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ABSTRACT

An earlier dislocation model for predicting the grain size effect on deformation twinning in nanocrystalline (nc) face-centred-cubic (fcc) metals has been found valid for pure metals but problematic for alloys. The problem arises from the assumption that the stacking-fault energy (γ_{SF}) is twice the coherent twin-boundary energy (γ_{fcc}), which is approximately correct for pure fcc metals, but not for alloys. Here we developed a modified dislocation model to explain the deformation twinning nucleation in fcc alloy systems, where $\gamma_{SF} \neq 2\gamma_{twin}$. This model can explain the differences in the formations of deformation twins in pure metals and alloys, which is significant in low stacking-fault energy alloys. We also describe the procedure to calculate the optimum grain size for twinning in alloy systems and present a method to estimate γ_{twin}.

1. Introduction

Nanostructured metals and alloys usually have very high strength, but low ductility [1–3]. Growth twins and deformation twins are two of a few approaches that can simultaneously improve the strength and ductility of nanostructured metals [4–7]. Lu et al. [8] used high density of growth nanotwins to significantly improve the strength of copper, without degrading its conductivity. Zhang et al. [9] fabricated a 330 stainless-steel thin film by magnetron sputtering deposition, with high hardness due to nanoscale twins. There are three main mechanisms for twins to improve mechanical properties. First, twin boundaries can effectively block dislocation slip, similar to grain boundaries, to increase the yield strength [10–12]. Second, defective twin boundaries could also serve as dislocation sources for further plastic deformation [13,14]. Third, the accumulation of dislocations on twin boundaries leads to higher strain hardening rate, which consequently improves the ductility [6,12,15]. In addition, twins are also reported to increase the strain rate sensitivity, which also helps improve ductility [16].

Deformation twinning has been studied extensively in recent decades. One of the fundamental issues is the formation mechanisms of deformation twins [4]. Corse-grained face-centred cubic (fcc) metals are believed to deform by twinning via the pole mechanism

[17], prismatic glide mechanism [18], faulted dipole mechanism [19], three-layer mechanism [20], etc. However, the formation mechanism of deformation twins in nanostructured metals has been reported to be different from those of coarse-grained metals. Experimental observations and MD simulation revealed multiple twinning mechanisms, including overlapping stacking-fault ribbons [21], partial emission from grain boundaries [22], low to zero macroscopic strain twinning via random emission of partials [23], grain boundary splitting and migration [24], sequential twinning [25], partial multiplication at twin boundaries [26] and dislocation rebound mechanism [16], etc.

Based on partial emission from grain boundaries, Zhu et al. [27,28] developed an analytical model to describe the normal and inverse grain size effect on the nucleation and growth of deformation twins in nanocrystalline fcc metals and found the existence of an optimum grain size for twinning, relating to critical stress. Later, Wu et al. [29], experimentally observed such grain size effect in nanocrystalline Ni. The optimum grain sizes predicted by the analytical model agreed surprisingly well with experimentally values for many nanocrystalline pure fcc metals [29,30]. One of the assumptions used in the model derivation was that stacking-fault energy was twice the coherent twin-boundary energy, i.e. $\gamma_{SF} = 2\gamma_{twin}$. However, in alloy systems, $\gamma_{SF} = 2\gamma_{twin}$ may be no longer valid, because alloy is not always homogeneous and the local bonding of atoms would have a preference that changes the relationship of γ_{SF} and γ_{twin} [31]. Therefore, the critical stress and optimum grain size for twinning can no longer be described reasonably by the model. Indeed significant discrepancy has been observed between the experimental data and the optimum grain size for twinning in nanocrystalline Cu–Zn alloys [30].

It has been reported that the stacking-fault energy and twin-fault (coherent twin boundary) energy may change independently for many alloys [32]. Therefore, independent variations of γ_{SF} and γ_{twin} need to be considered in modelling the formation of deformation twins in nanocrystalline alloys. Although γ_{twin} is important for the formation of deformation twins in alloy systems, it is difficult to find γ_{twin} data for most alloys [33]. Meanwhile, some researchers utilised inaccurate methods to calculate γ_{twin}, and those results were not dependable [34].

In this paper, we modified the early nucleation model for deformation twins for pure fcc metals to make it suitable for alloy systems. We also studied the effect of the ratio $2\gamma_{SF}/\gamma_{twin}$ on the optimum grain size for twinning when it deviated from 1, the case for pure fcc metals. The model was applied to the Cu–Zn system and Cu–Al systems, in which some experimental data were available.

2. Model development

In recent studies, both simulation results [24,35] and experimental data [36–38] showed that deformation twins in nanocrystalline metals were largely formed by the emissions of Shockley partials from grain boundaries. Based on these observations, the earlier analytical model for deformation twinning described the twin nucleation in two steps: (1) stacking-fault generation across the whole grain by a partial dislocation from a dissociated lattice dislocation, and (2) twinning partial emission on an adjacent slip plane. This two-step theory agreed well with some experimental observations [39,40]. Because the nanostructured materials are usually produced by severe plastic deformation techniques [39–41], which produce high density of dislocations at grain boundaries, the emission of partial
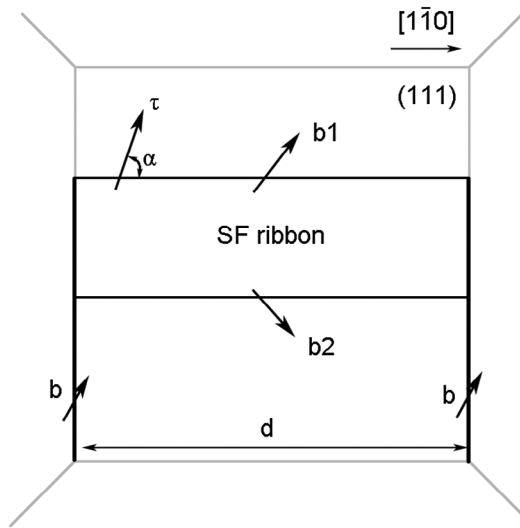
Figure 1. A schematic illustration of the dislocation model for deformation twinning nucleation in screw system.

dislocations do not need to overcome the energy barriers as described in the generalised planar fault energy curve. In addition, to keep the current model simple, we do not consider the influence of short-range order, which has influence in the movement of dislocations in some alloy systems [42–44]. In other words, only stacking-fault energy, shear modulus and lattice parameters are involved in the analytical model for pure metals [27]. In the model derivation for alloys, we follow the same steps, but also introduce the ratio $\gamma_{SF}/\gamma_{twin}$.

In the fcc systems, there exist three scenarios in which a lattice dislocation can dissociate into two partials to nucleate a twin: the screw system, 60° I system and 60° II system [28]. In our earlier study [27], compared with screw system and 60° I system, 60° II system needs a much higher shear stress to be activated, thus the probability of the 60° II system to form a deformation twin is much lower. In the following, we only analyse the screw system and 60° I system.

2.1. Screw system

In this section, we would like to analyse the screw system in detail, as shown in Figure 1. Assuming the grains in a sample are randomly oriented and the orientation distribution is the same for grains in all size ranges. To move the first partial dislocation from grain boundary, the critical external resolved shear stress τ_p can be described as [28]:

$$\tau_p = \frac{1}{\cos(\alpha - 30°)}\left[\frac{\sqrt{6}\gamma_{SF}}{a} + \frac{Ga(4 - v)}{8\sqrt{6}\pi(1 - v)d}\ln\left(\frac{\sqrt{2}d}{a}\right)\right] \qquad (1)$$

where γ_{SF} is stacking-fault energy; α is the angle between shear stress and the partial dislocation; a is lattice parameter; v is Poisson's ratio; G is shear modulus; d is the grain size.

Following the same procedure, we obtain the critical resolved shear stress τ_l to move a lattice screw dislocation [28]:

$$\tau_l = \frac{Ga}{2\sqrt{2}\pi(1-v)d\cos(\alpha)} \ln \frac{\sqrt{2}d}{a} \tag{2}$$

After a partial dislocation slip produces a stacking-fault, the slip of a twinning partial on adjacent slip plane will generate a two-layer twin nucleus, and the stacking-fault is replaced by two twin boundaries. For pure fcc metals, stable twin-boundary energy (γ_{twin}) is about half the stacking-fault energy [45]. In an alloy system, the relationship $\gamma_{SF} = 2\gamma_{twin}$ no longer exists [33,34]. Therefore, additional energy barrier for the nucleation of a twin can be described as:

$$\Delta E = 2\gamma_{twin} - \gamma_{SF} \tag{3}$$

Substituting (3) into (1) yields the critical external shear stress to form a twin:

$$\tau_{twin} = \frac{1}{\cos(\alpha - 30°)}\left[\frac{\sqrt{6}(2\gamma_{twin} - \gamma_{SF})}{a} + \frac{Ga(4-v)}{8\sqrt{6}\pi(1-v)d}\ln\left(\frac{\sqrt{2}d}{a}\right)\right] \tag{4}$$

We introduce a new coefficient λ, named alloy factor, defined as:

$$\lambda = \frac{2\gamma_{twin}}{\gamma_{SF}} \tag{5}$$

Equation (4) can be rewritten as:

$$\tau_{twin} = \frac{1}{\cos(\alpha - 30°)}\left[\frac{\sqrt{6}(\lambda - 1)\gamma_{SF}}{a} + \frac{Ga(4-v)}{8\sqrt{6}\pi(1-v)d}\ln\left(\frac{\sqrt{2}d}{a}\right)\right] \tag{6}$$

The trailing partial, with a burgers vector $\mathbf{b_2}$ (see Figure 1) is driven by external shear stress and stacking-fault energy, which can be written as [28]:

$$\tau_{trail} = \frac{1}{\cos(\alpha + 30°)}\left[\frac{\sqrt{6}Ga(8+v)}{48\pi(1-v)d}\ln\left(\frac{\sqrt{2}d}{a}\right) - \frac{\gamma_{SF}}{a}\right] \tag{7}$$

Only if the twinning partial prevails over the trailing partial ($\tau_{trail} > \tau_{twin}$) will it successfully form a deformation twin [28]. Thus setting $\tau_{trail} = \tau_{twin} = \tau_c$, we will obtain the optimum size of grains for twinning:

$$\frac{1}{d_c}\ln\left(\frac{\sqrt{2}d_c}{a}\right) = \frac{48\pi\gamma_{SF}}{Ga^2}\left[\frac{(1-v)(\lambda - 1)\cos(\alpha + 30°) + (1-v)\cos(\alpha - 30°)}{(8+v)\cos(\alpha - 30°) - (4-v)\cos(\alpha + 30°)}\right] \tag{8}$$

$$\tau_c = \frac{\gamma_{SF}}{a}f(\alpha) \tag{9}$$
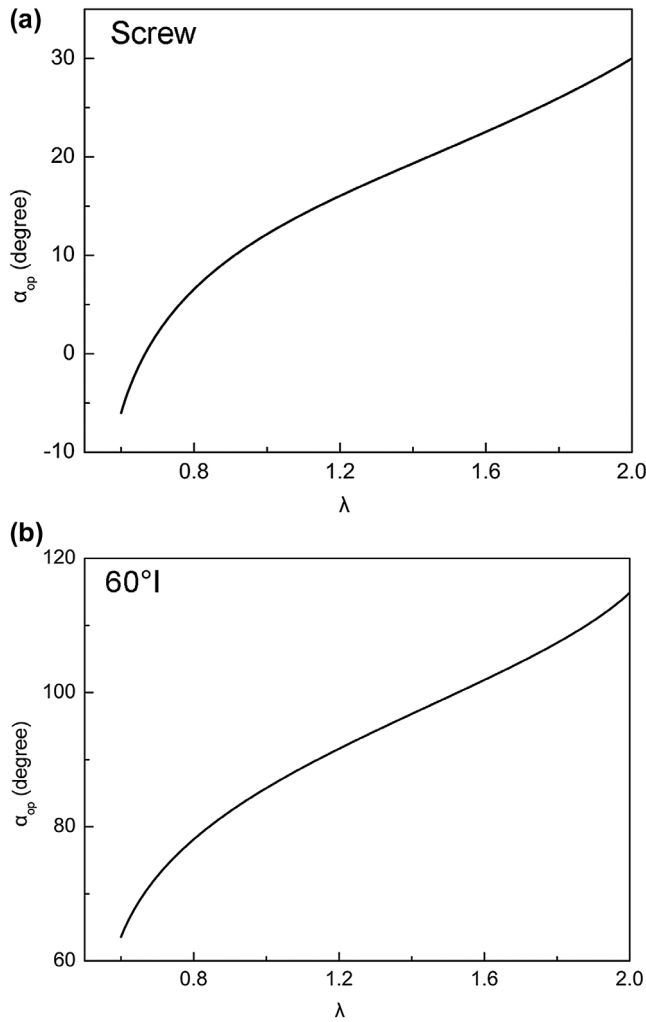
where

(a)

(b)

Figure 2. (a) The relationship between α_{op} (defined in Figure 1) and $\lambda = 2\gamma_{twin}/\gamma_{SF}$ for the screw system; (b) The relationship between α_{op} and $\lambda = 2\gamma_{twin}/\gamma_{SF}$ for the 60° I system.

$$f(\alpha) = \frac{12\sqrt{2}}{\cos(\alpha)}\left[\frac{(\lambda - 1)\cos(\alpha + 30°) + \cos(\alpha - 30°)}{(8 + \nu)\cos(\alpha - 30°) - (4 - \nu)\cos(\alpha + 30°)}\right] \quad (10)$$

Because $f(\alpha)$ varies less than 0.03% when Poisson's ratio ν varied from 0.27 to 0.44 [28], we can set $\nu = 0.33$. For a known λ value, setting $\mathrm{d}f(\alpha)/\mathrm{d}\alpha = 0$, we can solve optimum α_{op} at which $f(\alpha)$ is at its minimum, and τ_c is smallest. α_{op} is only related to λ. Their relationship is plotted as Figure 2(a). After acquiring α_{op} with a specific λ, substituting α_{op} back to Equation (8), the optimum grain size for twinning d_{op} at a specific λ can be obtained.

2.2. 60° I system

Following similar procedure, we can derive the critical stress, optimum stress orientation α_{op} and optimum grain size d_{op} for the 60° I system. τ_p, τ_l, τ_{trail} and τ_{twin} are derived as:

$$\tau_p = \frac{1}{\sin(\alpha)}\left[\frac{\sqrt{6}\gamma_{SF}}{a} + \frac{Ga}{2\sqrt{6\pi}d}\ln\left(\frac{\sqrt{2}d}{a}\right)\right] \tag{11}$$

$$\tau_l = \frac{Ga(4-3v)}{8\sqrt{2}(1-v)d\cos(\alpha-60°)}\ln\left(\frac{\sqrt{2}d}{a}\right) \tag{12}$$

$$\tau_{twin} = \frac{Ga}{2\sqrt{6\pi}d\sin(\alpha)}\ln\left(\frac{\sqrt{2}d}{a}\right) + \frac{\sqrt{6}(\lambda-1)\gamma_{SF}}{a\sin(\alpha)} \tag{13}$$

$$\tau_{trail} = \frac{\sqrt{6}}{\cos(\alpha-30°)}\left[\frac{Ga(8-5v)}{48\pi(1-v)d}\ln\left(\frac{\sqrt{2}d}{a}\right) - \frac{\gamma_{SF}}{a}\right] \tag{14}$$

Setting $\tau_{trail} = \tau_{twin} = \tau_c$, the critical size and critical stress is:

$$\frac{1}{d_c}\ln\left(\frac{\sqrt{2}d_c}{a}\right) = \frac{48\pi\gamma_{SF}}{Ga^2}\left[\frac{(1-v)\sin(\alpha) + (1-v)(\lambda-1)\cos(\alpha-30°)}{(8-5v)\sin(\alpha) - 4(1-v)\cos(\alpha-30°)}\right] \tag{15}$$

$$\tau_c = \frac{\gamma_{SF}}{a}f(\alpha) \tag{16}$$

where

$$f(\alpha) = \frac{3\sqrt{2}(4-3v)}{\cos(\alpha-60°)}\left[\frac{(v-1)\cos(\alpha-30°) + \sin(\alpha)}{(8-5v)\sin(\alpha) - 4(1-v)\cos(\alpha-30°)}\right] \tag{17}$$

Following the same procedure for the screw system, we can obtain the relationship between λ and optimum angle α_{op} (plotted in Figure 2(b)), as well as the relationship between λ and optimum grain size d_{op}.

3. Results and discussion

3.1. Optimum grain size for deformation twinning

The average optimum grain size can be described as [4]:

$$d_{op}^{average} = (d_{op}^{screw} + d_{op}^{60°I})/2 \tag{18}$$

Assuming the lattice parameter $a = 0.363$ nm, shear modulus $G = 44$ GPa and $v = 0.33$, we can calculate the optimum size variation with λ (from 0.6 to 2.0) in the screw and 60° I
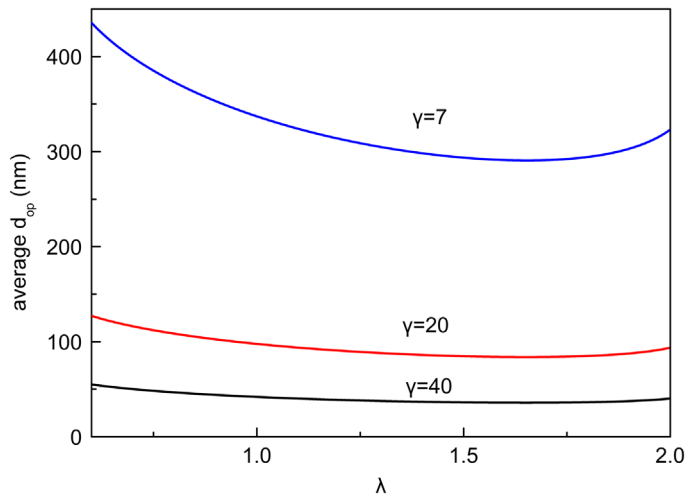
Figure 3. (colour online) The variation of optimum grain size with λ for varying stacking-fault energies for a hypothetical fcc Alloy system.

systems. As plotted in Figure 3, the average optimum size decreases almost monotonically with increasing λ in the range of 0.6–2.0. It is obvious that the optimum grain size decreases with increasing γ_{SF}, which is in the same trend as in our earlier model [27]. Figure 4 also shows that λ has a larger influence on the optimum grain size for twinning for alloys with smaller stacking-fault energy. For example, in the range from 0.6 to 2.0, λ can cause an optimum grain size to vary by ~30% at γ_{SF} = 7 mJ/m², but causes very little variation at γ_{SF} = 40 mJ/m². Therefore, for alloy systems with low stacking-fault energy, the influence of λ on the optimum grain size for twinning needs to be considered, and this explains experimental observation in the Cu–Zn systems [30].

3.2. Calculation for optimum grain size

To our knowledge, there has been no report on the optimum grain size for twinning of the Cu–Al system. In this section, we will calculate the optimum grain size based on our alloy model. γ_{SF} and γ_{twin} of pure Cu, Cu–5.0%Al and Cu–8.3%Al can be obtained from literature [34], and λ are 1, 1.60 and 1.57 for these three alloys (calculated from the data reported in the reference). Knowing λ, we can acquire the critical angle, α_{op}, by derivative of Equation (10). Because the shear modulus varies very little for Cu–Al system [46], we use G = 44GPa in the calculation for all three alloys. The parameters for calculation are listed in Table 1, and the results calculated by our model are presented in Table 2.

τ_{twin} (black line) and τ_{trail} (red line) for screw system are plotted in Figure 4. Since the τ_{twin} and τ_{trail} are plotted at the optimum angle, at which minimum shear stress is required for the nucleation of a deformation twin, the critical size in Figure 4 is also the optimum grain size for twinning. Similarly, the optimum grain size of 60° I system can also be obtained. After calculating the average d_{op} of two systems, the optimum grain size of Cu, Cu–5.0%Al and Cu–8.3%Al can be found as ~37, ~74 and ~260 nm using Equation (18). Among the three compositions we calculated, Cu–8.3%Al has the lowest stacking-fault energy, the
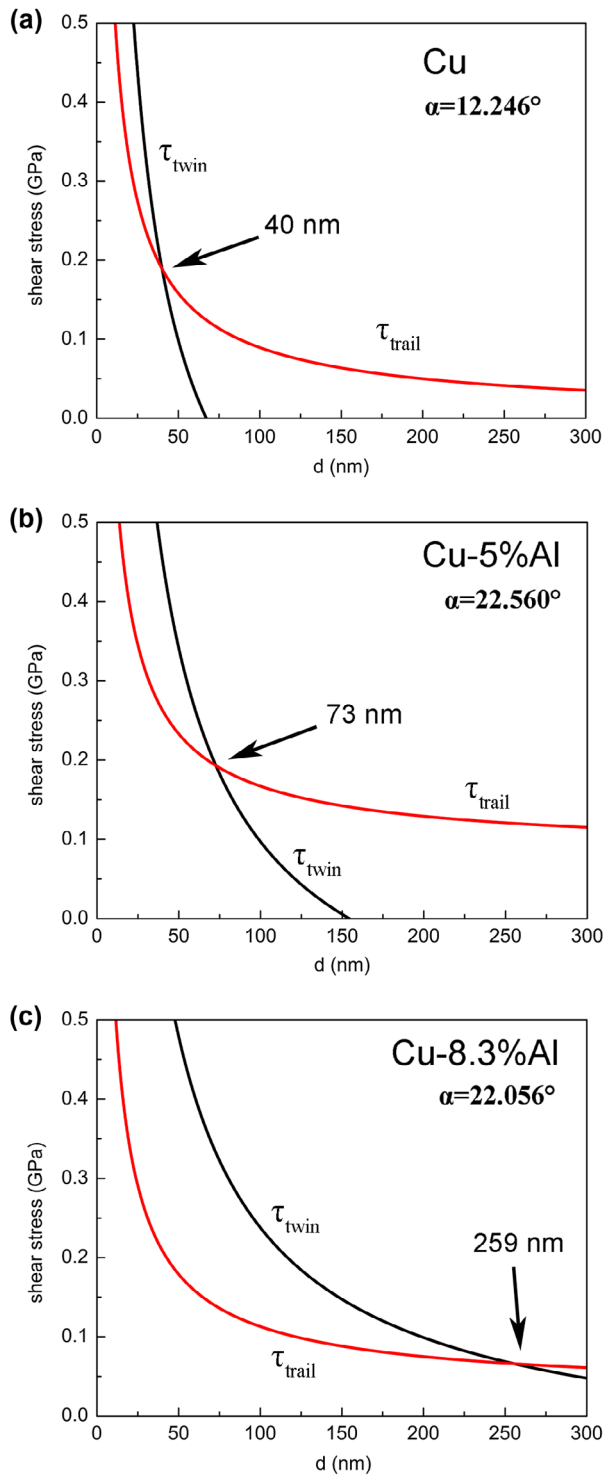
Figure 4. (colour online) Critical grain size for twin nucleation at the optimum angle *a* for screw system in Cu–Al systems: (a) Cu; (b) Cu–5%Al; (c) Cu–8.3%Al.

Table 1. The parameters for Cu–Al calculation [34,46].

Compositions	γ_{SF} (mJ/m²)	$2\gamma_{twin}$ (mJ/m²)	λ	Lattice parameter (nm)	Poisson's ratio
Cu	40	40	1	0.365	0.31
Cu–5%Al	20	32	1.60	0.364	0.325
Cu–8.3Al	7	11	1.57	0.364	0.33

Table 2. Calculated results.

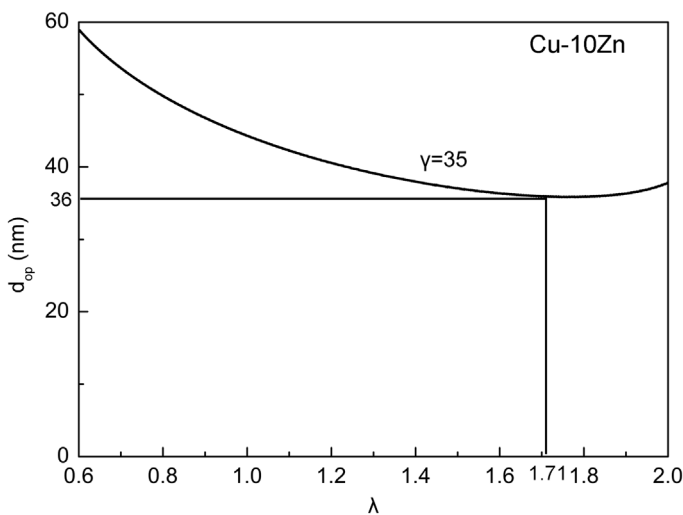| Compositions	a_{op} (screw)	d_{op} (screw) (nm)	a_{op} (60° I)	d_{op} (60° I) (nm)	d_{op} (previous model) (nm)	d_{op} (modified model) (nm)
Cu	12.246°	40	86.088°	34	37	37
Cu–5%Al	22.560°	73	101.946°	69	96	71
Cu–8.3%Al	22.056°	259	101.100°	225	335	242

Figure 5. d_{op} vs. λ for Cu–10Zn.

modified d_{op} is 30% smaller than the result calculated by the earlier model (using $\lambda = 1$), which is consistent with our earlier discussion that the alloy effect is more significant in low stacking-fault energy materials. Although we do not have the optimum grain size data for Cu–Al systems, the observation in Cu–Zn systems, whose alloy factor is also larger than 1, show that optimum grain size is smaller than what is calculated by the previous model [30]. This is consistent with the current alloy model for twin nucleation.

3.3. Estimation for twin forming energy

Because the data of stable twin-boundary energy are lacking in the literature, our model presents a method to estimate twin-boundary energy (γ_{twin}), with the help of experimentally observed optimum grain size. The experimentally observed optimum sizes are 35 and 45 nm for Cu–10Zn and Cu–15Zn, respectively [30]. The stable stacking-fault energies are 35 and 25 mJ/m² for Cu–10Zn and Cu–15Zn [33]. Thus, this model gives us a simple method to estimate γ_{twin} of Cu–Zn system.
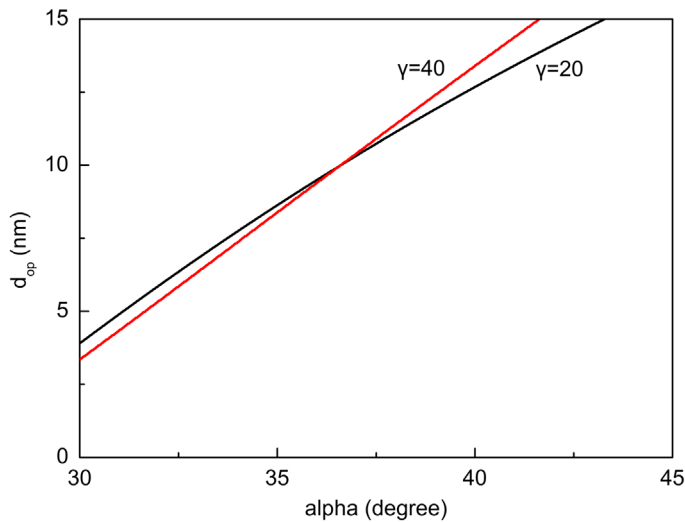
Figure 6. (colour online) The optimum grain size vs. angle α in 60° I dislocation system.

To estimate γ_{twin} of the system, we need to find the λ of the system, taking Cu–10Zn as an example. We plot the optimum grain size vs. λ (Figure 5) at stable stacking-fault energy that is 35 mJ/m². Though the experimental observed optimum grain size is ~35 nm for Cu–10Zn, the calculated result of our model is ~36 nm. We drew a horizontal line from 36 nm, and the x-coordinate of intersection is 1.71, thus λ is 1.71 for Cu–10Zn. Similarly, we can find λ as 1.78 for Cu–15Zn. With λ values, we can estimate the γ_{twin} for these two different systems as 20 and 14 mJ/m², respectively.

3.4. Influence of orientation

For simplicity, we have assumed in our model that the grains are randomly oriented and only consider the optimum angle, which represents the direction that needs the least shear stress. However, for the deformation of textured nanostructured alloys, the shear stress angle α is no longer random [47,48]. Under this circumstance, the effect of shear stress angle α may need to be considered, and will have obvious influence on the optimum grain size.

Taking Cu and Cu–5%Al system as an example, stacking-fault energy (20 mJ/m²) of Cu–5%Al is lower than Cu (40 mJ/m²), which means the optimum size of Cu–5%Al is always larger than Cu based on our model, if the direction of stress is its optimum angle. However, after considering the influence of orientation, the optimum grain size of Cu–5%Al could become smaller than Cu in a specific α range (from 30° to 35° for 60° I system), as shown in Figure 6. This is because in this range, the shear stress for Cu–5%Al is much bigger than Cu and twinning occurs due to the large shear stress.

4. Conclusion

By modifying an earlier partial emission-based pure metal model, we were able to describe the nucleation of deformation twinning in nanostructured alloys. Considering varying ratio

of γ_{SF} to γ_{twin} in alloys, we have derived a modified optimum grain size and critical stress for deformation twinning, by introducing the alloy factor $\lambda = 2\gamma_{twin}/\gamma_{SF}$. Our model indicates that λ has an influence on the optimum grain size, especially for low stacking-fault energy alloys. It also provides a new relationship among γ_{SF}, γ_{twin} and d_{op}, for which one can estimate the twin-fault energy. We also reveal that the optimum grain size can vary with texture and the orientation of applied stress. In addition, we would like to point out that the current model cannot be applied in fcc alloy systems with short-range order of alloy elements.

Disclosure statement

No potential conflict of interest was reported by the authors.

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