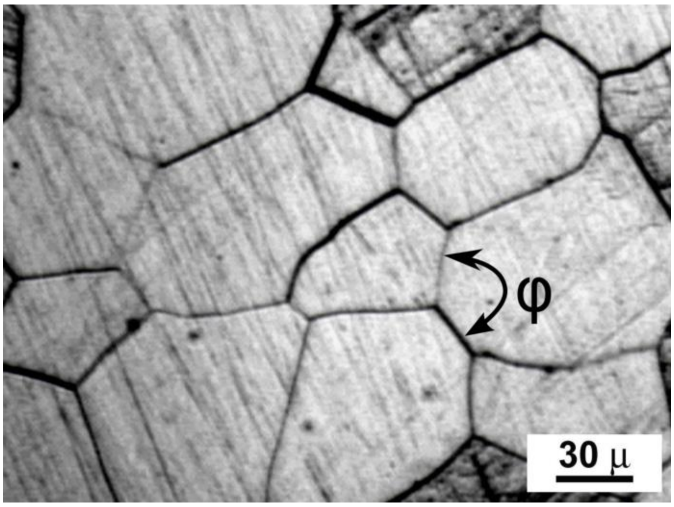
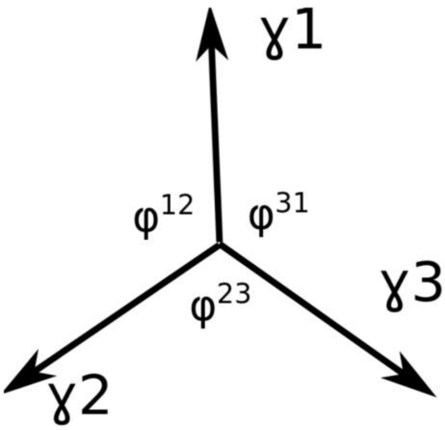
1. Inside a poly-crystal, there are numerous grains. What is interesting is that all the contact angles (φ) between two grains are usually very close to 2π/3. Can you explain why this is the case?



Solution:



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

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

And

$$\gamma_2 sin\,(\varphi^{12}) = \gamma_3 sin\,(\varphi^{31})$$

When the grain boundary energies are almost isotropic,

$$\gamma_1 \approx \gamma_2 \approx \gamma_3$$

You will have:

$$\varphi^{12} = \varphi^{23} = \varphi^{31} \approx \frac{2}{3}\pi$$

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

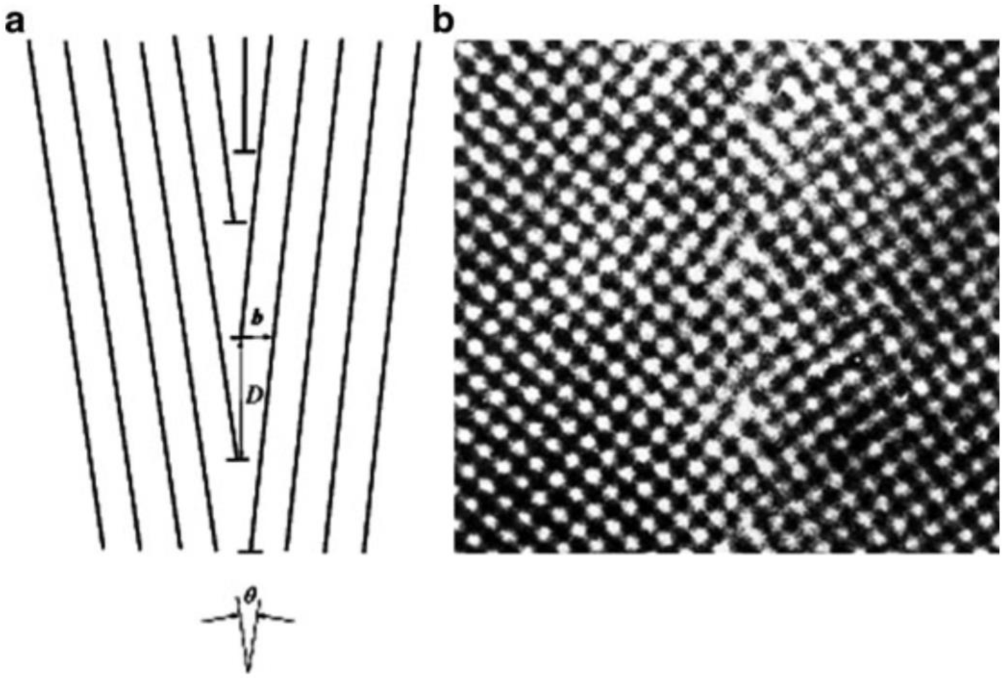


Figure 1: Schematic illustration and HRTEM image of [110] low-angle grain boundary in molydenum.

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 tilt angle θ becomes larger.

Solution:

a) According to geometrical considerations

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

And

$$D = \frac{b}{2\sin\left(\frac{\theta}{2}\right)}$$

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.