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The role of Ta on twinnability in nanocrystalline Cu–Ta alloys

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ABSTRACT

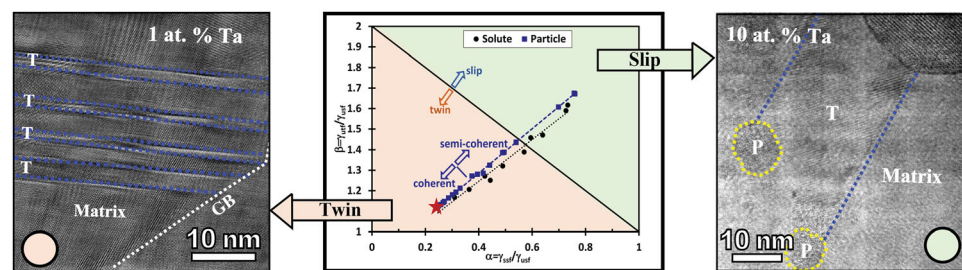
Nanostructured Cu–Ta alloys show promise as high-strength materials in part due to their limited grain growth. In the present study, we elucidate the role of Ta on the transition from deformation twinning to dislocation-mediated slip mechanisms in nanocrystalline Cu through atomistic simulations and transmission electron microscopy characterization. In particular, computed generalized stacking fault energy curves show that as Ta content increases there is a shift from twinning to slip-dominated deformation mechanisms. Furthermore, heterogeneous twinnability from microstructural defects decreases with an increase in Ta. The computed effect of Ta on plasticity is consistent with the HRTEM observations.

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KEYWORDS

Nanocrystalline; twinning; dislocation; TEM



IMPACT STATEMENT

We show for the first time using atomistic simulations and TEM that, similar to grain size, the Ta nano-particles can be used to tailor the governing deformation mechanisms in NC-alloys.

Metals with a mean grain size (d) below 100 nm, i.e. nanocrystalline (NC) materials, have garnered significant interest due to their superior mechanical properties as compared with coarse-grained materials.[1] A large number of experimental and computational studies have explored how grain boundary mediated plasticity and microstructural length scale affect the mechanical behavior of NC materials.[2–4] For example, the Hall–Petch [5,6] relationship describes the experimentally observed increase in yield strength with decreasing grain size down to diameters as small as 20 nm [1,2]; this behavior is generally followed by a plateau/negative slope region for grain sizes below a critical size (e.g. 8–15 nm for Cu [7]). This inverse Hall–Petch effect has been directly attributed to changes in the governing deformation

mechanisms away from traditional dislocation glide and pile-up processes.[8] Fundamental changes in deformation mechanisms are also known to cause many other intriguing and unexpected physical responses of NC metals, including altered strain rate and pressure dependence of deformation,[9] superplasticity,[10] and low-temperature creep,[11] to name a few.[12] Generally, these unique deviations in behavior are solely attributed to a continual reduction in grain size and an increase in the fraction of grain boundaries and triple junctions, which leads to experimentally reported mechanisms of deformation twinning, GB rotation/sliding and viscous flow.[13–15] Plastic instability [2,3,16,17] due to loss in the strain hardening behavior and grain growth (under both monotonic and cyclic loading) [18–20] have also

been observed in various pure NC materials at small grain sizes. The ability to utilize such unique deformation responses advantageously depends heavily on our ability to recognize and to engineer them within NC metals. That is, by restricting or promoting specific deformation mechanisms, it may be possible to elicit or tune unprecedented physical responses in these materials.

Recently, quasi-static and dynamic yield strengths of greater than 1 GPa were measured in bulk samples of a NC Cu–Ta, which could not be explained by grain size strengthening alone.[21] The increase in strength was attributed to the thermal decomposition of a non-equilibrium Cu-rich Cu–Ta solid solution over a range of temperatures (700–900°C), which led to the formation of a high density of small coherent Ta-rich atomic clusters (~ 2 nm in diameter).[21] The presence of these Ta precipitates within grains and along grain boundaries resulted in strength levels approximately two times higher than those predicted by Hall–Petch hardening alone.[22] These studies suggest that the presence of Ta-based clusters play a commanding role in defining the deformation response as compared with the NC grain size alone. However, there is no direct experimental evidence to date of how and why Ta has such a pronounced effect. This work shows for the first time that the mean Ta particle size and distribution, much like grain size, can be used to tailor the governing deformation mechanisms in NC immiscible alloys.

In this letter, the role that Ta particles play in altering the slip and deformation twinning response in previously reported NC Cu–Ta alloys is examined using a combination of generalized stacking fault energy (GSFE) surfaces along with high-resolution transmission electron microscopy (TEM) characterization. The GSFE curves are often employed to measure and understand the competition between dislocation slip and twinning, often referred to as the *twinnability* of the material.[23] Here, we used a large-scale atomic/molecular massively parallel simulator (LAMMPS) [24] along with a semi-empirical embedded atom potential (EAM) developed by Pun et al. [25] to compute the GSFE energy curves. This EAM potential was parameterized using an extensive database of energies and configurations from density functional theory (DFT) calculations of energy differences between various crystal structures of pure Cu and pure Ta, the formation energies of coherent Cu–Ta interfaces, and the binding energy of several ordered compounds, such as $L1_2$ –Cu₃Ta, $L1_0$ –CuTa, $L1_1$ –CuTa, B_2 –CuTa and $L1_2$ –Ta₃Cu.[25] More details on the validation of the EAM potential at different temperatures can be found in [25].

The relaxed GSFE curves (Figure 1(a)) were computed in LAMMPS using a rectangular slab structure having x , y , and z axes oriented along the $[11\bar{2}]$, $[11\bar{1}]$, and $[\bar{1}10]$ directions, respectively, with a $(11\bar{1})$ plane stacking sequence of ABCAB|CABC, see Figure 1(b). The simulation cell/supercell dimensions were $17.7\text{ nm} \times 12.5\text{ nm} \times 1\text{ nm}$ (Figure 1(g) and 1(h)). To compute GSFE curves, a 3 nm vacuum was added along the y direction while a periodic boundary condition was maintained along the other two directions. Then, the upper half crystal of the $(11\bar{1})$ plane was displaced along the x direction by a partial Burger's distance of $(a/\sqrt{6})$ to create a stable stacking fault (γ_{ssf}) with a stacking sequence of ABCAB|ABCA, as shown in Figure 1(d). From this point, either a trailing partial of the dissociated dislocation is nucleated or another partial dislocation of leading type on the adjacent plane is nucleated to form a microtwin (Figure 1(f)). For the emission of a trailing partial, Rice [26] showed that the required critical stress is a function of energy difference ($\gamma_{\text{usf}} - \gamma_{\text{ssf}}$) and the stacking sequence can be restored to ABCAB|CABC (Figure 1(b)). In the next step, the displacement was carried out on the adjacent $(11\bar{1})$ plane along the $[11\bar{2}]$ direction to create a microtwin (twin fault, γ_{utf}) with a stacking sequence of ABCABA|CAB, see Figure 1(f). During each incremental shear displacement, the structure was relaxed using a conjugate gradient algorithm with force and energy criteria of $10^{-12}\text{ meV/\AA}$ and 10^{-12} meV , respectively. To quantify the role of Ta on predominant deformation mechanisms (twin versus slip transition), the GSFE curves were computed for the Cu matrix with distinct Ta particle sizes, ranging from 0 to 10 nm in radius. While the Cu–Ta system is known to be a phase separated (immiscible) material,[27] GSFE curves for several non-equilibrium Cu–Ta solid solution (up to 10 at% Ta) were also computed, because these solid solutions can be expected to experimentally occur and persist over moderate temperature ranges.[28] In the case of solid solution Cu–Ta, Ta atoms were free to relax in all directions whereas Cu atoms were free to move along the $[11\bar{1}]$ direction only.

All GSFE curves with different Ta solute concentrations and Ta particle sizes are presented in Figure 2(a) and 2(b), respectively. The first local maximum corresponds to the unstable stacking fault energy (γ_{usf}), which is correlated to the energy barrier for the leading partial to propagate. In the case of Cu–Ta solid solutions, the γ_{usf} decreases with the addition of Ta solute. In contrast, the value of γ_{usf} was found to increase with the addition of Ta particles to the Cu matrix. Overall, in both cases, the stable stacking fault energy and unstable twinning fault energy (γ_{ssf} and γ_{utf} , respectively) increase

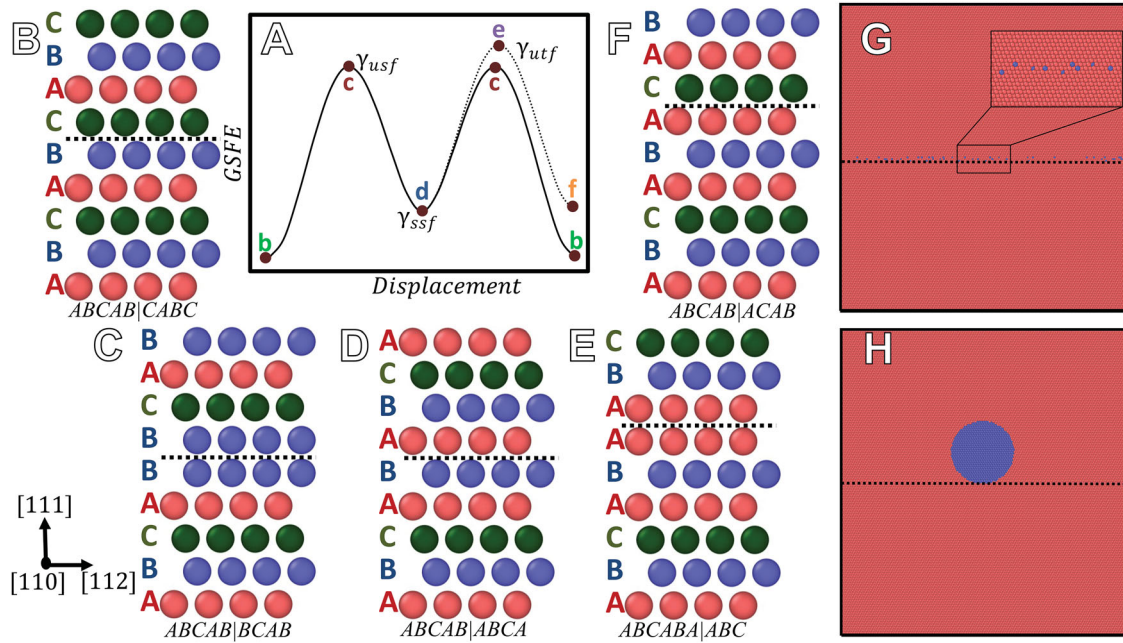


Figure 1. (a) Illustrative model for the GSFE calculation: (b) a perfect crystal with ABCAB|CABC stacking; (c) an unstable stacking fault (γ_{usf}) with ABCAB|BCAB stacking; (d) a stable stacking fault (γ_{ssf}) with ABCAB|ABCA stacking left behind by the leading partial; (e) an unstable twinning fault (γ_{utf}) with ABCABA|ABC stacking; (f) 2 layers microtwin with ABCABA|CAB stacking; (g) supercell with a random doping of Ta atoms; and (h) supercell with one Ta particle. Note that the red, blue and green atoms are A, B, and C stacking, respectively. In (g) and (h), the red and blue atoms correspond to copper and tantalum atoms, respectively. The dotted line in this figure represents the shear plane. For a twin fault to nucleate, the shear plane has to move by one atomic layer.

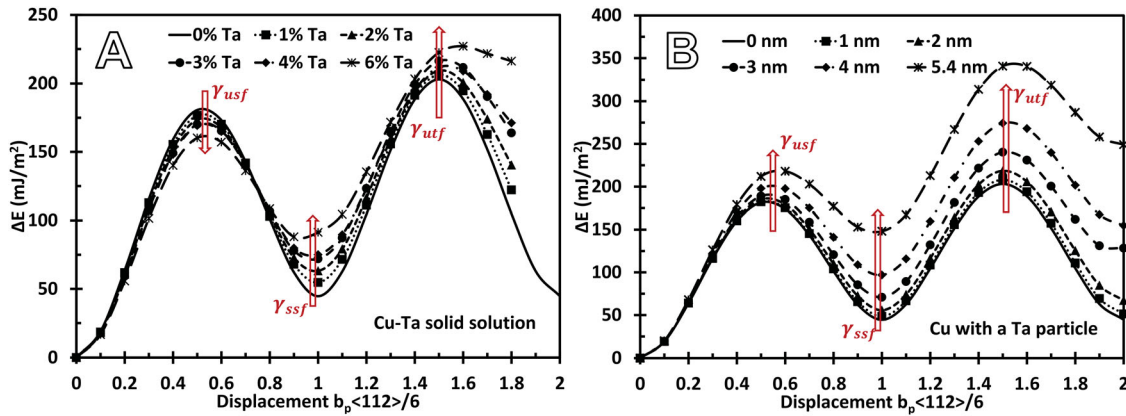


Figure 2. GSFE as a function of shear displacement along the [112] direction for (a) Cu–Ta solid solution alloys and (b) the Cu matrix with various sized Ta particles (radius). In both cases, we observed an increase in γ_{ssf} and γ_{utf} with addition to Ta.

with the addition of Ta. The ratios $\alpha = \gamma_{ssf} / \gamma_{usf}$ and $\beta = \gamma_{utf} / \gamma_{usf}$ can provide an insight into the observed changes in all three intrinsic properties (γ_{usf} , γ_{ssf} , and γ_{utf}) for different solute concentrations or particle sizes, as shown in Figure 3(a). If the ratio α , which is a ratio of the stable and unstable stacking fault energies, is close to one, then the energy barrier for a trailing partial is very low and the stacking fault width is very small, e.g. Al ($\alpha = \sim 0.97$).^[29] On the other hand and in the case of a pure Cu, the ratio α was found to be 0.24 (Figure 3(a), red

star), i.e. the energy barrier for a trailing partial is higher and, hence, the stacking fault width or extended partial can be observed across a grain size of 50 nm.^[30] However, the ratio α (Figure 3(a)) increases with the addition of Ta as a solid solution or in particle form, i.e. the stacking fault width decreases with a decrease in the energy barrier for the trailing partial (Figure 2). Furthermore, as the particle size increases, it is expected that the particle interface transitions from coherent to semi-coherent with respect to the Cu matrix ^[31]; this results in the

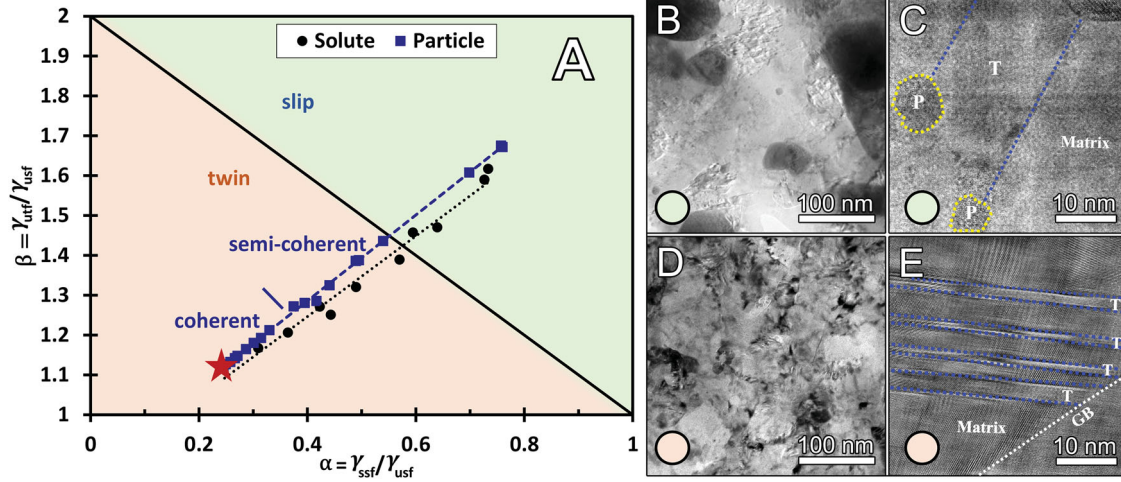


Figure 3. (a) Transition of deformation from slip to deformation twinning with increasing concentration of Ta (circle) and increasing particle size (diamond) in α - β coordinates. Note: Red star is a point with no Ta. Points under the ideal black line can form twins, while over the line, twinning is difficult. As the concentration of Ta as well as the Ta particle size increases, there is a transition from twinning to slip. Around a 2 nm radius particle size, there is a transition from a coherent boundary to a semi-coherent boundary for the particle as predicted by Eshelby.[31] TEM/HRTEM micrographs of (b, c) NC Cu-10 at% Ta (processed at 800°C) and (d, e) NC Cu-1 at% Ta (processed at 700°C). While the deformation in (b, c) is primarily dislocation-mediated (restricted by Ta particles, yellow outline), deformation in (d, e) occurs through twinning. The HRTEM images were taken in the $\langle 110 \rangle$ zone axis. For more details, please refer to the supplementary document which includes FFT images to indicate the nature of the feature (i.e.) twin boundaries.

ratio α increasing from 0.24 with no Ta to 0.30 for a Cu matrix with a 2 nm radius particle, see Figure 3(a). Similarly, as shown in Figure 3(a), a transition from twinning towards slip-dominated mechanisms occurs when the ratio α increases to approximately 0.69 for a 5.4 nm radius particle and 0.57 for the NC Cu-6% Ta solid solution.

The ratio of the unstable twinning fault energy to the unstable stacking fault energy, $\beta = \gamma_{\text{utf}}/\gamma_{\text{usf}}$, can also help explain the role of Ta on deformation twinning in NC Cu-Ta alloys. For pure Cu, the ratio β is close to unity (~ 1.11), i.e. the energy barrier for a twin fault is smaller and hence, nucleating a twin fault is relatively easy. However, as the value of β increases, the energy barrier (Figure 2) as well as the stress required to nucleate twin increases. In the present study, the ratio β increases with both increasing Ta solute concentrations or increasing Ta particle sizes (Figure 3(a)). For example, Figure 3(a) shows that the ratio β is 1.11, 1.18, and 1.60 for Cu with no Ta, Cu with 2 nm radius semi-coherent Ta particle, and Cu with 5.4 nm radius Ta particle size, respectively. This suggests that similar to grain size as discussed in [14,15], Ta particles can be used to tailor twinnability, with coherent particles increasing the density of deformation twinning and incoherent particles promoting dislocation-based plasticity. This is also true for the dissolved Ta content in solid solution. This has practical significance as the deformation response and microstructure of these materials will

depend heavily on the choice of bulk consolidation processing variables such as composition, temperature, and or pressure/degree of deformation.

TEM observations confirm this hypothesis. Figure 3 shows TEM results which compares the twin and dislocation contents in two different NC Cu-Ta alloys synthesized and consolidated through high-energy ball milling and equal channel angular processing. For additional processing details and sample preparation details, refer to the supplementary documents. Figure 3(b)-(e) shows ECAE processed bulk samples for NC Cu-10 at% Ta (800°C, Figure 3(b)-(c)) and NC Cu-1 at% Ta (700°C, Figure 3(d)-(e)), where the lighter areas represent Cu and darker areas represent the Ta phase. These two processing conditions were chosen as the mean grain size and their distributions are comparable (NC Cu-10% Ta has a mean grain size of 118 nm and NC Cu-1% Ta has a mean grain size of 126 nm). As the grain sizes of the alloys are comparable (Figure S1), the effect of Ta concentration on the deformation mechanism can be isolated. While both alloys contain Ta-rich particles, the NC Cu-10 at% Ta alloy has a higher density of both smaller (diameter < 10 nm) and larger particles (diameter of 50–100 nm) compared with the NC Cu-1 at% Ta sample.[9] Using HRTEM characterization along the $\langle 110 \rangle$ zone axis, we show that in (Figure 3(c)), the Ta-based particles (outlined using yellow dotted lines) can be seen at the end of a twin (outlined using blue dotted lines)

blocking the twin boundary from growing on either end. On the other hand, the twin boundaries (outlined using blue dotted lines) in Figure 3(e) are not constrained by the Ta-based particles. For more details, please refer to the supplementary document which includes fast Fourier transform (FFT) images to indicate the nature of the feature (i.e.) twin boundaries, see Figure S2. The average twin density per unit area obtained over multiple regions is $\sim 1 \times 10^{12} \text{ m}^{-2}$ for NC Cu-10 at% Ta and is $\sim 4 \times 10^{12} \text{ m}^{-2}$ for the NC Cu-1 at% Ta sample. These experimental observations are in good agreement with the computational results where the NC Cu-10 at% Ta alloy is expected to exhibit dislocation-dominated plasticity and the NC Cu-1 at% Ta alloy is expected to exhibit twin-dominated deformation.

Last, the role of Ta on homogeneous and heterogeneous twin nucleation as compared with dislocation nucleation in NC Cu-Ta can be inferred from the ratios α and β computed from GSFE calculations. As described by Cai et al., [23] the homogeneous twinning ability (T_{OR} , OR stands for crystal orientation) in NC Cu due to the influence of orientation and GSFE is given by

$$T_{OR} = \tan^{-1} \left(\frac{\beta - 1}{\alpha - 1} \right) + \frac{\pi}{4}, \quad (1)$$

Tadmor and Hai [29] proposed a simple criterion for inhomogeneous or heterogeneous nucleation of twins from crack tips in the absence of strain rate and temperature. This criterion is expected to be valid because thermal activation does not play an important role in deformation twinning.[32] Moreover, extending to high rates, materials twin more easily at high strain rates compared with lower strain rates, so this criterion is expected to be the lower bound for predicting twin

nucleation.[32] Hence, twins nucleate at the tips of moving cracks where stresses and strain rates are high.[33] Therefore, twinnability from an ideal crack tip (T_{CT}) without temperature and strain rate is

$$T_{CT} = [1.136 - 0.151\alpha]/\sqrt{\beta}. \quad (2)$$

Similarly, Asaro and Suresh [34] proposed a criterion for heterogeneous twin nucleation (T_{GB}) from a grain boundary, i.e.

$$T_{GB} = \sqrt{(3 + 2\alpha)/\beta}. \quad (3)$$

In all three cases, the condition when $T > 1$ favors a twin partial emission over the trailing partial. For pure Cu, the twinning criteria values are 1.76, 1.03, and 0.62 for T_{GB} , T_{CT} , and T_{OR} , respectively; these agree well with published literature values of 1.55, 0.95, and 0.58 for T_{GB} , [34] T_{CT} [29] and T_{OR} , [23] respectively. Hence, heterogeneous deformation twins nucleate from crack tips and grain boundaries. Furthermore, the above three criteria for twinning tendency from different nucleation sites can be understood through an intrinsic twinnability factor η ($\eta = (\gamma_{usf} - \gamma_{ssf})/(\gamma_{utf} - \gamma_{ssf})$), which only depends on the material's intrinsic properties γ (stacking fault energies, Figure 2). Figure 4 shows the effect of Ta concentration on the twinnability for homogeneous (T_{OR}) twin formation, which is more predominant than for heterogeneous (T_{CT} and T_{GB}) twin formation, i.e. $T_{OR} \propto \beta/\alpha$; whereas T_{CT} & $T_{GB} \propto \alpha/\beta$ (where $\beta > 1$ and $\alpha < 1$). Hence, as the percentage of Ta increases (right to left on Figure 4), the rate of decrease in twinnability is greater for a homogeneous twins (T_{OR}) compared with heterogeneous twins (T_{CT} and T_{GB}) for both solid solution (Figure 4(a)) and Ta particle size (Figure 4(b)). Our result predicts that the formation of

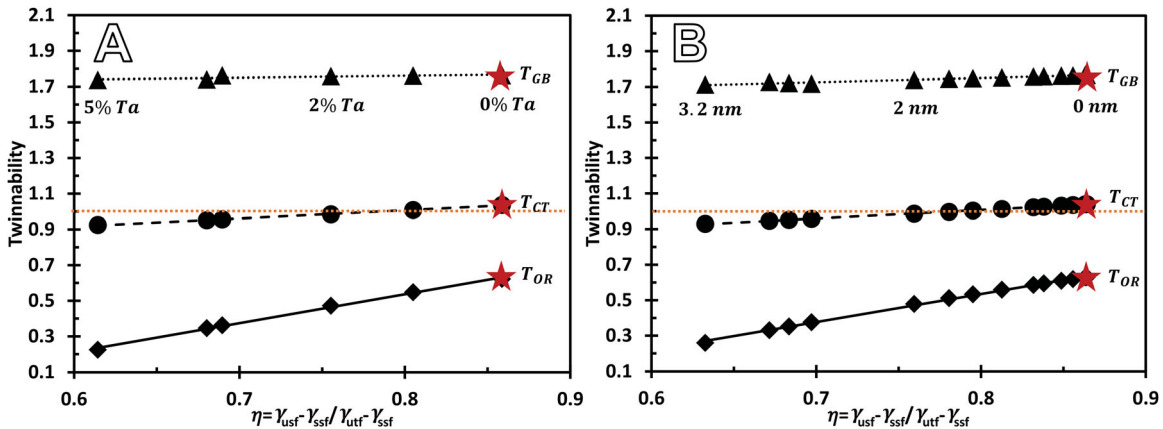


Figure 4. Twinnability as a function of intrinsic twinnability factor η for (a) solid solution of Ta atoms and (b) different sizes of tantalum particle. Red star points indicate pure Cu (no Ta). Diamond points are for homogeneous twins, while circles and triangles are for heterogeneous twins from a crack tip and a grain boundary, respectively. With an increase in the concentration of Ta, there is a decrease in homogeneous twins.

trailing partials is favored over that of twinning partials from crack tips ($T_{CT} < 1$) for a given Ta particle size of 1.8 nm in radius ($T_{CT} = 0.94$) and for 3 at% Ta atoms ($T_{CT} = 0.95$). There is no transition from a twinning partial to trailing partial in case of heterogeneous twin nucleation at the grain boundary.

In summary, we elucidate the role of Ta on the transition from twinning to slip-dominated deformation mechanisms in Cu-Ta alloys through atomistic simulations and TEM experiments. In particular, we computed GSFE curves and showed that as Ta content increases, there is a shift from a twin-dominated towards a dislocation-dominated deformation mechanism. Thus, similar to grain size as discussed in [14,15], Ta particles can be used to tailor twinnability, with coherent particles increasing the density of deformation twinning and incoherent particles promoting dislocation-based plasticity. Furthermore, heterogeneous twinnability from microstructural defects such as grain boundaries decreases with an increase in Ta content. The observed effect of Ta on plasticity is consistent with the TEM observations.

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Disclosure statement

No potential conflict of interest was reported by the author.

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