacking fault energies of aluminum alloys—density functional theory calculations, *Metals* 8 (10) (2018) 823.
- [53] Y. Kulkarni, R.J. Asaro, Are some nanotwinned fcc metals optimal for strength, ductility and grain stability? *Acta Mater.* 57 (16) (2009) 4835–4844.
- [54] Z.H. Jin, P. Gumbsch, E. Ma, K. Albe, K. Lu, H. Hahn, H. Gleiter, The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centred cubic metals, *Scr. Mater.* 54 (6) (2006) 1163–1168.

- [55] Z.H. Jin, P. Gumbsch, K. Albe, E. Ma, K. Lu, H. Gleiter, H. Hahn, Interactions between non-screw lattice dislocations and coherent twin boundaries in face-centered cubic metals, *Acta Mater.* 56 (5) (2008) 1126–1135.
- [56] M. Chassigne, M. Legros, D. Rodney, Atomic-scale simulation of screw dislocation/coherent twin boundary interaction in Al, Au, Cu and Ni, *Acta Mater.* 59 (4) (2011) 1456–1463.
- [57] G. Voronoi, Nouvelles applications des paramètres continus à la théorie des formes quadratiques. Deuxième mémoire. Recherches sur les paralléloèdres primitifs, *J. für die reine und Angew. Math.* 1908 (134) (1908) 198–287.
- [58] A. Stukowski, Visualization and analysis of atomistic simulation data with OVITO—the open visualization tool, *Model. Simul. Mater. Sci. Eng.* 18 (1) (2009) 015012.
- [59] J. Monk, B. Hyde, D. Farkas, The role of partial grain boundary dislocations in grain boundary sliding and coupled grain boundary motion, *J. Mater. Sci.* 41 (23) (2006) 7741–7746.
- [60] H. Van Swygenhoven, P.M. Derlet, A. Hasnaoui, Atomic mechanism for dislocation emission from nanosized grain boundaries, *Phys. Rev. B* 66 (2) (2002) 024101.
- [61] H. Van Swygenhoven, P.M. Derlet, A.G. Froseth, Stacking fault energies and slip in nanocrystalline metals, *Nat. Mater.* 3 (6) (2004) 399–403.
- [62] F. Sansoz, J.F. Molinari, Incidence of atom shuffling on the shear and decohesion behavior of a symmetric tilt grain boundary in copper, *Scr. Mater.* 50 (10) (2004) 1283–1288.
- [63] F. Sansoz, J.F. Molinari, Mechanical behavior of Σ tilt grain boundaries in nanoscale Cu and Al: a quasicontinuum study, *Acta Mater.* 53 (7) (2005) 1931–1944.
- [64] G.J. Tucker, M.A. Tschopp, D.L. McDowell, Evolution of structure and free volume in symmetric tilt grain boundaries during dislocation nucleation, *Acta Mater.* 58 (19) (2010) 6464–6473.
- [65] Y. Wei, A.F. Bower, H. Gao, Enhanced strain-rate sensitivity in fcc nanocrystals due to grain-boundary diffusion and sliding, *Acta Mater.* 56 (8) (2008) 1741–1752.
- [66] T. Zhang, K. Zhou, Z.Q. Chen, Strain rate effect on plastic deformation of nanocrystalline copper investigated by molecular dynamics, *Mater. Sci. Eng.* 648 (2015) 23–30.
- [67] N. Lu, K. Du, L. Lu, H.Q. Ye, Transition of dislocation nucleation induced by local stress concentration in nanotwinned copper, *Nat. Commun.* 6 (1) (2015) 7648.
- [68] T. Zhu, J. Li, A. Samanta, A. Leach, K. Gall, Temperature and strain-rate dependence of surface dislocation nucleation, *Phys. Rev. Lett.* 100 (2) (2008) 025502.
- [69] D. Bufford, H. Wang, X. Zhang, High strength, epitaxial nanotwinned Ag films, *Acta Mater.* 59 (1) (2011) 93–101.
- [70] T.A. Furnish, A.M. Hodge, On the mechanical performance and deformation of nanotwinned Ag, *APL Mater.* 2 (4) (2014) 046112.
- [71] R.T. Ott, J. Geng, M.F. Besser, M.J. Kramer, Y.M. Wang, E.S. Park, R. LeSar, A.H. King, Optimization of strength and ductility in nanotwinned ultra-fine grained Ag: twin density and grain orientations, *Acta Mater.* 96 (2015) 378–389.
- [72] H. Zhang, J. Geng, R.T. Ott, M.F. Besser, M.J. Kramer, Effect of temperature on the nano/microstructure and mechanical behavior of nanotwinned Ag films, *Metall. Mater. Trans. A* 46 (9) (2015) 4078–4085.
- [73] O. Anderoglu, A. Misra, H. Wang, F. Ronning, M.F. Hundley, X. Zhang, Epitaxial nanotwinned Cu films with high strength and high conductivity, *Appl. Phys. Lett.* 93 (8) (2008) 083108.
- [74] O. Anderoglu, A. Misra, H. Wang, X. Zhang, Thermal stability of sputtered Cu films with nanoscale growth twins, *J. Appl. Phys.* 103 (9) (2008) 094322.
- [75] M. Mieszala, G. Guillonéau, M. Hasegawa, R. Raghavan, J.M. Wheeler, S. Michler, J. Philippe, Orientation-dependent mechanical behaviour of electrodeposited copper with nanoscale twins, *Nanoscale* 8 (35) (2016) 15999–16004.
- [76] N.M. Heckman, L. Velasco, A.M. Hodge, Influence of twin thickness and grain size on the tensile behavior of fully nanotwinned CuAl alloys, *Adv. Eng. Mater.* 18 (6) (2016) 918–922.
- [77] N.M. Heckman, L. Velasco, A.M. Hodge, Tensile behavior of fully nanotwinned alloys with varying stacking fault energies, *MRS Commun.* 7 (2) (2017) 253–258.
- [78] G.-D. Sim, J.A. Krogstad, K.Y. Xie, S. Dasgupta, G.M. Valentino, T.P. Weihs, K.J. Hemker, Tailoring the mechanical properties of sputter deposited nanotwinned nickel-molybdenum-tungsten films, *Acta Mater.* 144 (2018) 216–225.
- [79] J.A. Bahena, N.M. Heckman, C.M. Barr, K. Hattar, B.L. Boyce, A.M. Hodge, Development of a heterogeneous nanostructure through abnormal recrystallization of a nanotwinned Ni superalloy, *Acta Mater.* 195 (2020) 132–140.
- [80] D. Bufford, Y. Liu, Y. Zhu, Z. Bi, Q.X. Jia, H. Wang, X. Zhang, Formation mechanisms of high-density growth twins in aluminum with high stacking-fault energy, *Mater. Res. Lett.* 1 (1) (2013) 51–60.
- [81] Q. Li, S. Xue, J. Wang, S. Shao, A.H. Kwong, A. Giwa, Z. Fan, Y. Liu, Z. Qi, J. Ding, H. Wang, J.R. Greer, H. Wang, X. Zhang, High-strength nanotwinned Al alloys with 9R phase, *Adv. Mater.* 30 (11) (2018) 1704629.
- [82] Y.F. Zhang, Q. Li, S.C. Xue, J. Ding, D.Y. Xie, J. Li, T. Niu, H. Wang, H. Wang, J. Wang, X. Zhang, Ultra-strong nanotwinned Al–Ni solid solution alloys with significant plasticity, *Nanoscale* 10 (46) (2018) 22025–22034.
- [83] S.M. Taheri Mousavi, H. Zhou, G. Zou, H. Gao, Transition from source- to stress-controlled plasticity in nanotwinned materials below a softening temperature, *npj Comput. Mater.* 5 (1) (2019) 2.
- [84] R.J. Asaro, S. Suresh, Mechanistic models for the activation volume and rate sensitivity in metals with nanocrystalline grains and nano-scale twins, *Acta Mater.* 53 (12) (2005) 3369–3382.
- [85] J.R. Rice, Dislocation nucleation from a crack tip: an analysis based on the Peierls concept, *J. Mech. Phys. Solids* 40 (2) (1992) 239–271.
- [86] M. Wagih, P.M. Larsen, C.A. Schuh, Learning grain boundary segregation energy spectra in polycrystals, *Nat. Commun.* 11 (1) (2020) 6376.
- [87] A. Misra, J.P. Hirth, R.G. Hoagland, Length-scale-dependent deformation mechanisms in incoherent metallic multilayered composites, *Acta Mater.* 53 (18) (2005) 4817–4824.
- [88] C.A. Schuh, T.C. Hufnagel, U. Ramamurty, Mechanical behavior of amorphous alloys, *Acta Mater.* 55 (12) (2007) 4067–4109.
- [89] P. Noell, J. Carroll, K. Hattar, B. Clark, B. Boyce, Do voids nucleate at grain boundaries during ductile rupture? *Acta Mater.* 137 (2017) 103–114.