Driving Force for Solidification

Topic 3

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MECH 636: Solidification Modelling

Definitions

- In the study of phase transformations we will be dealing with the changes that can occur within a given system e.g. an alloy that can exist as a mixture of one or more phases
- A phase can be defined as a portion of the system whose properties and composition are homogeneous and which is physically distinct from other parts of the system
- The components of a system at the different elements or chemical compound which make up the system

Gibbs Free Energy

$$G = H - T\,S$$

Enthalpy — Temperature — Entropy

Entropy: measure of randomness of the system

$$H = E + PV$$

measure of heat content of the system = Internal Energy + Pressure Volume

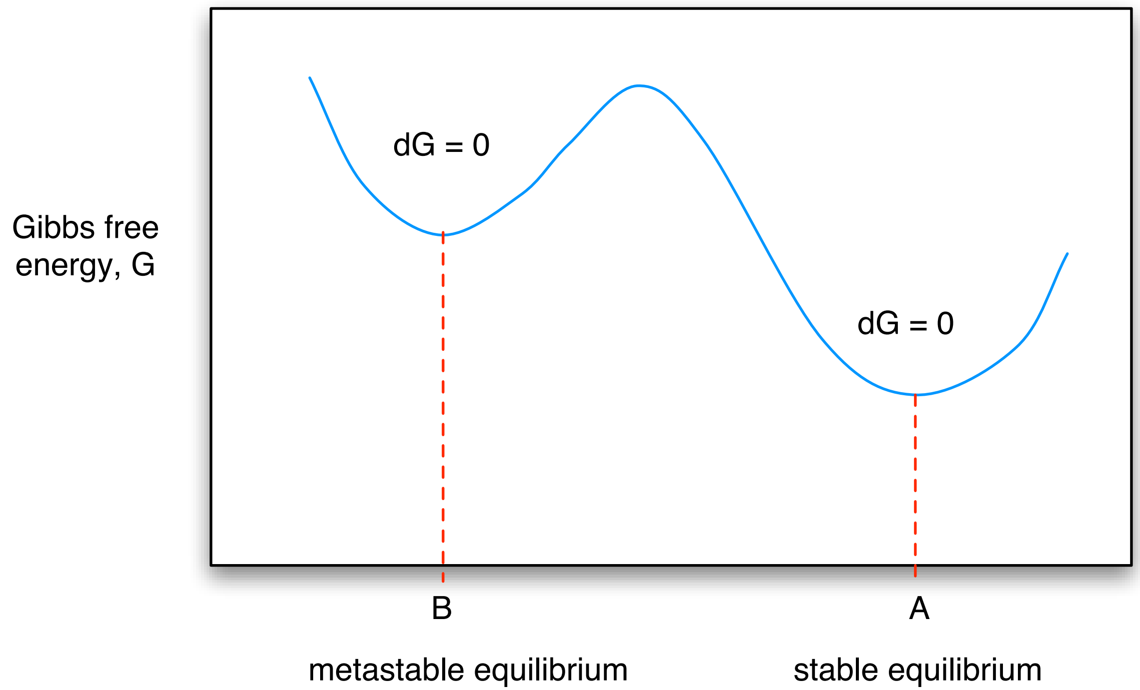
Internal Energy = Kinetic + Potential Energy

for condensed phases $PV \approx 0$ and thus $H \approx E$

A system is in equilibrium when it is at its most stable state when it has the lowest value of the Gibbs free energy

$$dG = 0$$

Equilibirum

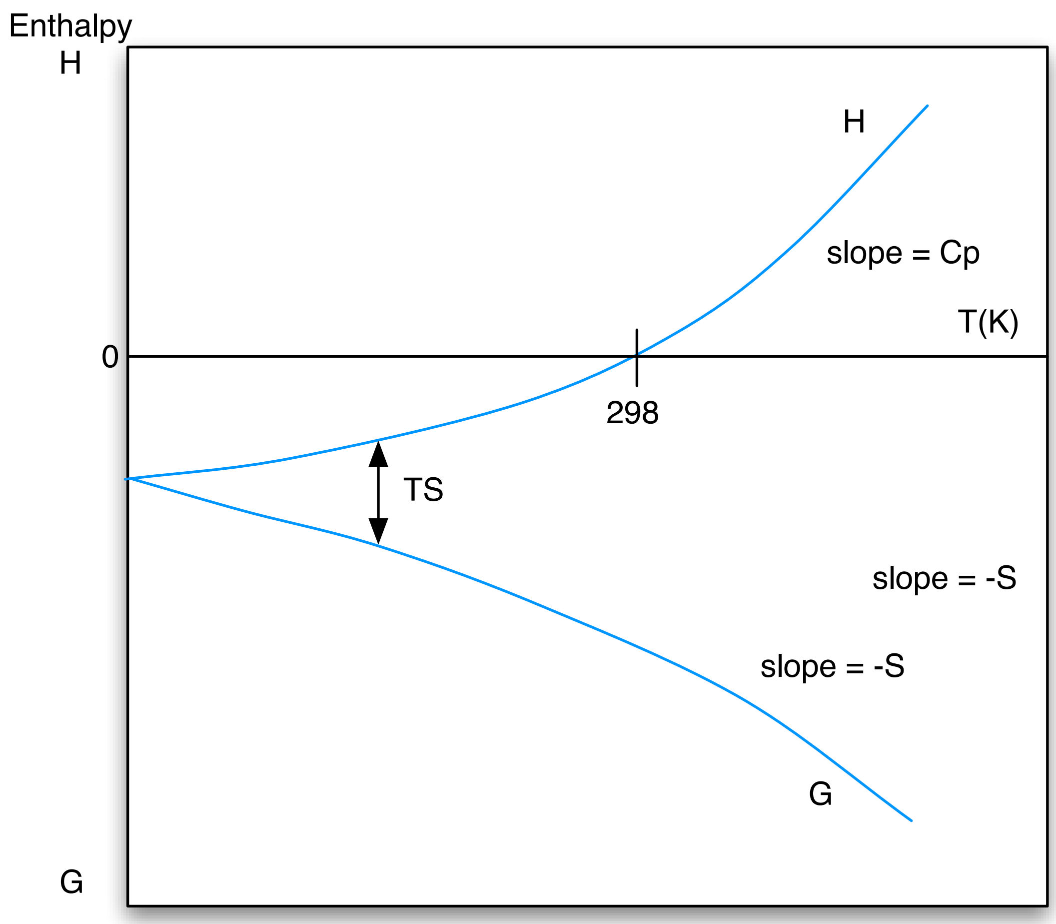


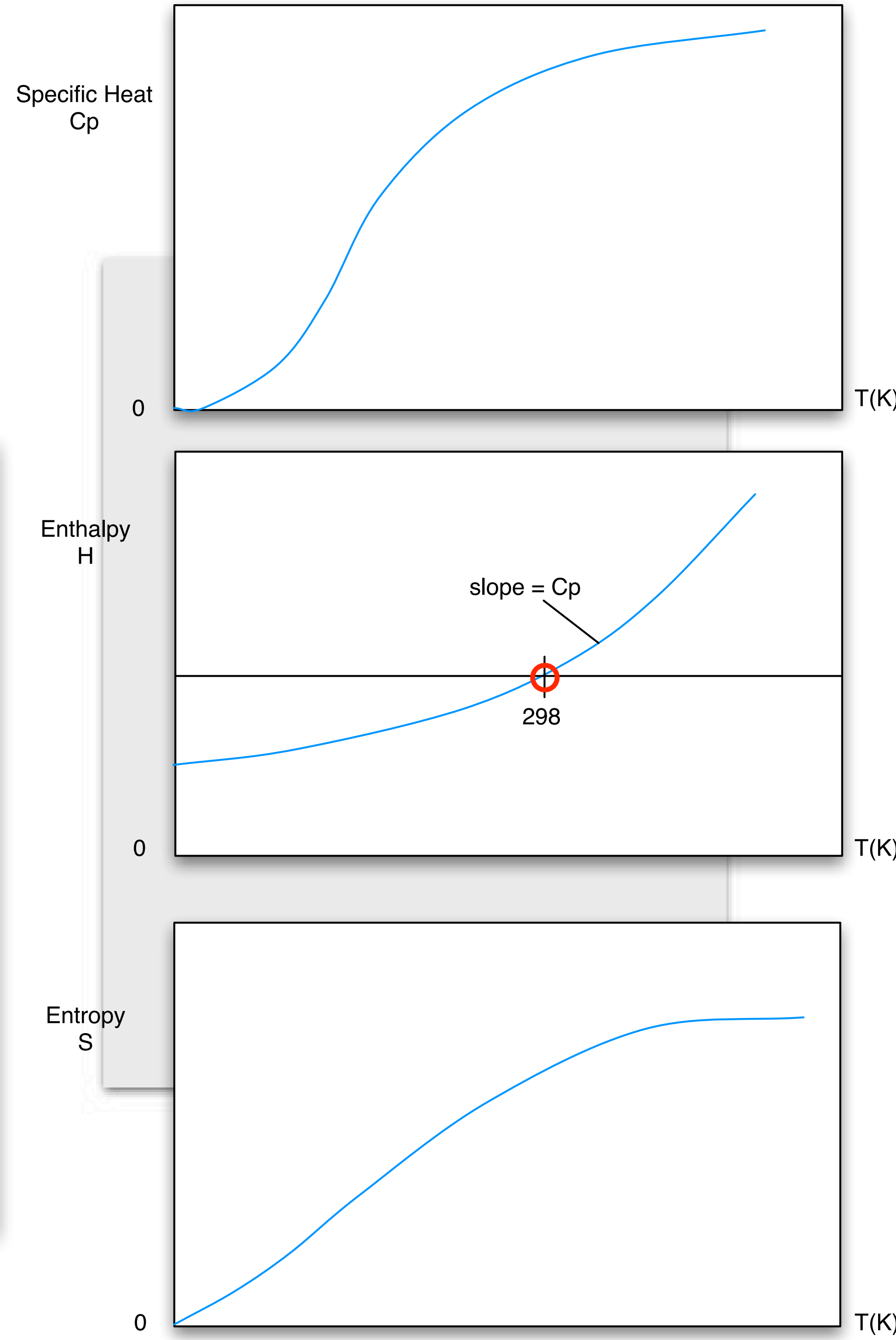
Any transformation that results in a decrease in Gibbs free energy is possible

$$\Delta G = G_2 - G_1 < 0$$

How fast does a phase transformation occur?

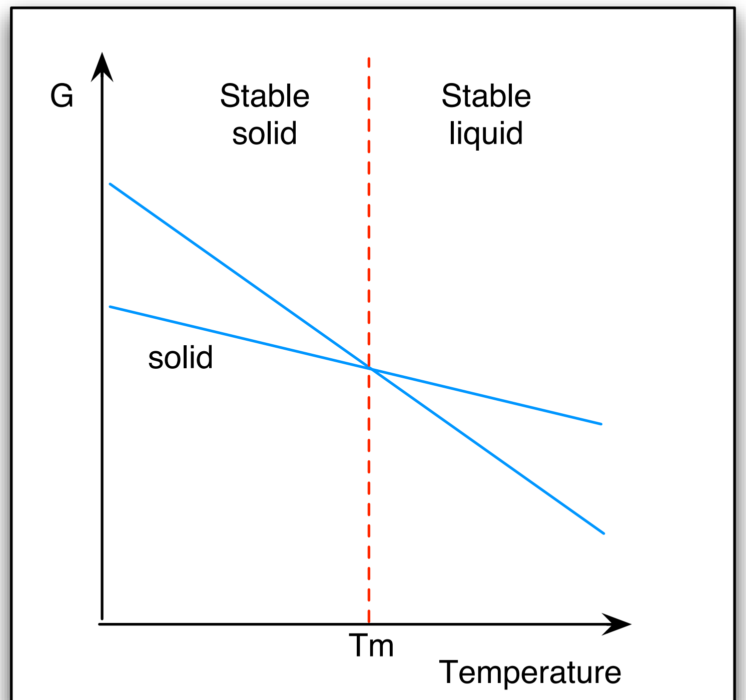
Free Energy Relations

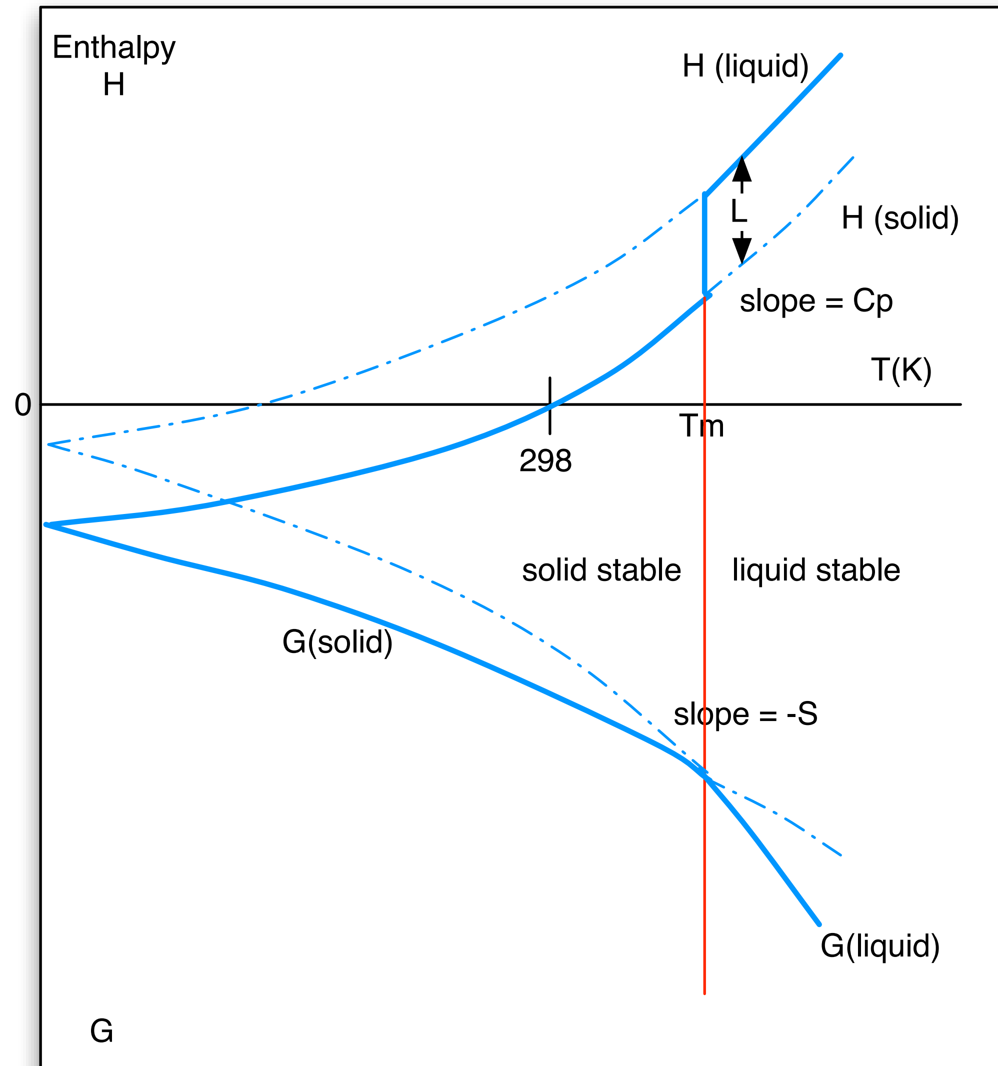




$$G = H - T\,S$$

Driving Force for Solidification





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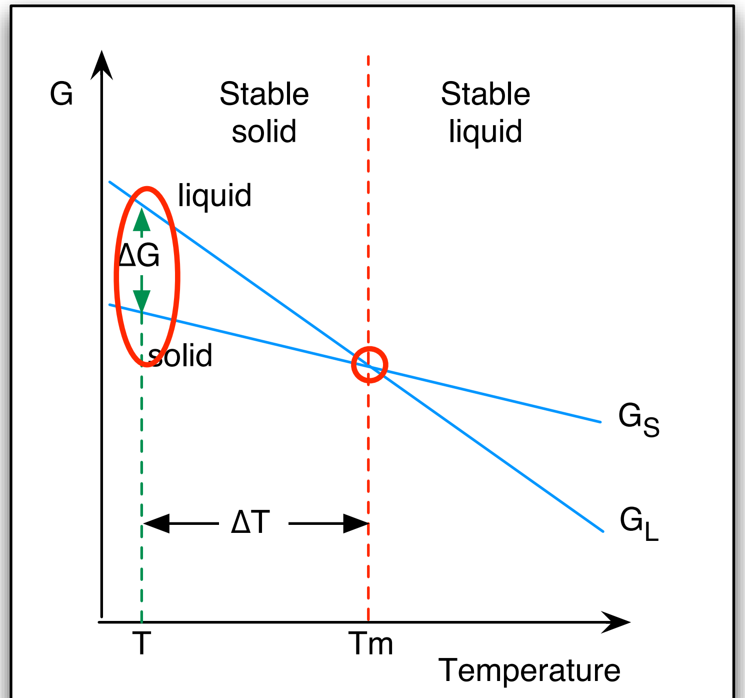


$$G_L = H_L - TS_L$$

$$G_S = H_S - TS_S$$

$$\Delta G = \Delta H - T\Delta S$$

$$\Delta H = H_L - H_S$$

$$\Delta S = S_L - S_S$$

At equilibrium $\Delta G = 0$

$$\Delta G = \Delta H - T_m \Delta S = 0$$

$$\Delta S_f = \frac{\Delta H_f}{T_m} = \frac{L}{T_m}$$

entropy of fusion (nearly a constant ≈ R)

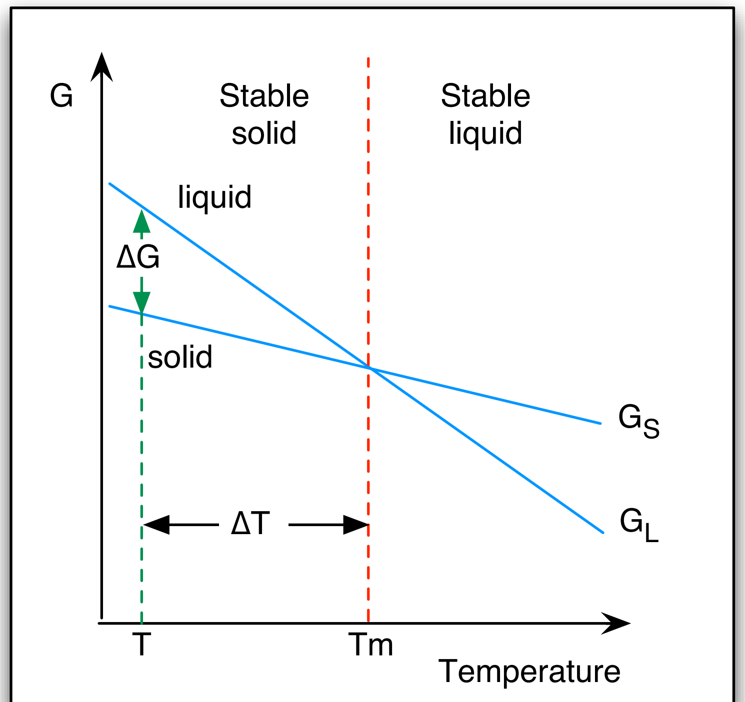
$$\Delta G \approx L - T\frac{L}{T_m}$$

for small ΔT we get

$$\Delta G \approx \frac{L\,\Delta T}{T_m} \approx \Delta S_f \Delta T$$

undercooling

Solidification



To get the solidification process started, the liquid phase must be undercooled, cooled to a temperature below the freezing point.

Once a nucleus forms, it can proceed to grow as fast as the latent heat of solidification and specific heat can be carried away.

Controlled by:
thermal conductivities
relative masses
shapes of the melt, the solid, and mold

Nucleation: occurs when a small piece of solid forms in the liquid and must attain a minimum critical size before it is stable

Growth: occurs as atoms from the liquid are attached to the tiny solid until no liquid remains