Part II : Interfaces
Module 4 : Equilibrium shapes of crystals

4 Equilibrium shapes of crystals

4.1 Motivation

Very small gold and salt crystals show facetted surfaces. Why?

See the following link for some nice micrographs.

`http://www.lassp.cornell.edu/sethna/CrystalShapes/Equilibrium_Crystal_Shapes.html`

4.2 Wulff construction and equilibrium shapes

Wulff plot is a nice way of representing the dependence of the interfacial energy on the surface plane orientation. In this method, we identify the lattice planes by their normals. Given a normal $\langle hkl \rangle$ and the surface energy γ_{hkl} associated with the surface plane with $\langle hkl \rangle$ as the normal, from an origin, we plot a point in the $\langle hkl \rangle$ direction at a distance which is equal to γ_{hkl}. The resultant plot is known as the Wulff plot. In the Figure 9 below, we show a schematic of such a Wulff plot.

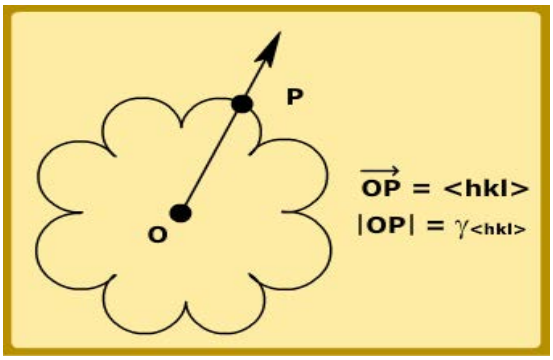

Figure 9: The Wulff plot constructed by placing points in various directions corresponding to the surface energy for a plane with that direction as the normal.

Given a Wulff plot, it is possible to identify the equilibrium shape. The equilirium shape is that shape which minimises $\sum A_i \gamma_i$ where A_i is the area of the $i-$th plane with an interfacial energy of γ_i. From the Wulff plot, it is clear that planes whose energies lie at the cusps of the Wulff plot have lower

energies; hence, if there be cusps in the Wulff plot, the equilibrium shape would consist of facets made up by such planes.

The general procedure to obtain the equilibrium shape from the Wulff plot is shown in Figure 10. At every point on the Wulff plot, we draw a tangent (which is perpendicular to the radial line). The inner envelope of such tangents gives us the equilbrium shape. If there are cusps in the Wulff plot, this construction give facetted equilibrium shapes.

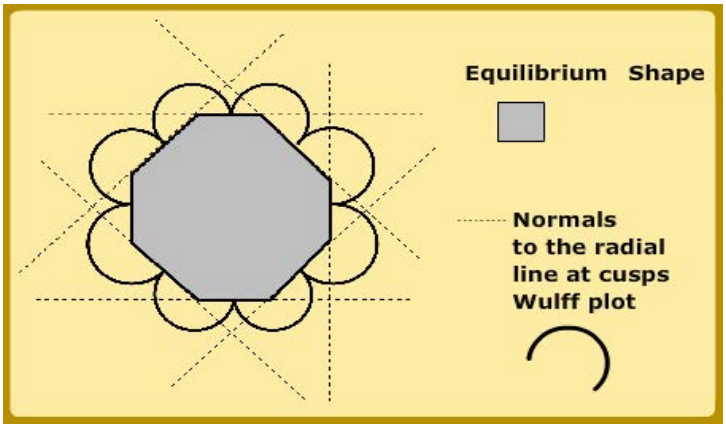

Figure 10: The Equilibrium shape identified from the Wulff plot. We draw the normals to the radial direction at every point. The inner envelope of the normals forms the equilibrium shape. Note that when there are cusps, the normals at the cusps form facetted interfaces as shown.

4.3 Tutorial problems and questions

1. Given the following Wulff plots (Figures. 11, 12, 13, and, 14), draw the corresponding equilibrium shapes of the crystals.

2. Given the following equilibrium shapes (Figures. 15, 16, and, 17) draw the simplest Wulff plots that would give rise to such equilibrium shapes.

4.4 Solutions to the tutorial

1. Given the Wulff plots (Figures. 11, 12, 13, and, 14), here are the corresponding equilibrium shapes (Figures. 18, 19, 20, and, 21).

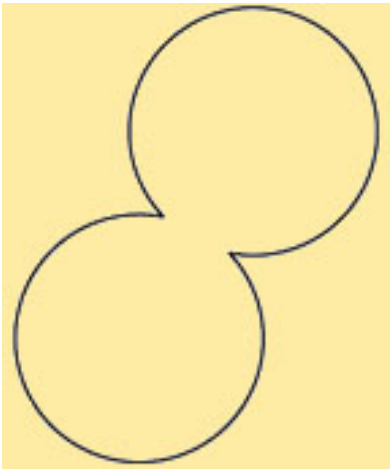

Figure 11: Schematic Wulff plot

2. the simplest Wulff plots (Figures. 22, 23, and, 24) that would give rise to equilibrium shapes shown in Figures. 15, 16, and, 17).

4.5 Supplementary information

In this section, we only considered the shape of a crystal in contact with its vapour. A construction known as Winterbottom construction is needed to identify the equilibrium shape of a crystal on a substrate.

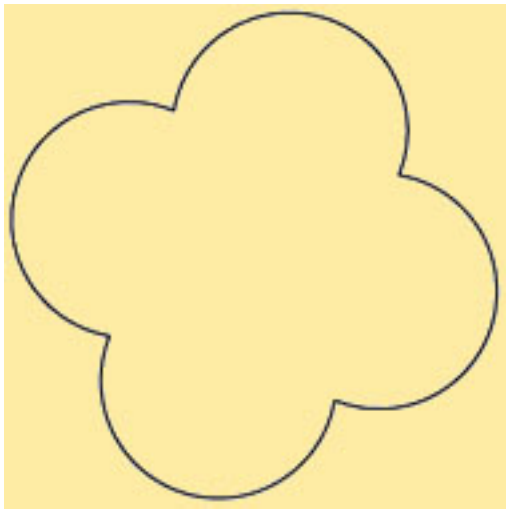

Figure 12: Schematic Wulff plot

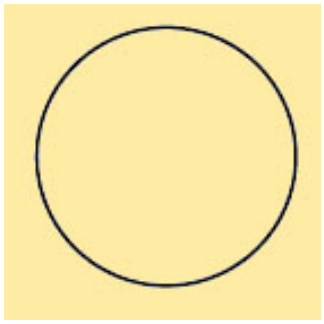

Figure 13: Schematic Wulff plot

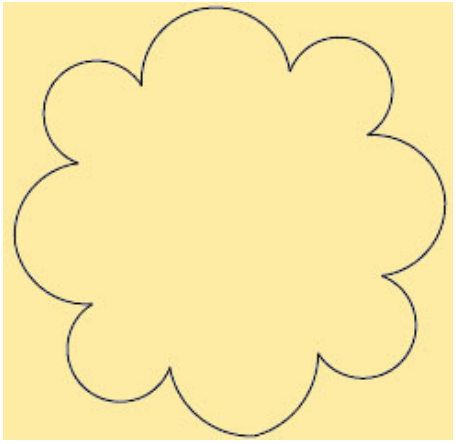

Figure 14: Schematic Wulff plot

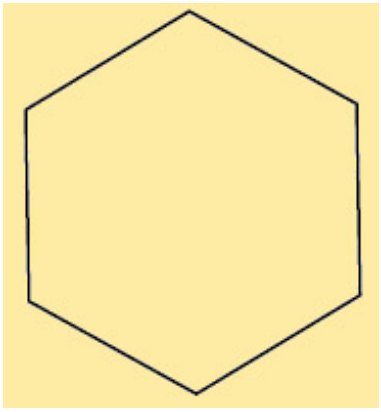

Figure 15: Equilibrium shape

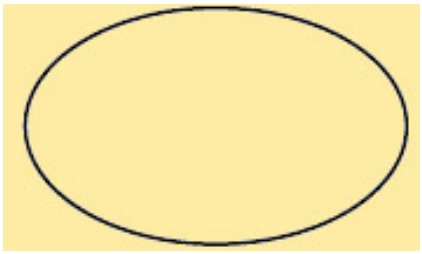

Figure 16: Equilibrium shape

Figure 17: Equilibrium shape

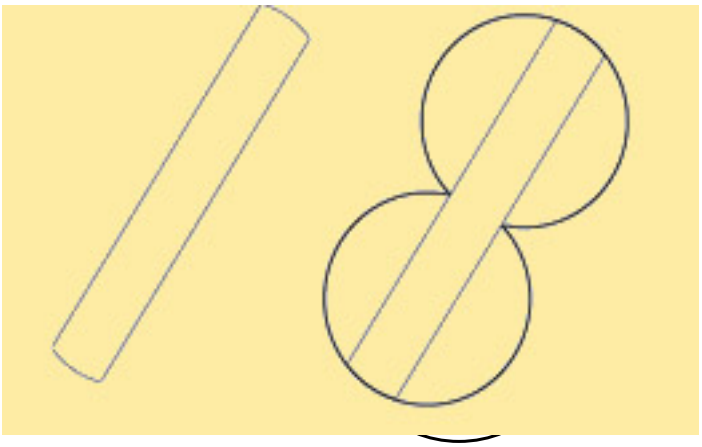

Figure 18: Wulff plot and equilibrium shape

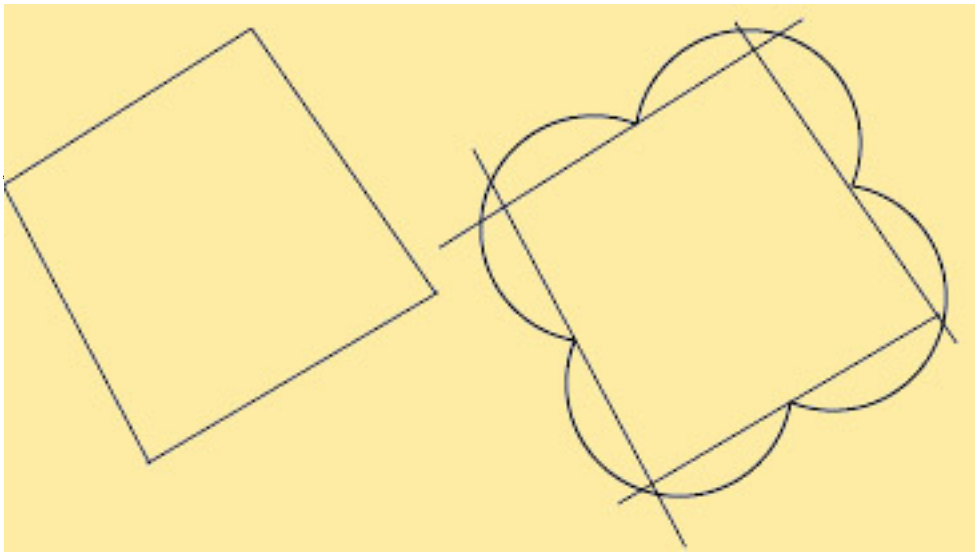

Figure 19: Wulff plot and equilibrium shape

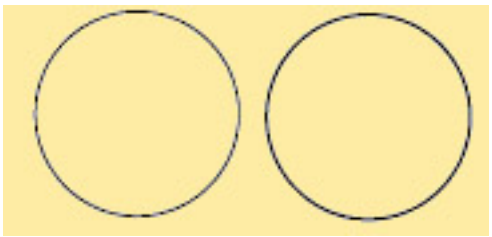

Figure 20: Wulff plot and equilibrium shape

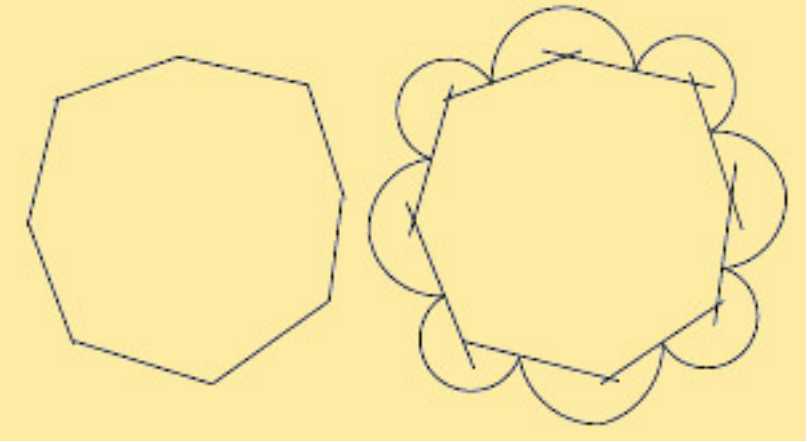

Figure 21: Wulff plot and equilibrium shape

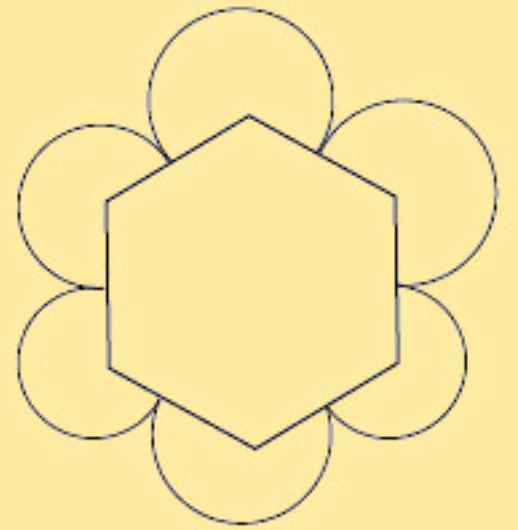

Figure 22: Simplest Wulff plot for the given equilibrium shape.

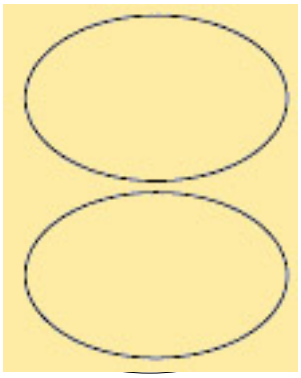

Figure 23: Simplest Wulff plot for the given equilibrium shape.

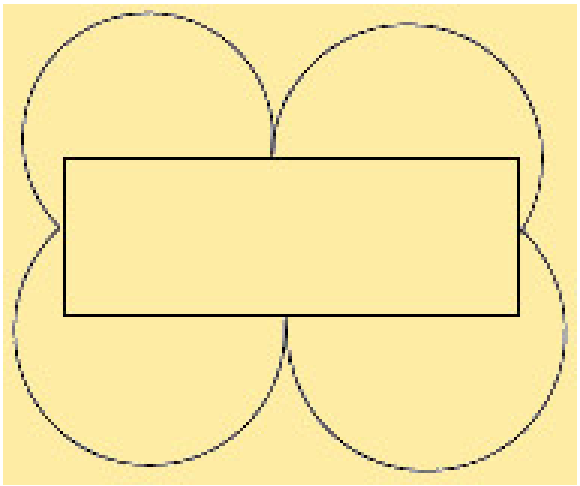

Figure 24: Simplest Wulff plot for the given equilibrium shape.

References

[1] David A. Porter, Kenneth E. Easterling, and Mohamed Y. Sherif, Phase transformations in metals and alloys, CRC press, Third edition, 2009.

[2] Peter Haasen, Physical metallurgy, Cambrdige University Press, Third edition, 1997.

[3] Guenter Gottstein, Physical foundations of materials science, New age international, First edition, 2006.

[4] Kenneth M. Ralls, Thomas H. Courtney, and John Wulff, Introduction to materials science and engineering, Wiley India Pvt. Ltd., 2011.

[5] V. Raghavan, Materials science and engineering: a first course, Prentice-Hall India Pvt. Ltd., Fifth edition, 2008.

[6] Robert E. Reed-Hill, Physical metallurgy principles, Affiliated East-West Press Pvt. Ltd., Second edition, 2008.

[7] Derek Hull and D J Bacon, Introduction to dislocations, Butterworth-Heinemann, Fifth edition, 2011.