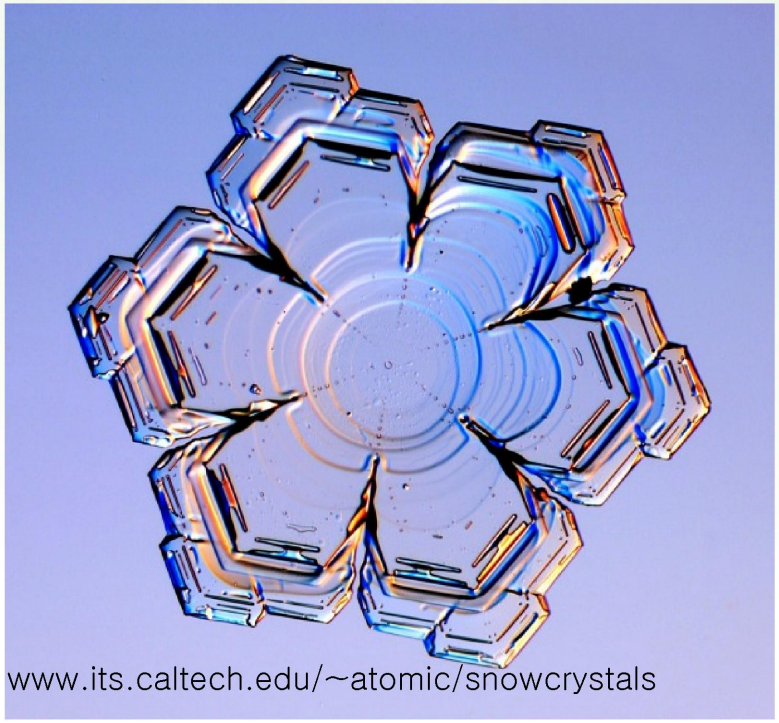
Wulff construction

The Wulff construction is to give the equilibrium shape of one material crystal with surrounding medium.



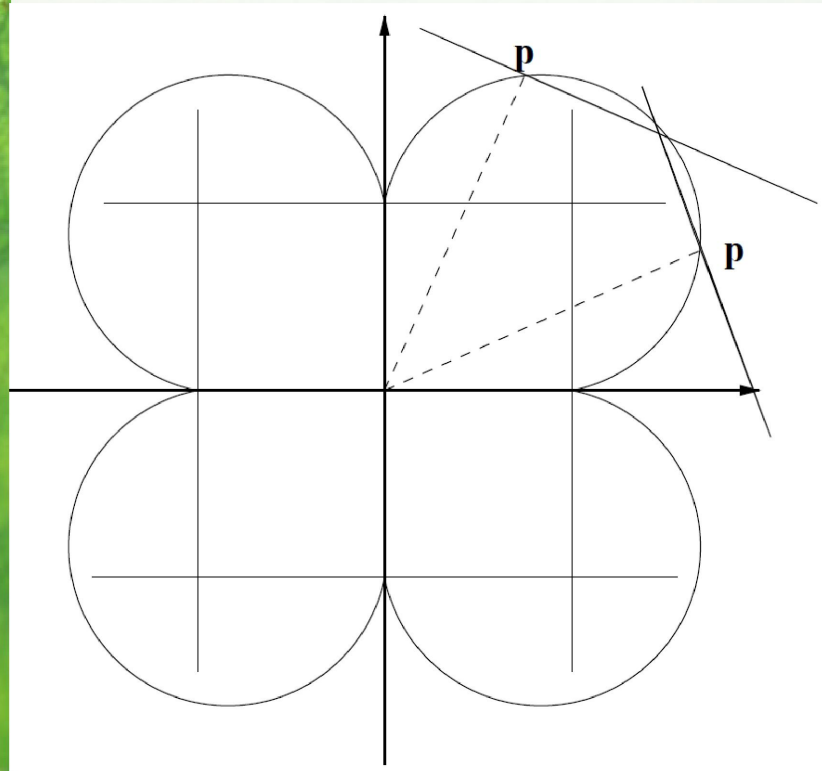
The equilibrium shape is determined by minimizing the total energy.

Wulff's geometric construction

Wulff's Theorem; Euler-Largange

Wulff construction

Wulff's geometric construction

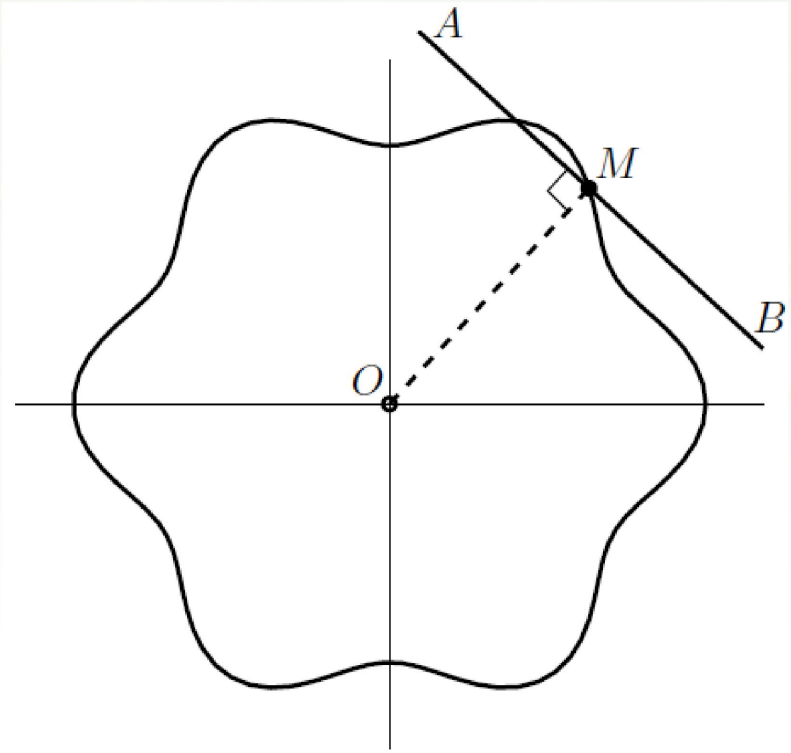


STEP1 Construct a polar plot of γ

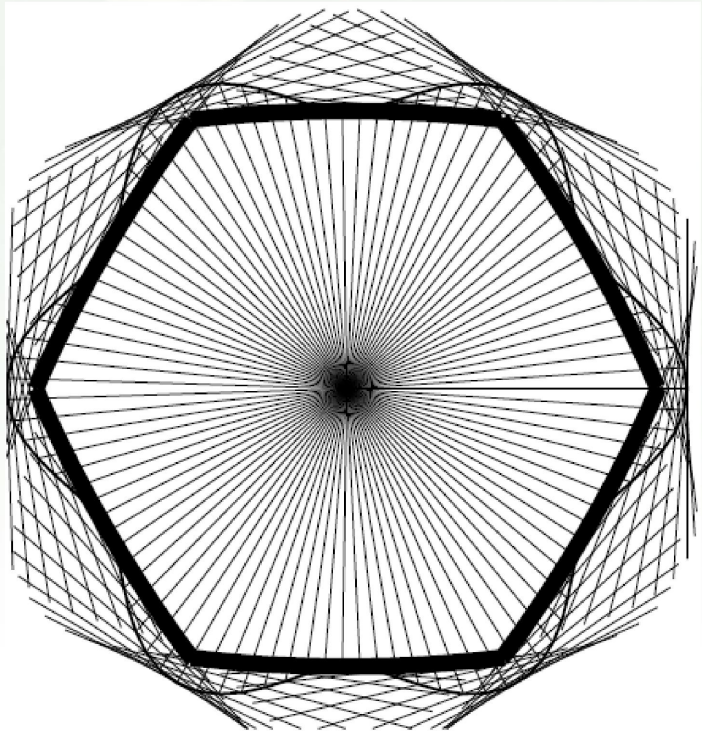
STEP2 For each point P on the polar, construct the plane through P and normal to the radial vector emanating from the origin to P.

STEP3 Construct all of the inner convex envelope of the planes.

Wulff construction



Interfacial free-energy density γ in the polar coordinates.

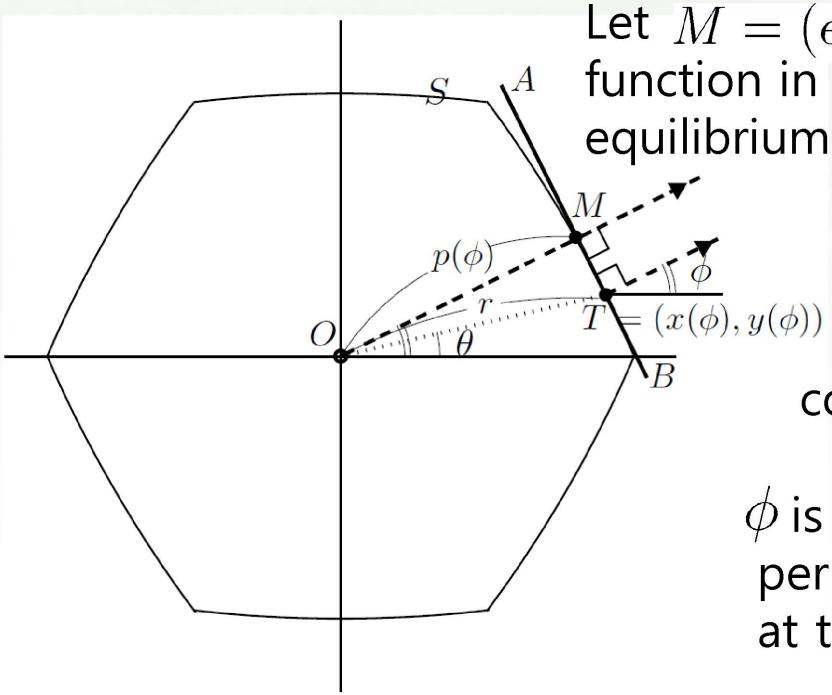


Equilibrium crystal shape

Wulff construction

Wulff's Theorem; Euler-Largange

In a crystal equilibrium, the distances of the faces from the center of the crystal are proportional to their surface free energies per unit area.



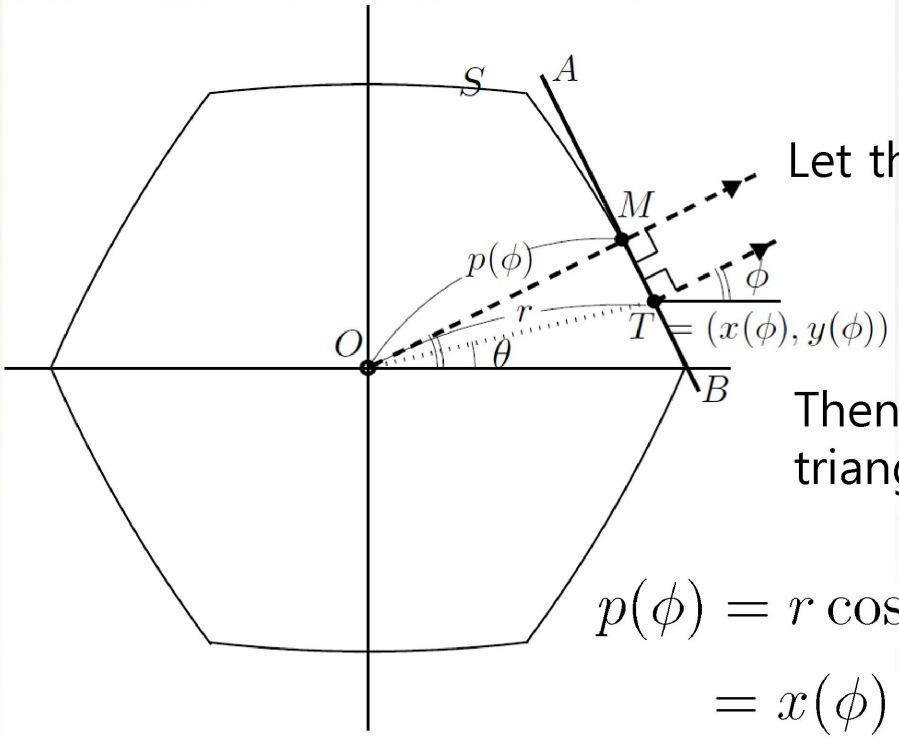
6-fold case

Let $M = (\epsilon(\theta), \theta)$ be a point on the interfacial energy function in polar coordinates. Then assume the equilibrium shape is known.

(r, θ) Polar coordinates of a point T of crystal boundary S. Thus, $T = (r, \theta)$ and let $T = (x(\phi), y(\phi))$ be the corresponding Cartesian coordinates.

ϕ is an angle between x-axis and the $\overline{AB}$ perpendicular line to the tangent line at the point T

Wulff construction



Let the length of the line segment $\overline{OM}$ be $p(\phi)$

Then $p(\phi)$ can be obtained from the right triangle $\triangle OTM$

$$p(\phi) = r\cos(\phi-\theta) = r\cos\phi\cos\theta + r\sin\phi\sin\theta$$
$$= x(\phi)\cos\phi + (\phi)\sin\phi.$$

We can express $(x(\phi), y(\phi))$ in terms of $p(\phi)$

Take a derivative to $p(\phi)$, then we have

$$p_\phi(\phi) = x_\phi(\phi)\cos\phi - x(\phi)\sin\phi + y_\phi(\phi)\sin\phi + y(\phi)\cos\phi.]$$

Wulff construction

Since the normal vector $(\cos\phi, \sin\phi)$ and the tangent vector (x_ϕ, y_ϕ) are orthogonal,

$$p_\phi = -x\sin\phi + y\cos\phi.$$

Then we have

$$x(\phi) = p(\phi)\cos\phi - p_\phi(\phi)\sin\phi,\ \ y(\phi) = p(\phi)\sin\phi + p_\phi(\phi)\cos\phi.$$

Let *F* and *A* be the total edge free energy and the area of crystal, respectively and be defined as

$$F = \int \epsilon(\phi)\sqrt{(x_\phi(\phi))^2 + (y_\phi(\phi))^2}d\phi,$$

$$A = \frac{1}{2}\int (x(\phi)y_\phi(\phi) - y(\phi)x_\phi(\phi))d\phi.$$

And rewrite this,

$$F = \int \epsilon(\phi)(p(\phi) + p_{\phi\phi}(\phi))d\phi,$$

$$A = \frac{1}{2}\int p(\phi)(p(\phi) + p_{\phi\phi}(\phi))d\phi.$$

Now we want to minimize F , with subject to a constant area constraint of A.

Wulff construction

Using the Lagrange multiplier λ we seek to minimize

$$F + \lambda A = \int \left(\epsilon(\phi) + \frac{\lambda}{2} p(\phi) \right) (p(\phi) + p_{\phi\phi}(\phi)) d\phi.$$

And then, the Euler-Lagrange equation is

$$\frac{\partial Q}{\partial p} - \frac{d}{d\phi} \left(\frac{\partial Q}{\partial p_\phi} \right) + \frac{d^2}{d\phi^2} \left(\frac{\partial Q}{\partial p_{\phi\phi}} \right) = 0,$$

where, $Q = \left(\epsilon + \frac{\lambda}{2} p \right) (p + p_{\phi\phi}).$

Use the above equations $p + p_{\phi\phi} = -\frac{1}{\lambda}(\epsilon + \epsilon_{\phi\phi})$

A solution of differential equation is $p(\phi) = -\frac{1}{\lambda}\epsilon(\phi).$

This result implies that in a crystal at equilibrium, the distances of the faces from the center of the crystal are proportional to their surface free energies per unit area