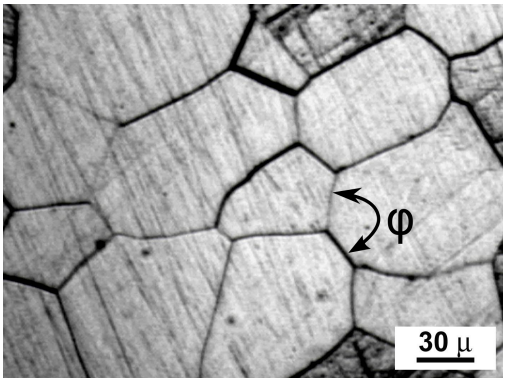
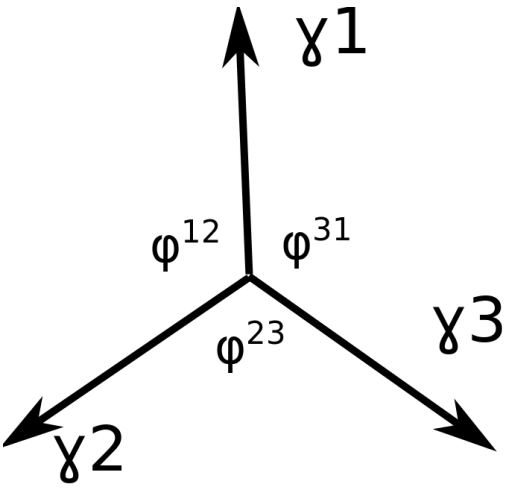
** Exercise 1 Grain boundary angles inside the crystal

Inside a poly-crystal, there are numerous grains. What is interesting is that all the contact angles (ϕ) between two grains are usually very close to $2\pi/3$. Can you explain why this is the case?



Solution to Exercise 1



Consider a junction. The three forces must be balanced (see the Young's equation):

$$\gamma_1 + \gamma_2 \cos(\phi^{12}) + \gamma_3 \cos(\phi^{31}) = 0,$$

and

$$\gamma_2 \sin(\phi^{12}) = \gamma_3 \sin(\phi^{31}).$$

When the grain boundary energies are almost isotropic, $\gamma_1 \approx \gamma_2 \approx \gamma_3$. And you will have

$$\phi^{12} \approx \phi^{23} \approx \phi^{31} \approx \frac{2}{3}\pi.$$

* Exercise 2 Small angle grain boundary

A small-angle tilt grain boundary can be described adequately by a vertical wall of dislocations.

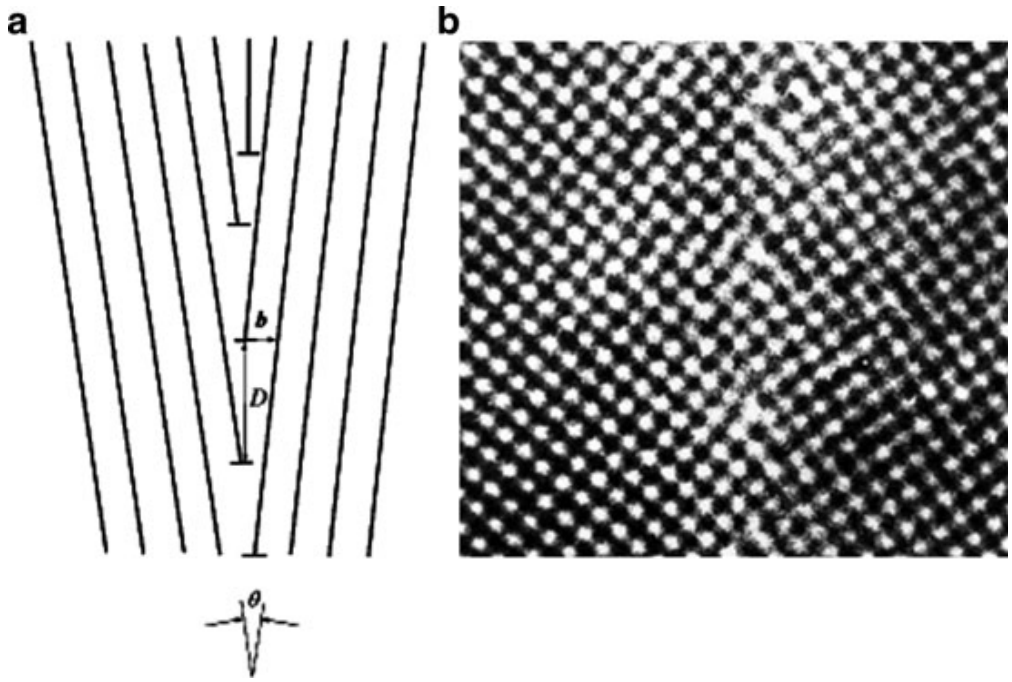


Figure 1: Schematic illustration and HRTEM image of [100] low-angle grain boundary in molybdenum.

(a) What is the average distance D between two dislocations? Given the angle of tilt θ and the lattice parameter b.

(b) The energy of a low-angle grain boundary can be approximated by

$$\gamma_{gb} \approx E_{\perp}/D,$$

where $E_{\perp}$ is the energy cost of a dislocation. Explain why this approximation will become more inaccurate when the angle of tilt θ becomes larger.

Solution to Exercise 2

Question (a).

According to geometrical considerations

$$D\sin(\theta/2) = b/2,$$

and

$$D = \frac{b}{2\sin(\theta/2)}.$$

Question (b).

As the tilt angle θ gets larger, the average distance between dislocations D becomes smaller. The smaller distances between dislocation arrays imply that the interactions between dislocations become larger and increase the dislocation energy cost. As a result, the structure will relax into a lower energy configuration, which does not resemble an array of dislocations.

The End.