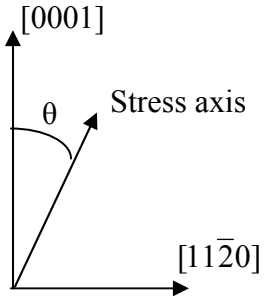
Department of Materials Science and Engineering
Massachusetts Institute of Technology
3.14 Physical Metallurgy – Fall 2003

Solutions to Problem Set #4

4.1 For a certain HCP metal, the shear stress required to activate twinning on a $(11\bar{2}1)$ plane is three times the shear stress to activate slip on the basal plane. Consider single crystals of this metal, pulled in tension on a stress axis that lies between [0001] and $[11\bar{2}0]$:

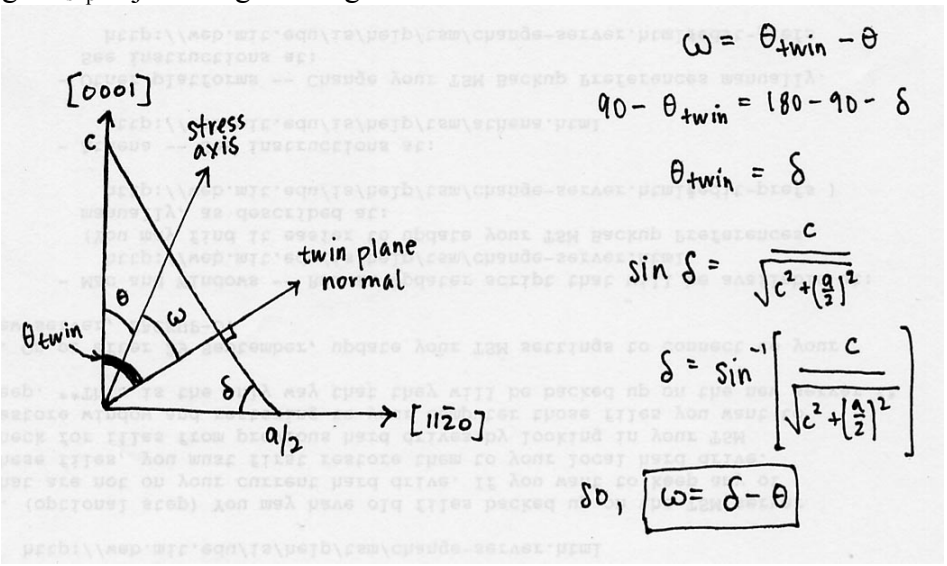


For some values of θ, twinning will be active, and for some θ slip will be active. Assuming that the twinning direction and slip direction are the same for all values of θ, calculate each of these ranges for an arbitrary assignment of c/a.

We need to find the values of θ for which $\frac{\tau_{twinning}}{\tau_{slip}} > 3$. In other words, what is the stress acting on the slip system and twinning system? We can use the Schmid factor construction to determine this. Lets call the angle between the twin plane normal and the stress axis ω.

$$\frac{\tau_{twinning}}{\tau_{slip}} = \frac{\cos\omega \cdot \cos\phi_{twin}}{\cos\theta_{slip} \cdot \cos\phi_{slip}}$$

Since they are acting in the same direction, $\cos\phi_{twin} = \cos\phi_{slip}$. Also, the slip plane is (0001), so that the angle θ_{slip} is just the given angle θ. Now we have to find ω which will be a function of c/a and θ.



Change between slip & twinning is when

$$\frac{\cos\omega}{\cos\theta} = 3 \rightarrow \frac{\cos(\delta-\theta)}{\cos\theta} = 3$$

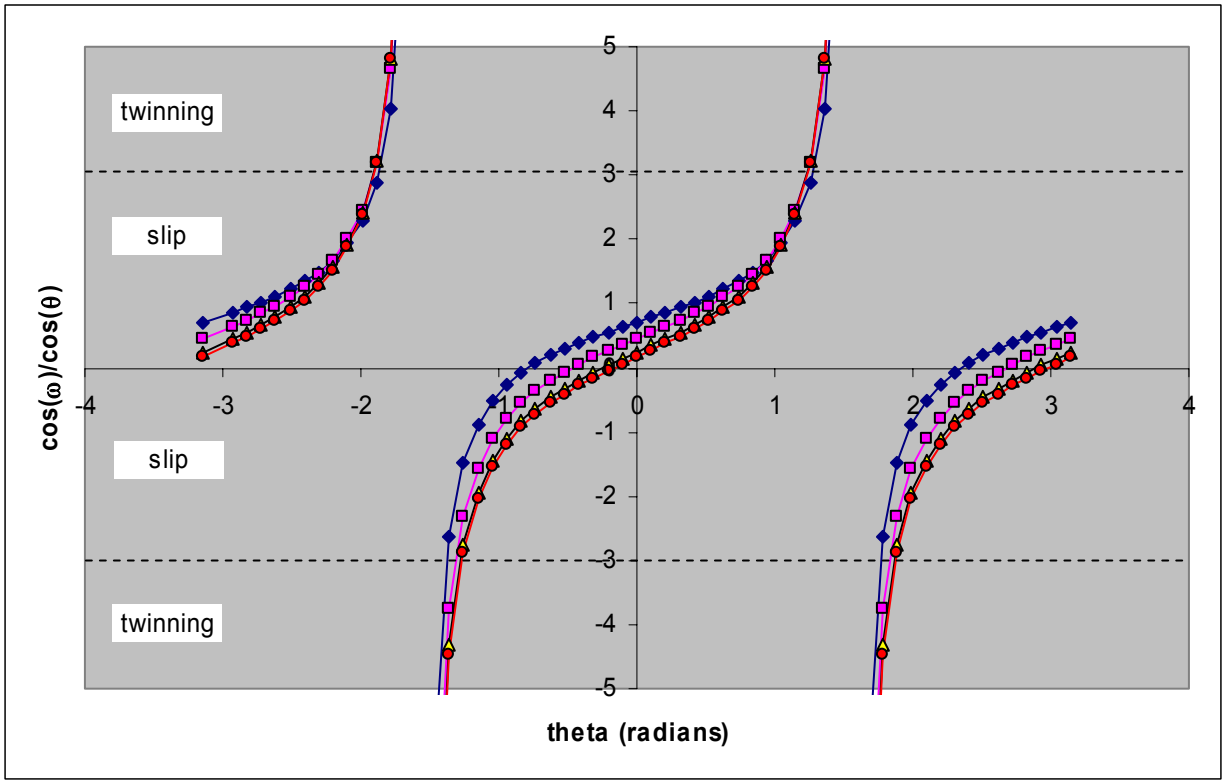
$$\cos(\delta-\theta) = 3\cos\theta$$

$$\cos\delta\cos\theta + \sin\delta\sin\theta = 3\cos\theta$$

$$\sin\delta\sin\theta = \cos\theta(3-\cos\delta)$$

$$\tan\theta = \frac{3-\cos\delta}{\sin\delta} \longrightarrow \theta = \tan^{-1}\left[\frac{3-\cos\left[\sin^{-1}\left(\frac{c}{\sqrt{c^2+\left(\frac{a}{2}\right)^2}}\right)\right]}{\frac{c}{\sqrt{c^2+\left(\frac{a}{2}\right)^2}}}\right]$$

Now, let's plot cosω/cosθ for several c/a ratios…



For the different c/a ratios in the plot, the angles between slip and twinning are:

c	a	δ (°)	θ (°)	θ(°)
1	2	45.00	72.86	-79.20
1	1	63.43	70.69	-75.45
2	1	75.96	70.62	-73.34
3	1	80.54	70.82	-72.69

(The transition also occurs when at $\theta = \theta + \pi$)

4.2 Calculate how much energy can be stored as dislocations by deforming a metal. State your answer as a fraction of the elastic energy you can store in the same metal if it can sustain 1% shear strain prior to yielding. State any assumptions you need in your calculation.

Elastic energy (per unit volume) = $\frac{1}{2}G\gamma^2 =$ $\boxed{5\times10^{-5}\,G}$ where G is the shear modulus.

Assumptions used in calculating the energy of dislocations:

- Dislocation density, $\rho = 10^{16}\ m^{-2}$

- $b = 2 \times 10^{-10}$ m

- Strain energy of dislocation will be described as = Gb^2 (ignores any prefactors)

Since the dislocation strain energy is actually energy per unit length, we need to multiply by the length of dislocations per unit volume (the dislocation density). Therefore:

$$\frac{\text{Energy}}{\text{volume}} = Gb^2\rho = G\left(2\times10^{-10}\,\text{m}\right)^2\left(10^{16}\,\text{m}^{-2}\right) = \boxed{4\times10^{-4}\,G}$$

Therefore, the ratio of the energy stored by the dislocations to the energy stored during elastic deformation is 8 (8 times more energy stored by dislocations).

Note: Answers could have obviously varied greatly depending on what dislocation density you assumed. Every order of magnitude difference in density results in an order of magnitude change in the relative weights of the two energy storage mechanisms.

4.3 When edge dislocations stack up into a low angle subgrain boundary, the misorientation is a function of their spacing, d:

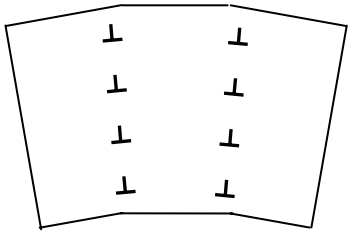
θ = b/d

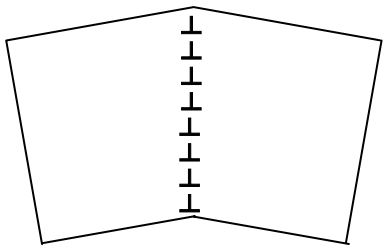
The energy of such a stack of dislocations is:

$$E = \frac{\mu b}{4\pi(1-\nu)}\theta$$

In the "second stage" of polygonization, low angle boundaries combine. Calculate the energy change when two low-angle boundaries combine into one, using the above equations.

Calculate the energy for the following 2 configurations:

(a) 

(b) 

(a) Each low-angle boundary has an angle of 5º, but there are two boundaries, so the total energy of this configuration is:

$$\mathrm{E} = 2 \cdot \frac{\mu b}{4\pi(1-\nu)}\left(\frac{5\pi}{180}\right)$$

(b) There one boundary (with twice as many dislocations with half the spacing) has an angle of 10º, so its energy is:

$$\mathrm{E} = \frac{\mu b}{4\pi(1-\nu)}\left(\frac{10\pi}{180}\right)$$

These energies are obviously the same → there is no energy change associated with coarsening of the subgrain structure.

4.4 On the basis of your calculation in 4.3, identify the driving force for coarsening of the subgrain structure in the second stage of polygonization.

The driving force for coarsening of the subgrain structure can be seen by considering the stress fields around the dislocations. The lateral spacing between boundaries is greater in (b), so the interaction energy between the boundaries decreases. In other words, the lateral repulsion between the dislocations in adjacent boundaries is lower by virtue of the 1/x decay of the stress field.