Modeling and Simulation of Isotropic Multi-Phase Systems

22.091, Introduction to Modeling and Simulation
Massachusetts Institute of Technology

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Overview

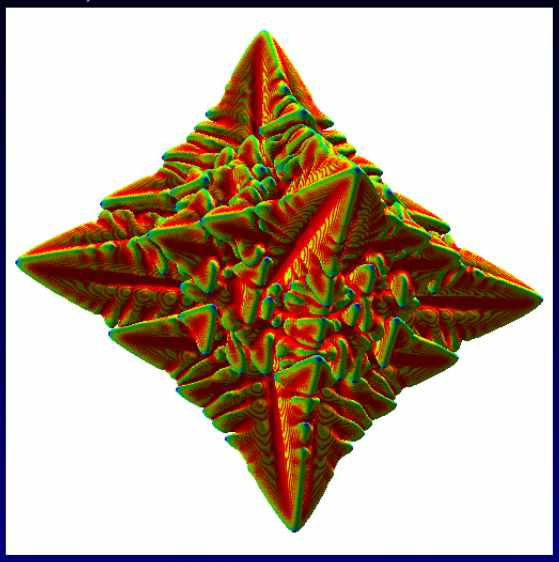
April 8: Interfaces at Equilibrium
- Interface curvature and pressure
- Wetting phenomena
- Minimal energy shapes
- Surface Evolver modeling tool

April 10: Interface Dynamics
- Brief Navier-Stokes intro
- Interfacial energy gradient and Marangoni shear
- Overview of modeling methodologies

April 12: Example of Reactions at Interfaces
- Electrochemistry intro: phenomena, instabilities
- Phase Field model of electrochemical reactions

October 22: Anisotropic Systems

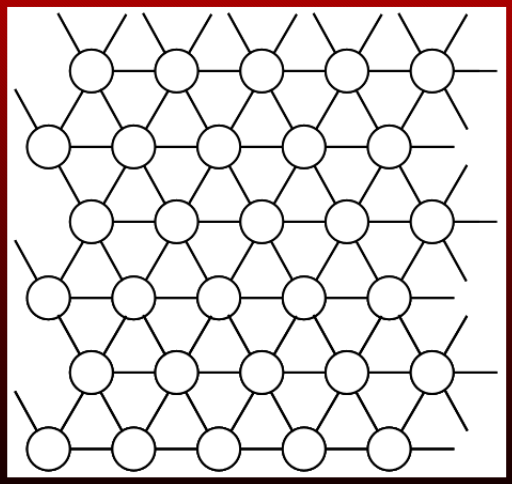
Crystal solidification, dendrites



James Warren, NIST

Surface/Interface Energy/Tension

Ball-and-stick solid example:



Multi-Phase Combinations:

- Solid-solid
- Solid-liquid
- Liquid-gas
- etc.

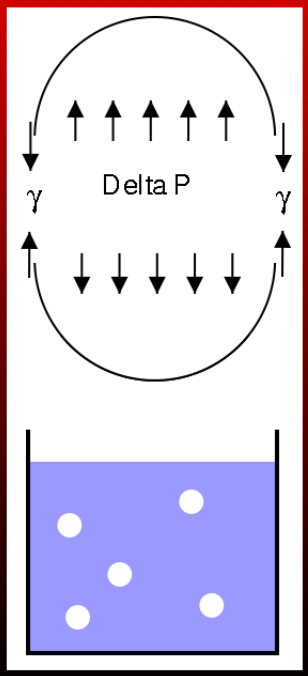
Surface Tension/Energy

- Surface/interface atoms are not in same bonding state as interior atoms
- Broken bonds lead to higher energy
- Energy/area = force/length

Surface Curvature

Tension in a curved surface results in unbalanced forces.
To balance: pressure difference

$\Delta P = \frac{\gamma}{R}$, 3-D: $\Delta P = \gamma\left(\frac{1}{R_1} + \frac{1}{R_2}\right)$



Alternatively: energy minimization leads to smaller interface until volume energy balances it.
For a gas-filled bubble in liquid:

$$E = 4\pi R^2\gamma + \frac{4}{3}\pi R^3\Delta P$$

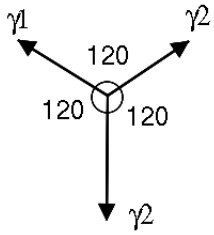
$$\frac{dE}{dR} = 0 \Rightarrow 8\pi R\gamma = 4\pi R^2\Delta P$$

$$\Delta P = \frac{\gamma}{2R}$$

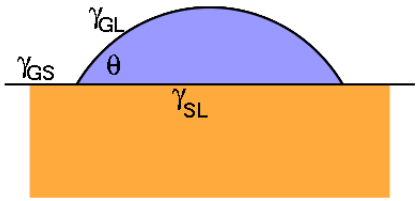
Wetting: Different Surface Energies

At a triple-junction, the forces balance:

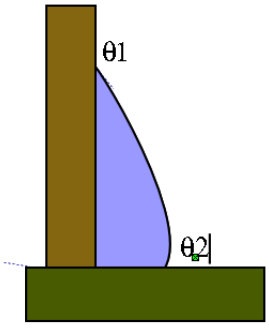
Grain bdrys/gas bubbles Liquid-solid-gas Liquid-gas-two solids



$\gamma 1 = \gamma 2 = \gamma 3$



$\gamma_{GS} = \gamma_{SL} + \gamma_{GL}\cos\theta$



Simulation: Surface Evolver

Basic principles:

- Construct surface out of triangles
- Calculate energy by integrating on triangles, edges
- Calculate derivatives of total energy with respect to vertex locations
- Move vertices to minimize energy, repeat last three steps

Example: cube.fe

- Simple surface: start with cube, iterate to a sphere

Example: mound.fe

- Mound of liquid on a surface
- Start with cube, iterate to a hemisphere
- Gravity: squishes the mound, but contact angle stays
- Table interface energy determines contact angle

Advanced Surface Evolver Examples

Minimal energy regular partition of 3-space: twointor.fe

- Unit cell of periodic system
- Two primitive cells
- Beat Kelvin tetrakaidecadedron partitioning by 0.3%!

Column of liquid solder: column.fe

- Solder droplet shape for flip-chip packaging
- Calculate restoring force in lateral and vertical directions

Solder droplet on optical fiber: wiredrop.fe

- Solder droplet shape
- Calculate capillary force in lateral and vertical directions
- Balance capillary force and elastic restoring force to calculate equilibrium fiber position