Materials Engineering

Phase transformation
Phase diagrams

Phase Transformation

Why is it important for us?

- Temperature, chemical composition and pressure can change the properties of materials
- Understanding what happens during heat treating processes
- Understanding the development of the microstructure

Phase Transformation

Today's topics

- Terminology of phase diagrams and phase transformations
- Thermodynamics of phase transformations
- Phase diagrams

Phase Transformation

Terminology

Component:

Pure metals and/or compounds of which an alloy is composed.
e.g. in a copper–zinc brass, the components are Cu and Zn

System:

Series of possible alloys consisting of the same components,
but without regard to alloy composition

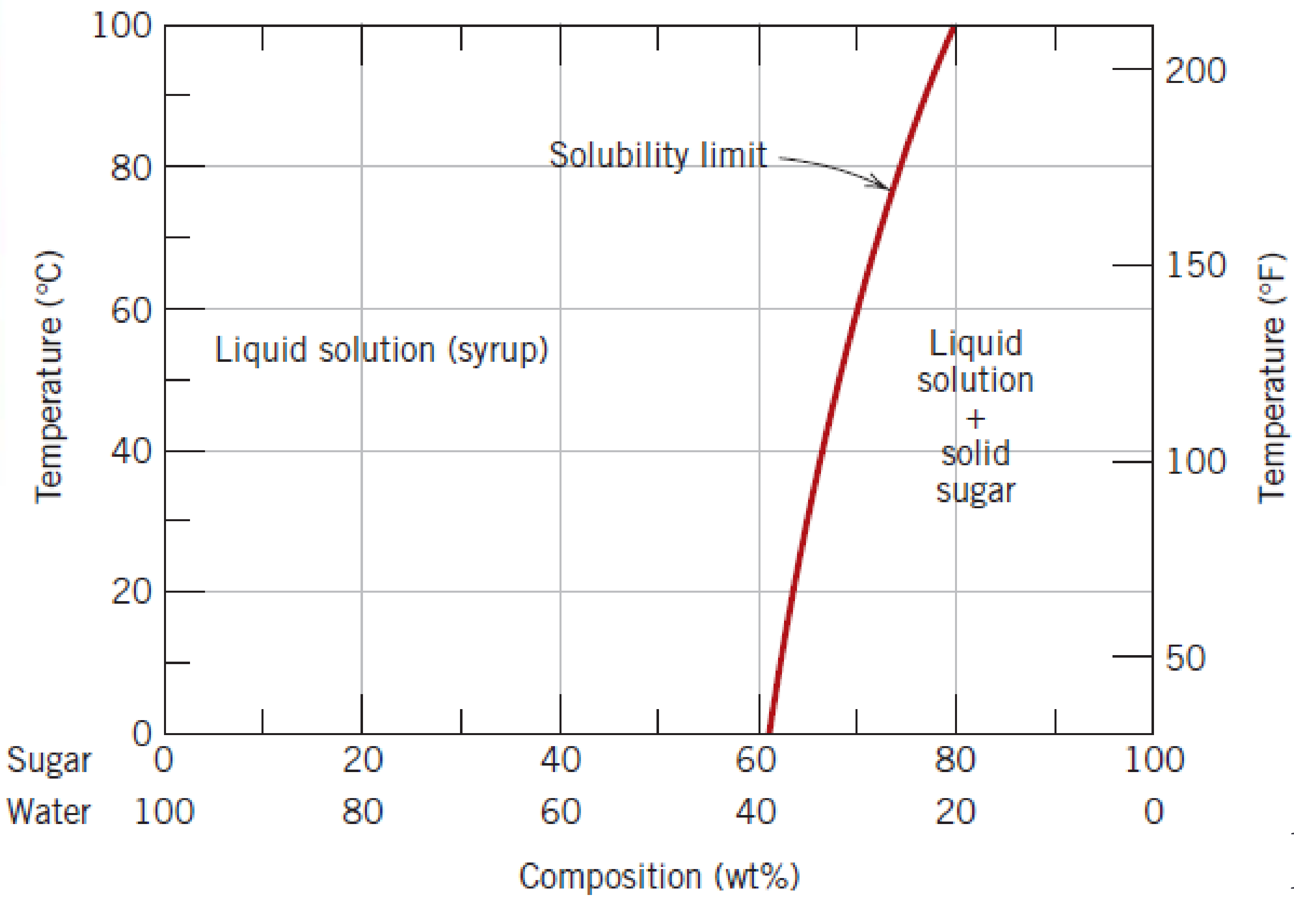
Solid solution

consists at least two different types of atoms
the solute atoms occupy either *substitutional* or *interstitial* positions in the solvent lattice

Phase Transformation

Solubility limit

A maximum concentration of solute atoms that may dissolve in the solvent to form a solid solution



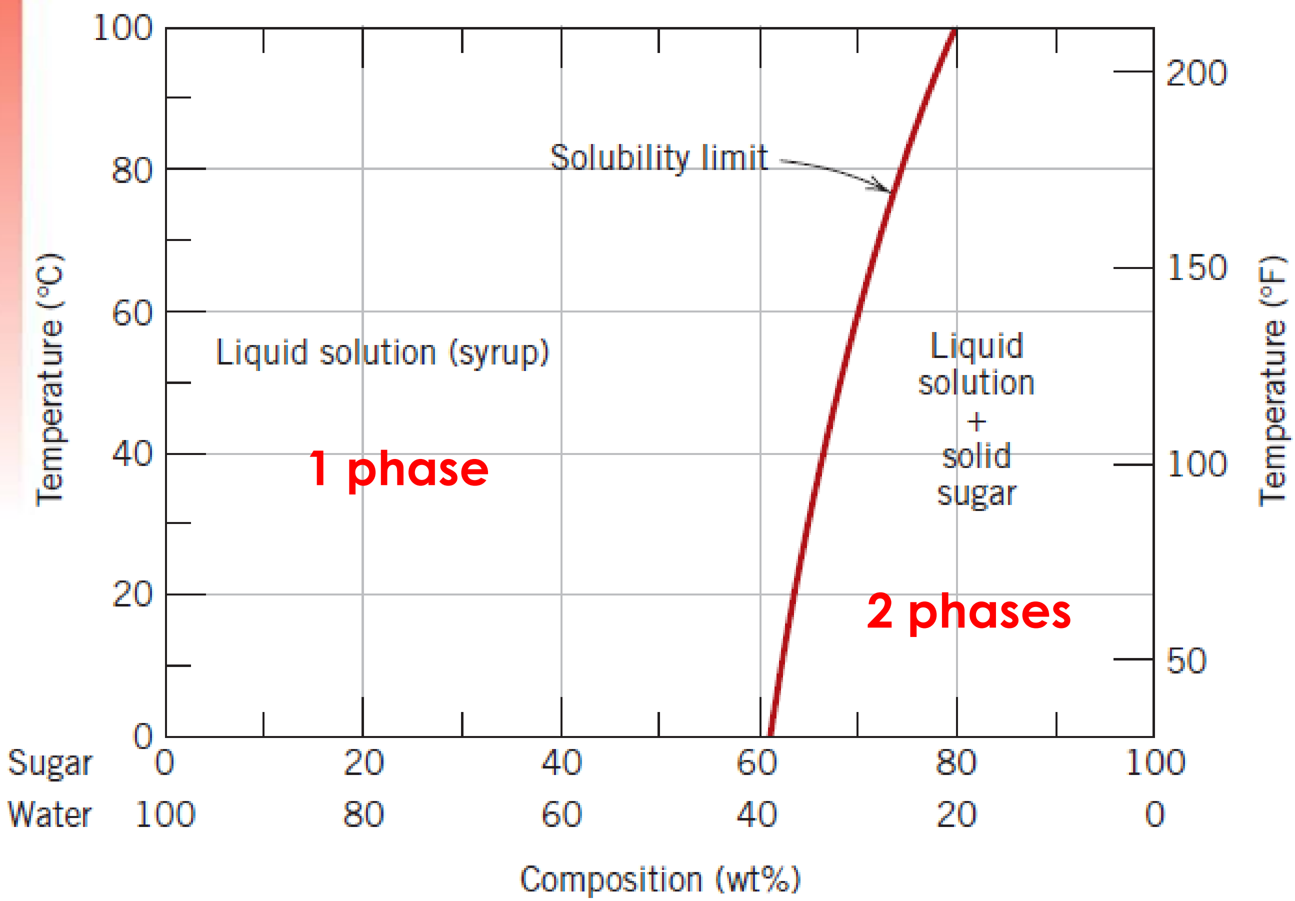
The solubility of sugar in a sugar–water syrup

Figures from Callister, Mat. Sci. and Eng. An Introduction, 8th edition

Phase Transformation

Phase

A homogeneous portion of a system that has uniform physical and chemical characteristics.



Own distinct properties

- Chemical composition
- State of matter
  (*e.g. water+ice*)
- Crystal structure
- …

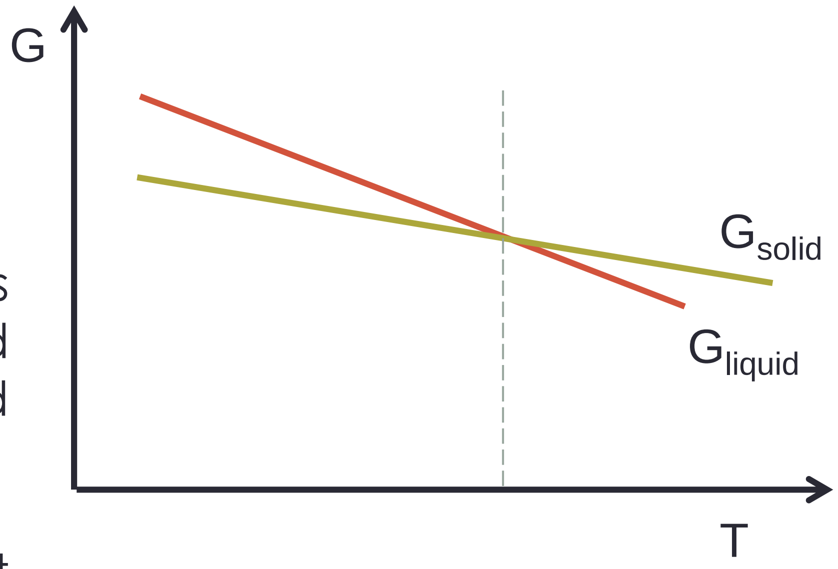
Homogeneous system:
single-phase system

Heterogeneous system:
two or more phases

Phase Transformation

Thermodynamics

Internal energy U: the energy needed to create the system
Enthalpy (H=U+pV): U+ energy required to make room for it by displacing its environment
Enthropy (S): expression of disorder or randomness, the energy not available for work
Helmholtz free energy (F=U-TS)
Gibbs free energy (free enthalpy)(G=H-TS)



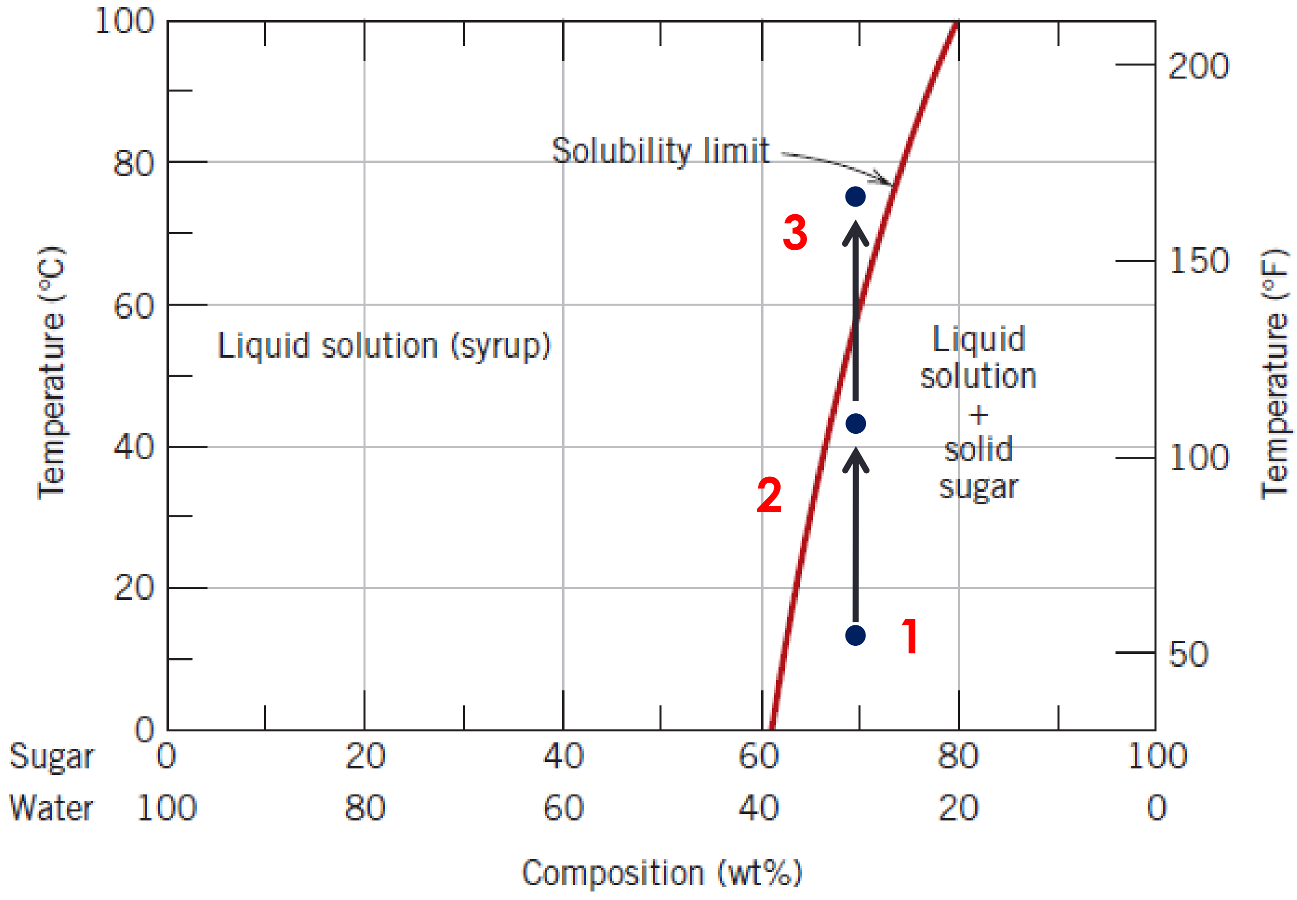
Equilibrium

A system is at equilibrium if its free energy is at a minimum under some specified combination of temperature, pressure, and composition.

The characteristics of the system do not change with time.

Phase Equilibrium

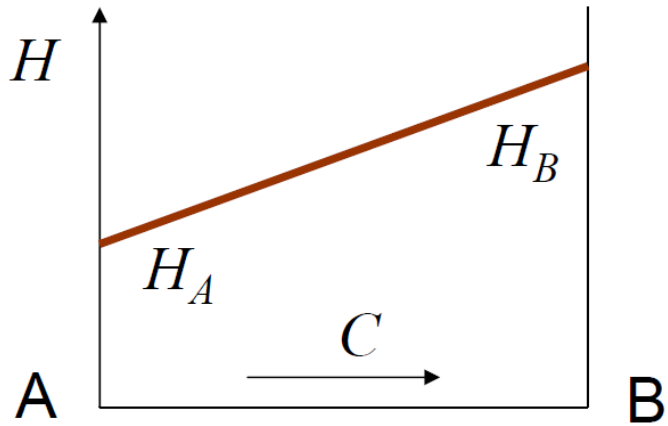
In an equilibrium system the ratio of phases are constant.



Phase Equilibrium

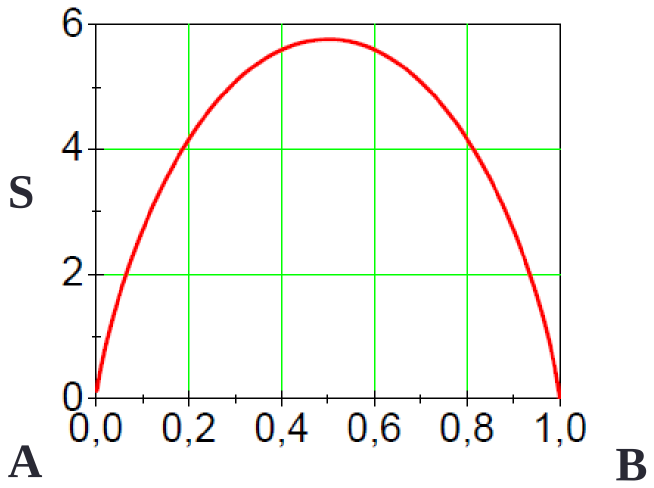
Equilibrium

Two component system (A-B)
(ideal solution: exchanging any two atoms does not change the enthalpy)



Entropy, S

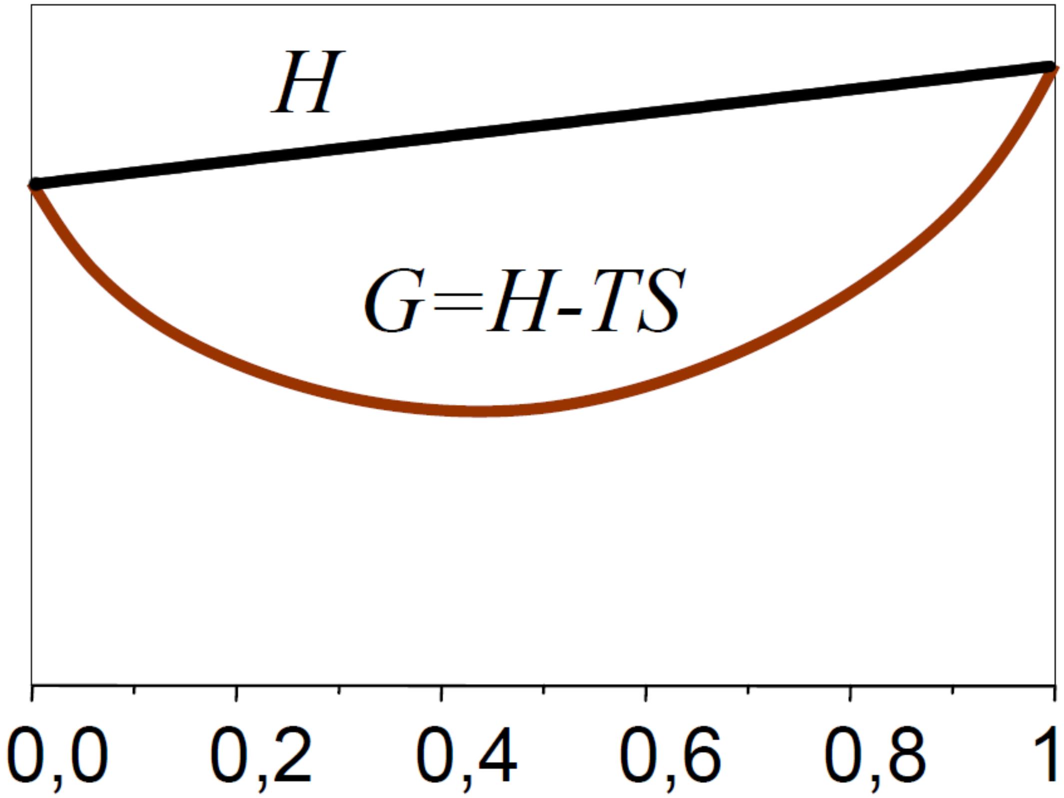
disorder or randomness
Processes reduce the state of order of the initial systems.



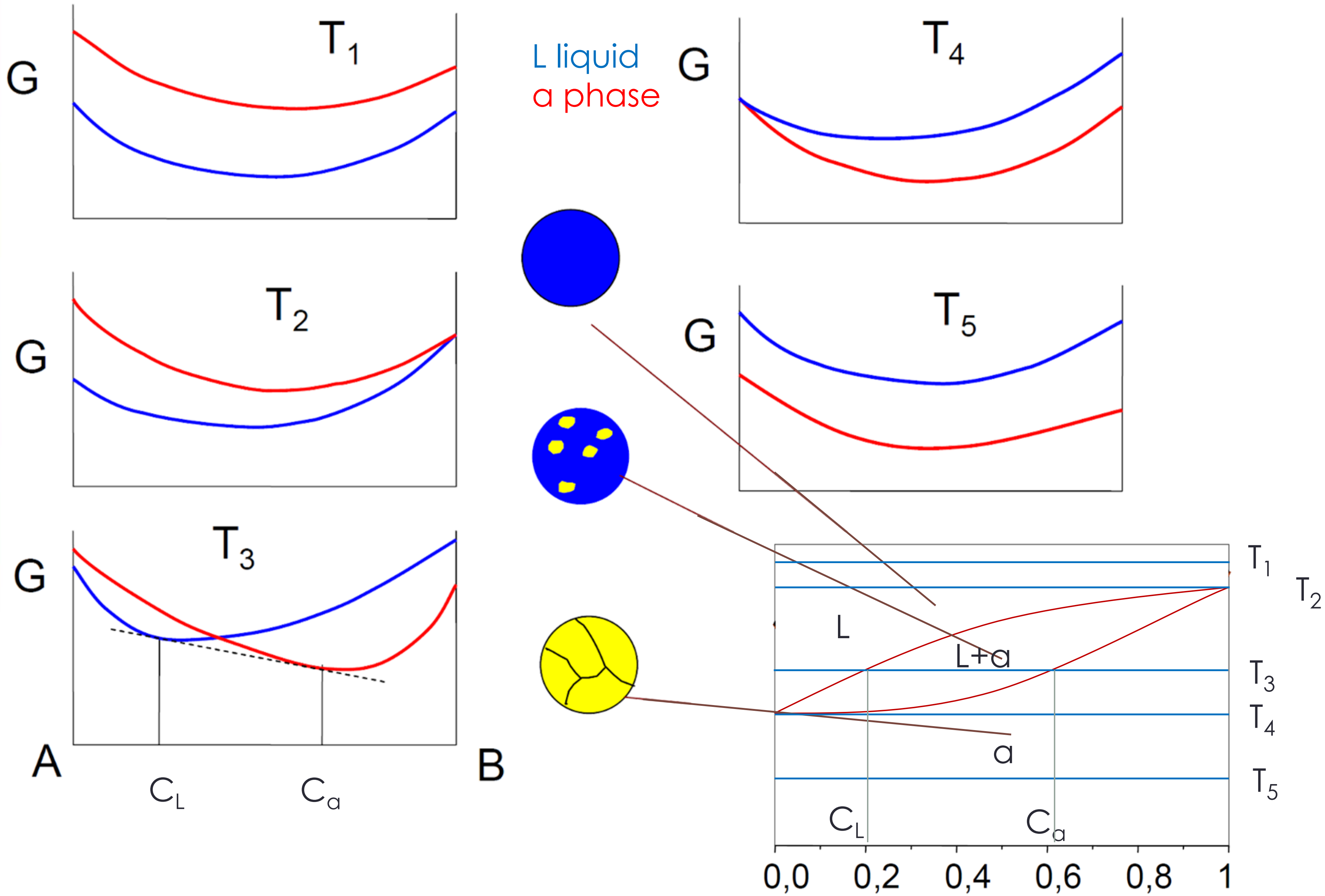
Phase Equilibrium

Equilibrium

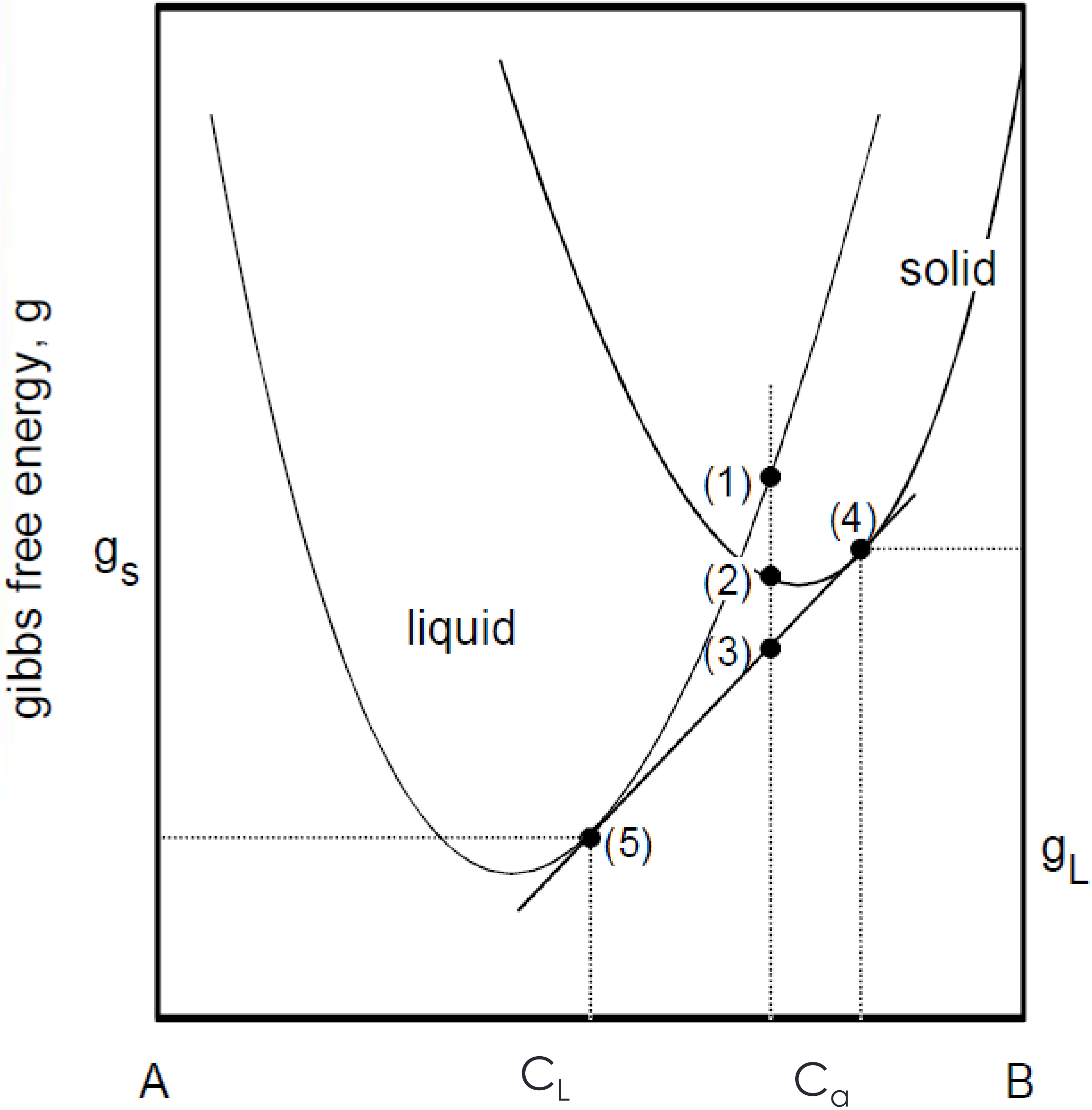
Two component system (A-B), ideal solution

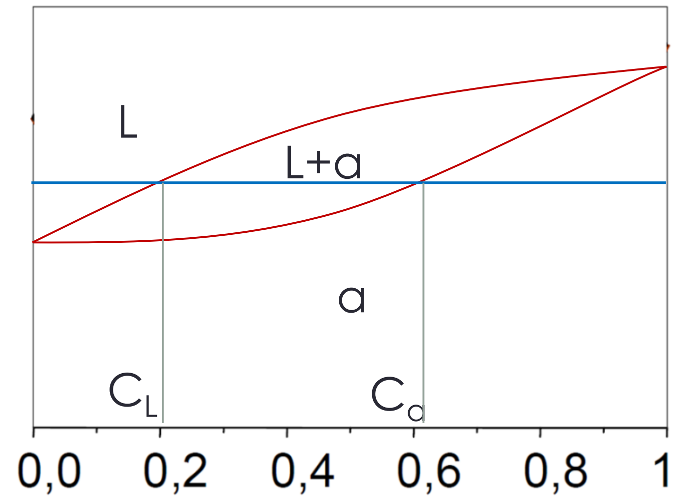


Phase Equilibrium



Phase Equilibrium





Phase Equilibrium

Metastable state

Often the state of equilibrium is never completely achieved because the rate of approach to equilibrium is extremely slow.

→ *non-equilibrium* or *metastable* state.

Metastable state or microstructure may persist indefinitely (changes only extremely slight)

Often, metastable structures are of **more practical significance** than equilibrium ones.

Phase Diagrams

Phase or equilibrium diagram

Information about the phase structure of a particular system.

Parameters
- Temperature
- Pressure
- Composition

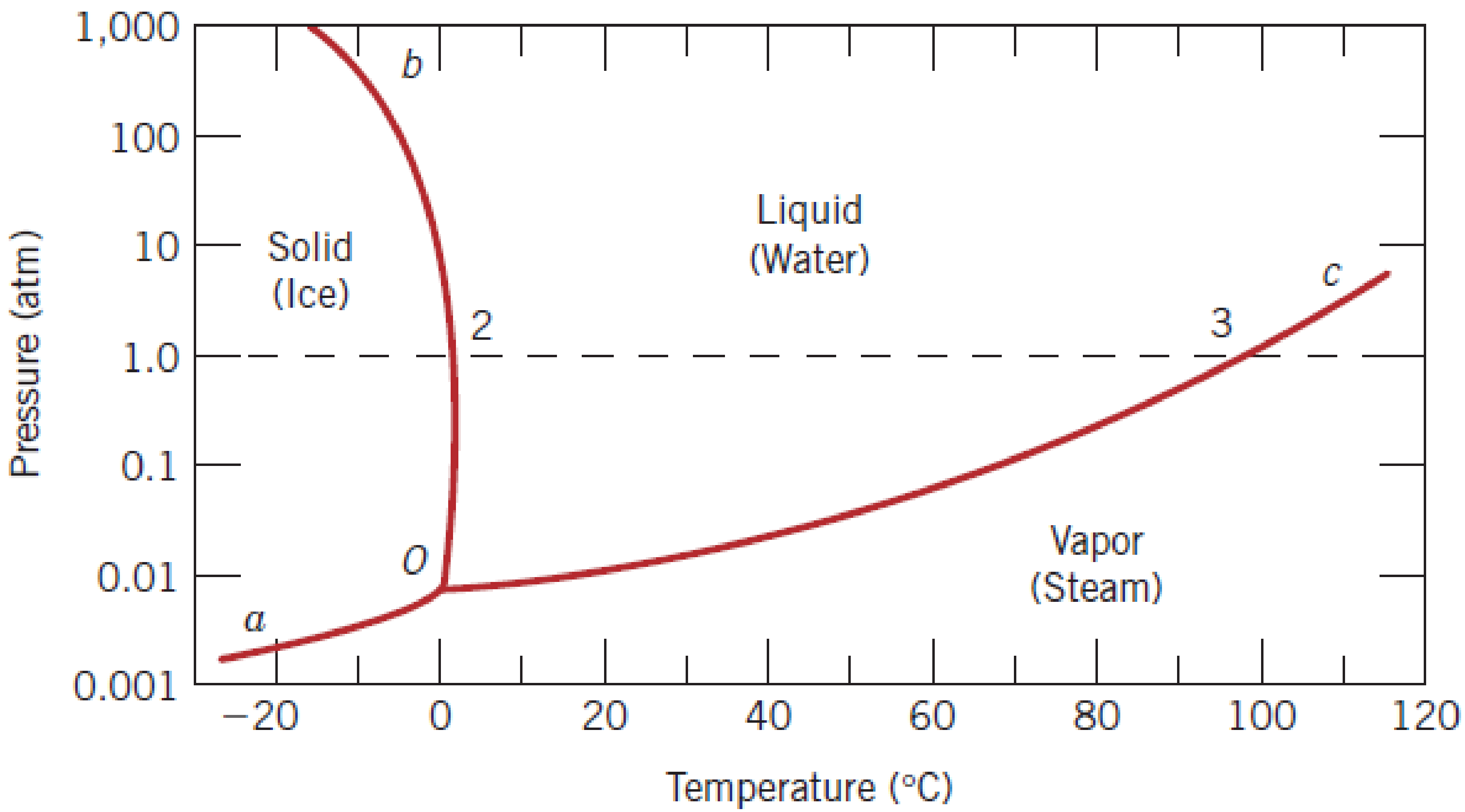
Informations
- State of the matter, crystal structure
- Phase composition
- Chemical composition of the phases

several different varieties
(e.g. composition-Temperature, pressure-Temperature)

Phase Diagrams

One-component (or unary) phase diagram

Simplest, one-component system p-T phase diagram



Pressure–temperature phase diagram for H_2O.

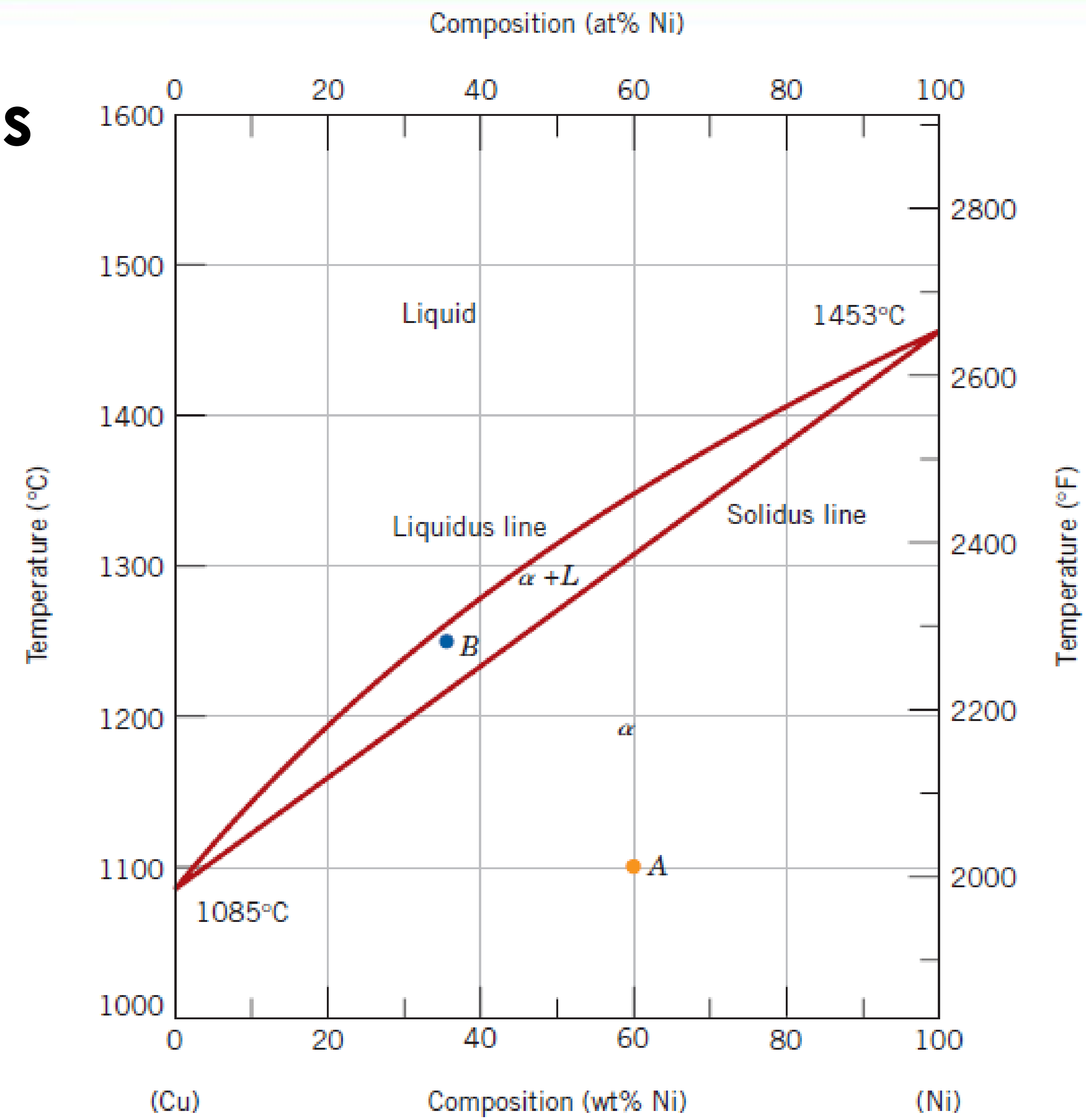
Note! phases at equilibrium

Phase Diagrams

Binary phase diagrams

composition-Temperature

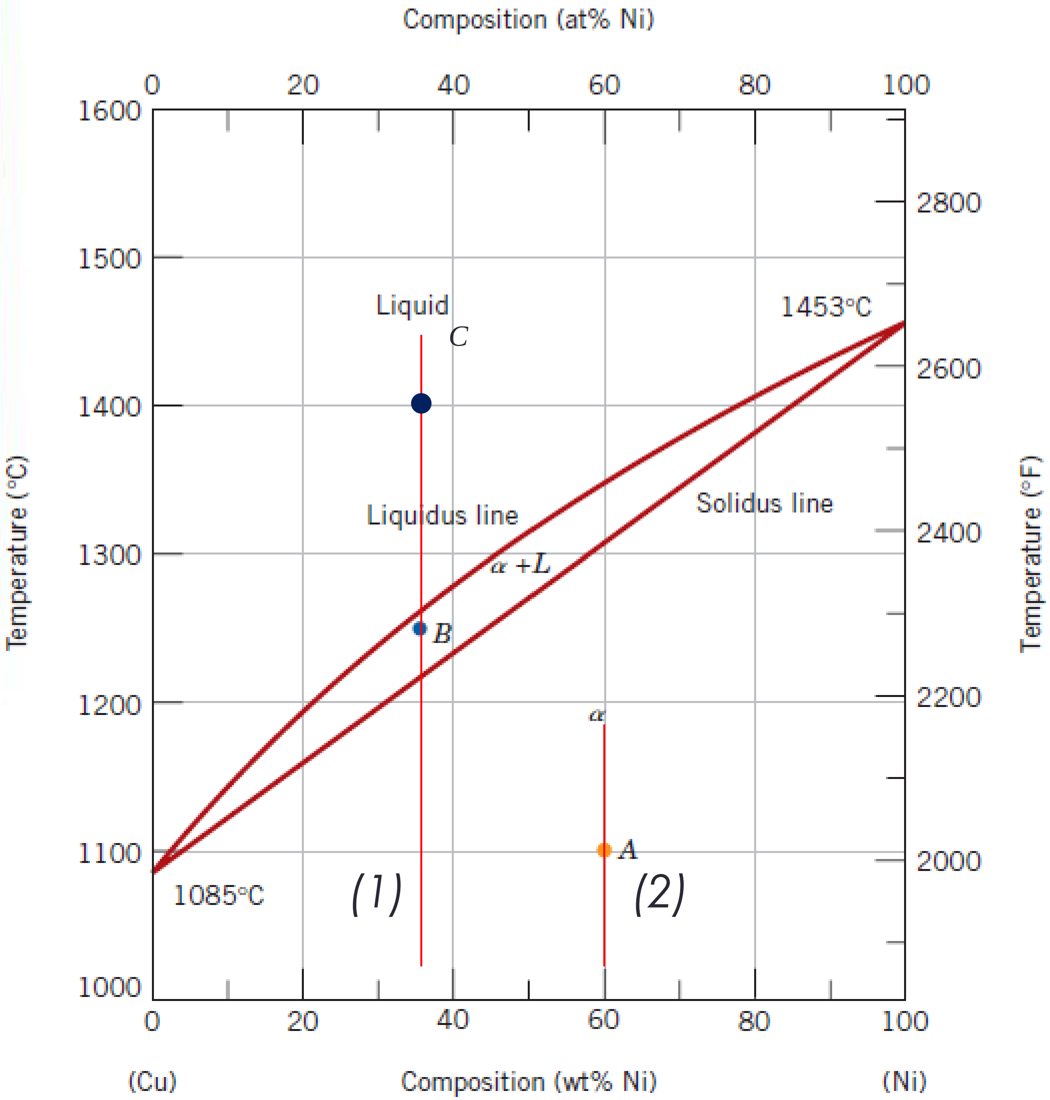
transition from one phase to another, or the appearance or disappearance of a phase.



Copper–nickel phase diagram

Phase Diagrams

Copper–nickel phase diagram



Alloy (2)

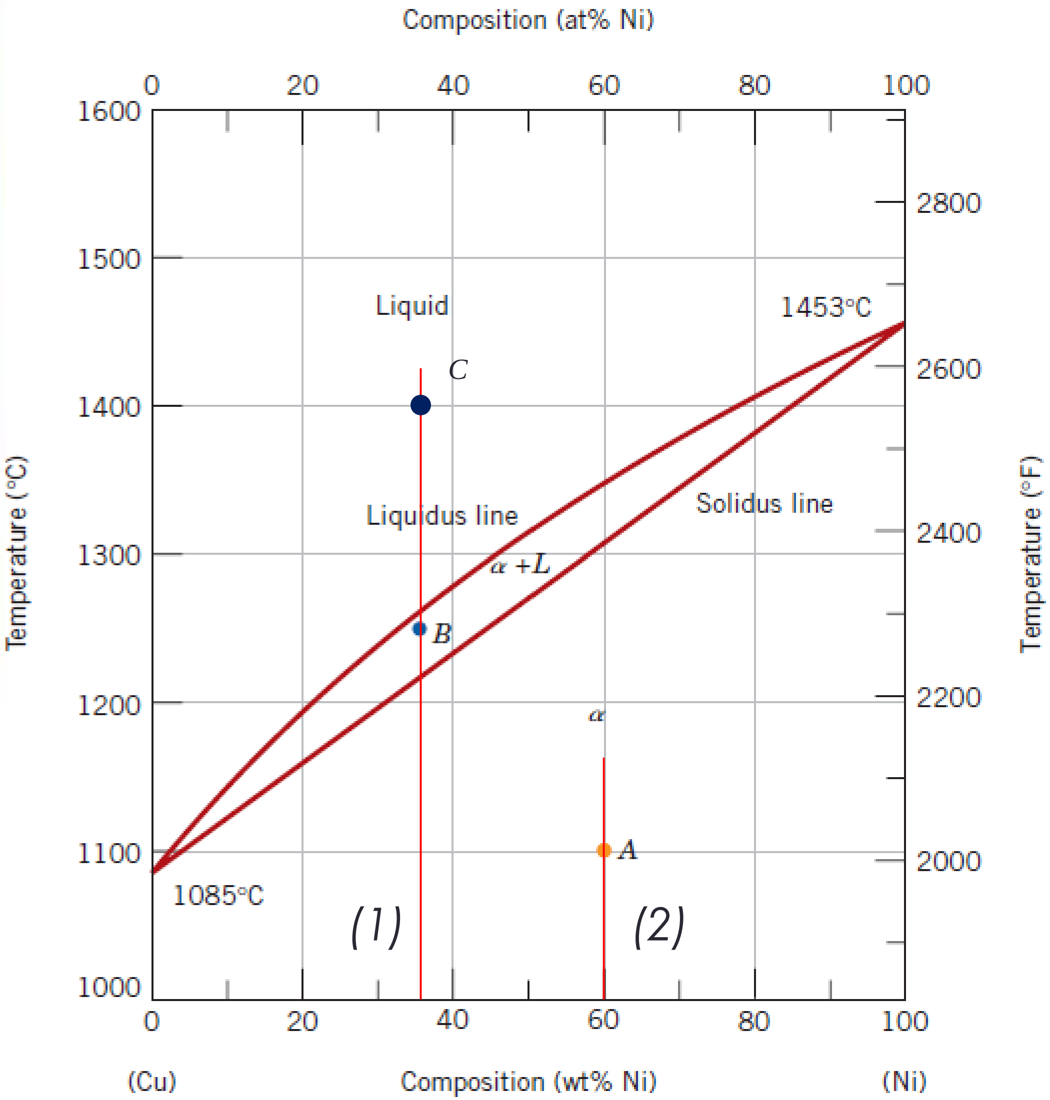
Point A:
T=1100°C
1 phase: a, solid sol. of Cu and Ni
C_{Ni}=60%, C_{Cu}=40%

Alloy (1)

Point C:
T=1400°C
1 phase: L, liquid
C_{Ni}=35%, C_{Cu}=65%

Phase Diagrams

Copper–nickel phase diagram



Alloy (1)

Point B:

T=1250°C

2 phases: a + L,

solid + liquid phase

Composition:

C_{Ni}=35%, C_{Cu}=65%

Mass fraction of phases

W_a=? %, W_L= ? %

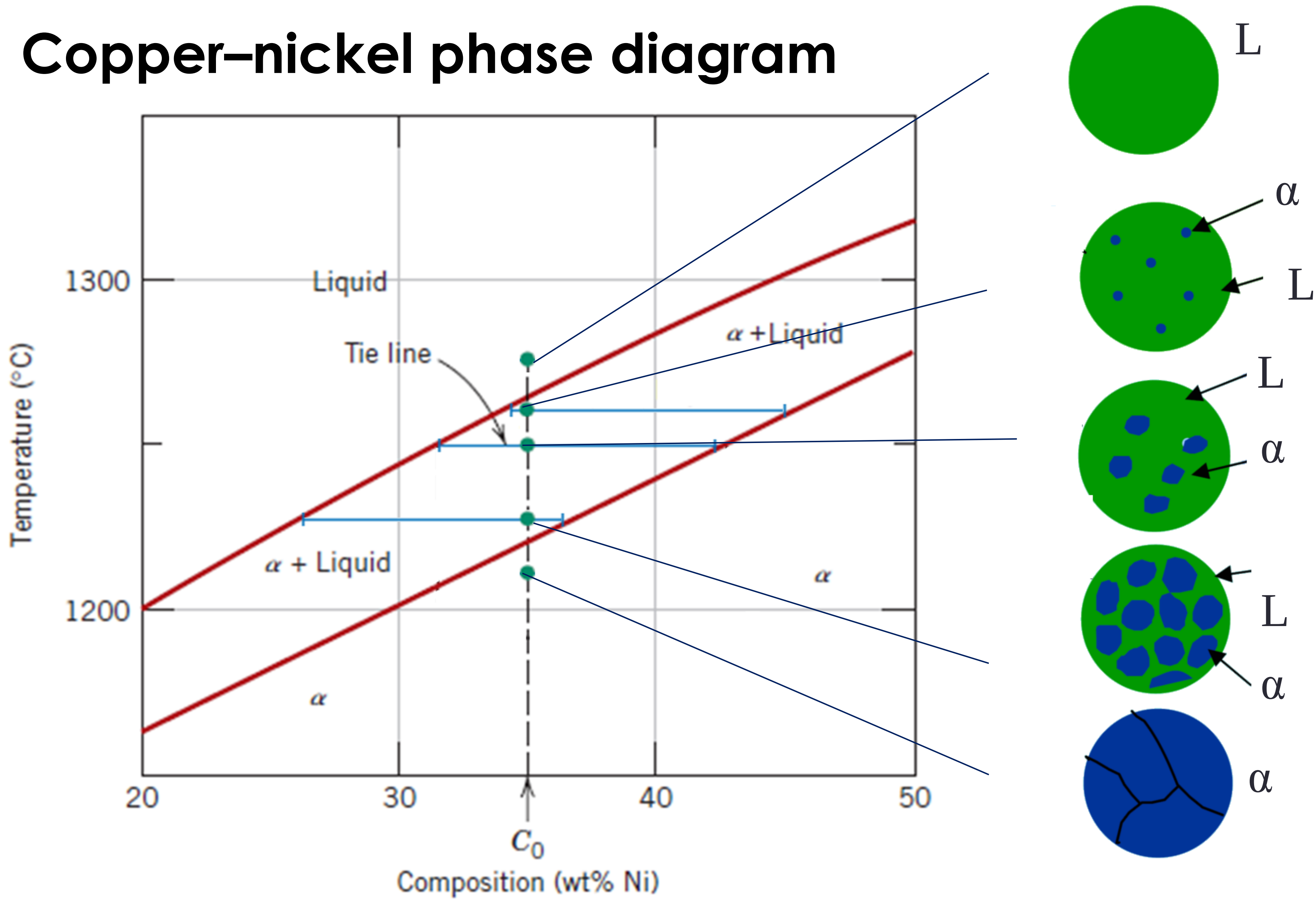
Composition of phases:

a: C_{Ni}=? %, C_{Cu}=? %

L: C_{Ni}=? %, C_{Cu}=? %

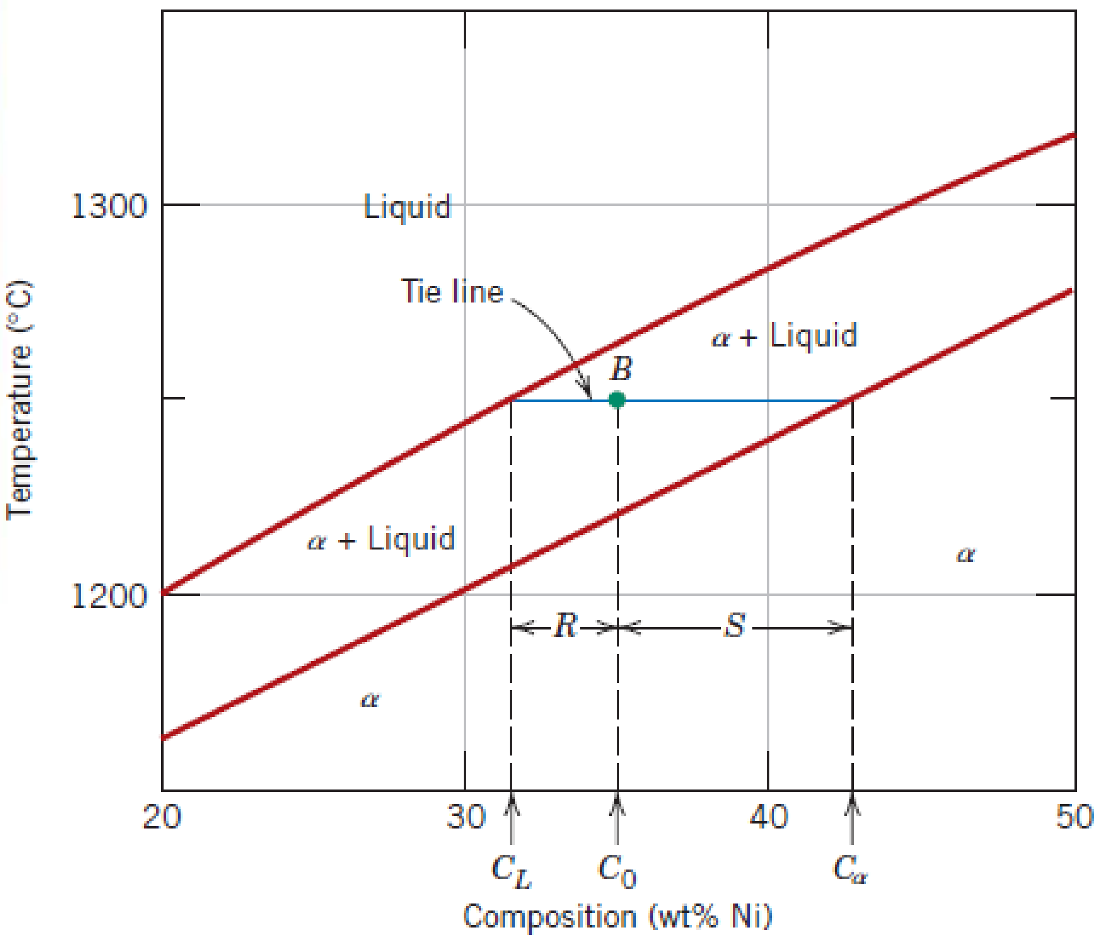
Phase Diagrams

Copper–nickel phase diagram

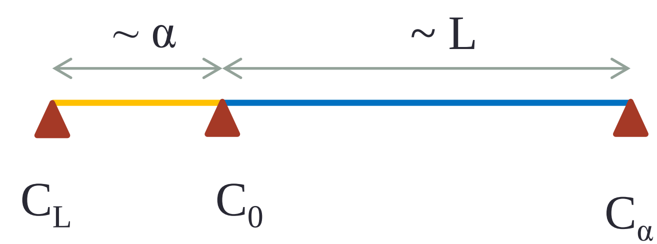


Phase Diagrams

Copper–nickel phase diagram



Lever rule

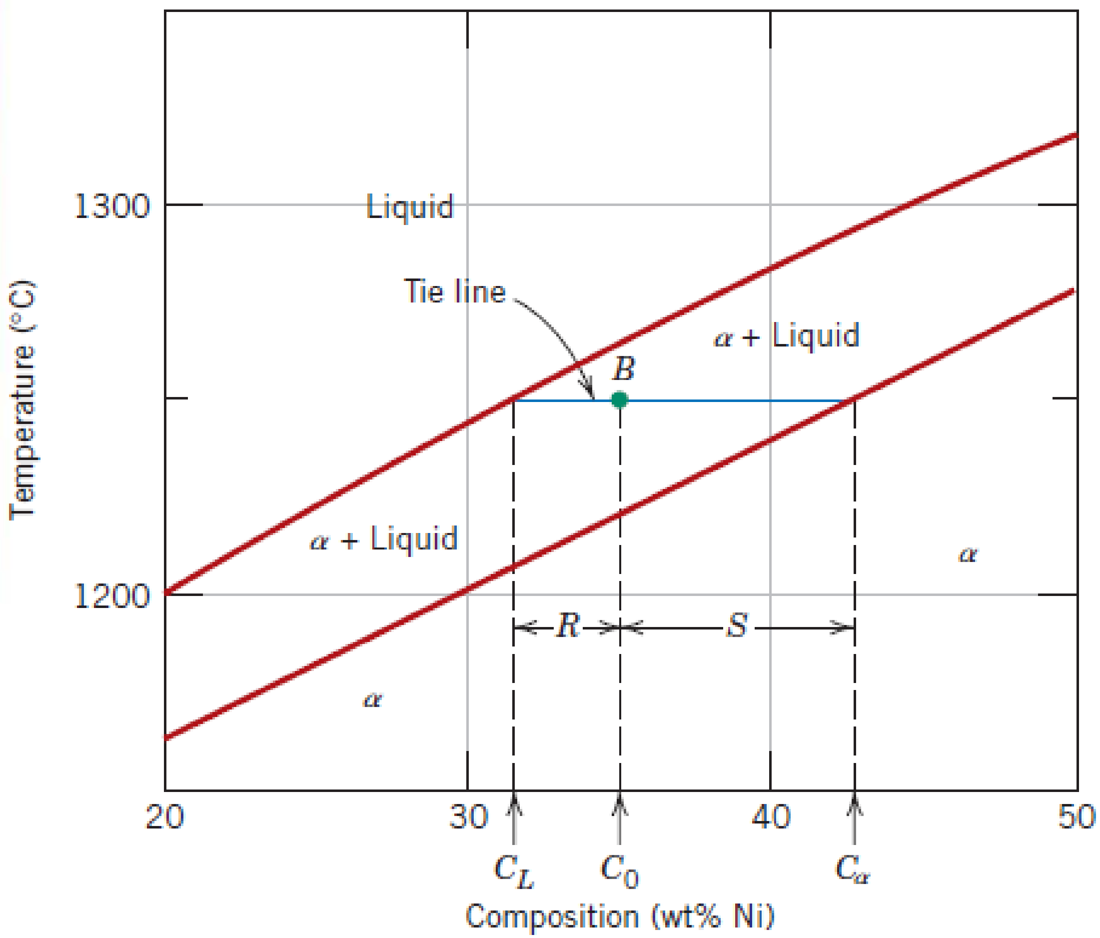


Mass fraction of phases

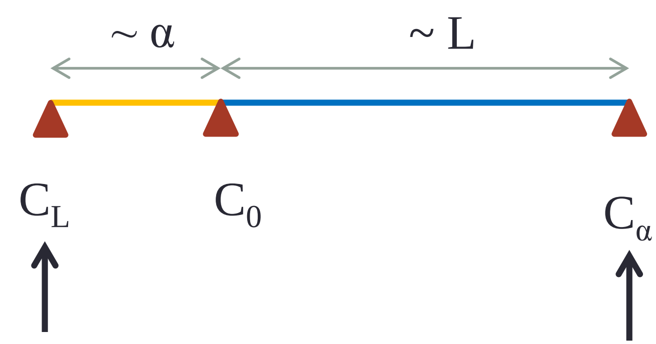
$$W_\alpha = \frac{C_0 - C_L}{C_\alpha - C_L} \qquad W_L = \frac{C_\alpha - C_0}{C_\alpha - C_L}$$

Phase Diagrams

Copper–nickel phase diagram



Composition of phases



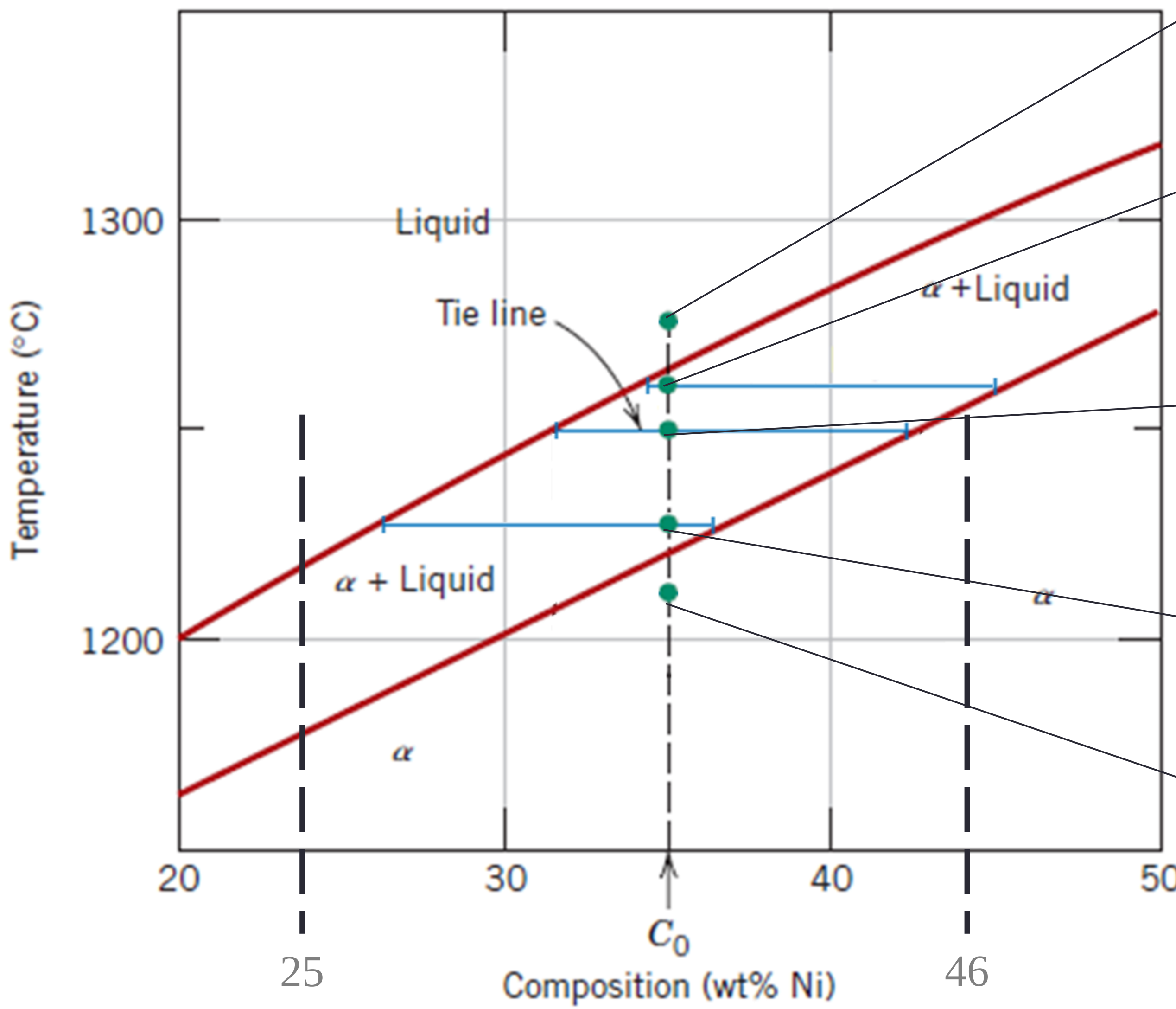
wt% of Ni
in liquid phase

wt% of Ni
in a phase

The chemical composition of the phases is changing with the temperature change.

Phase Diagrams

Copper–nickel phase diagram



Liquid phase: 35% Ni
α phase: -

Liquid phase: 34% Ni
α phase: 46% Ni

Liquid phase: 32% Ni
α phase: 43% Ni

Liquid phase: 35% Ni
α phase: 37% Ni

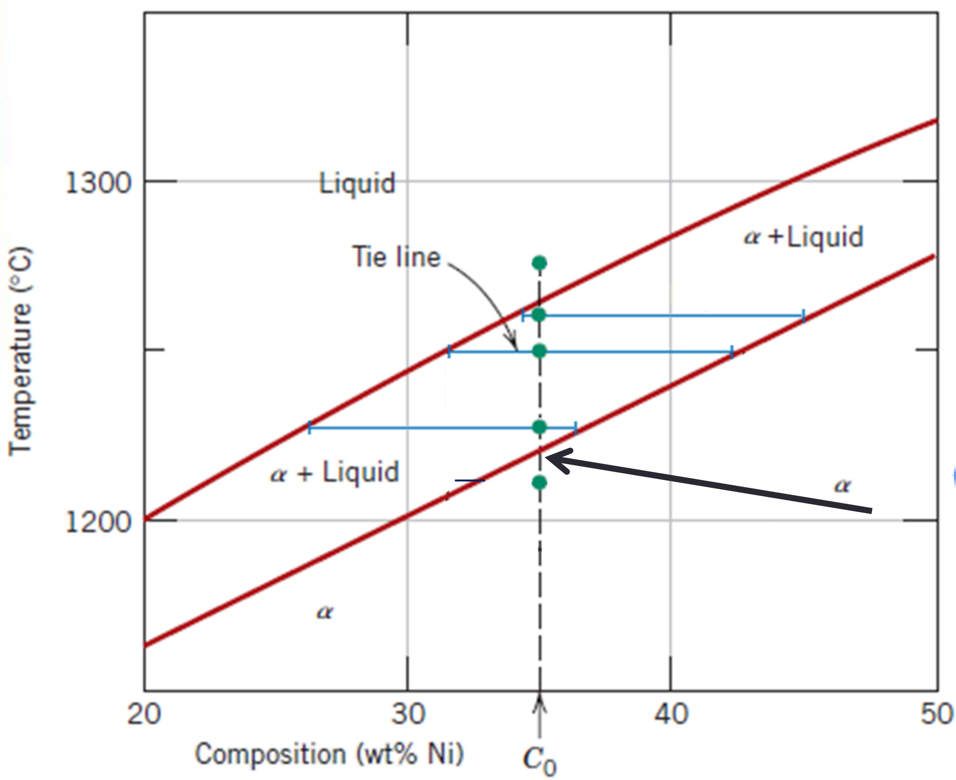
Liquid phase: -
α phase: 35% Ni

Phase Diagrams

Inhomogeneous and equilibrium phase

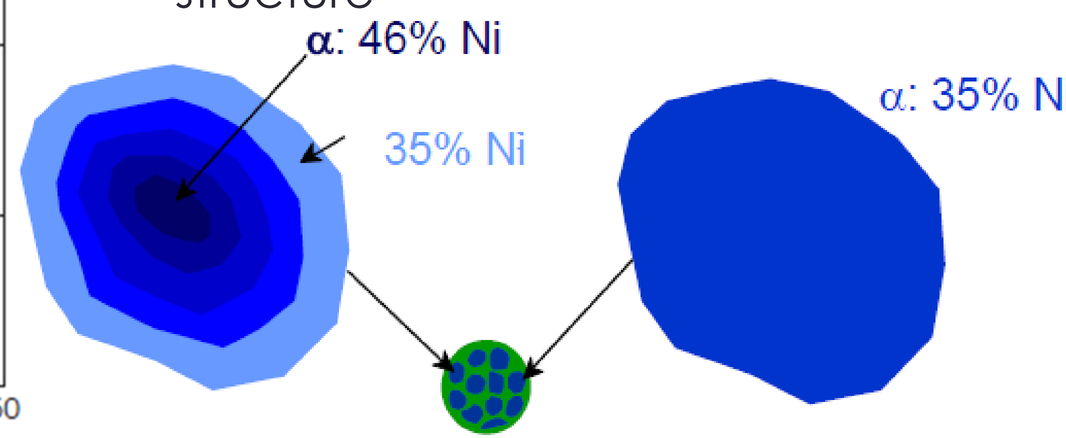
Equilibrium solidification:

- only for extremely slow cooling rates.
- diffusional processes (diffusion rates are lower for lower temperatures and for solid phases)



High cooling rate
Inhomogeneous structure

Low cooling rate
Equilibrium structure



Phase Diagrams

Inhomogeneous and equilibrium phase

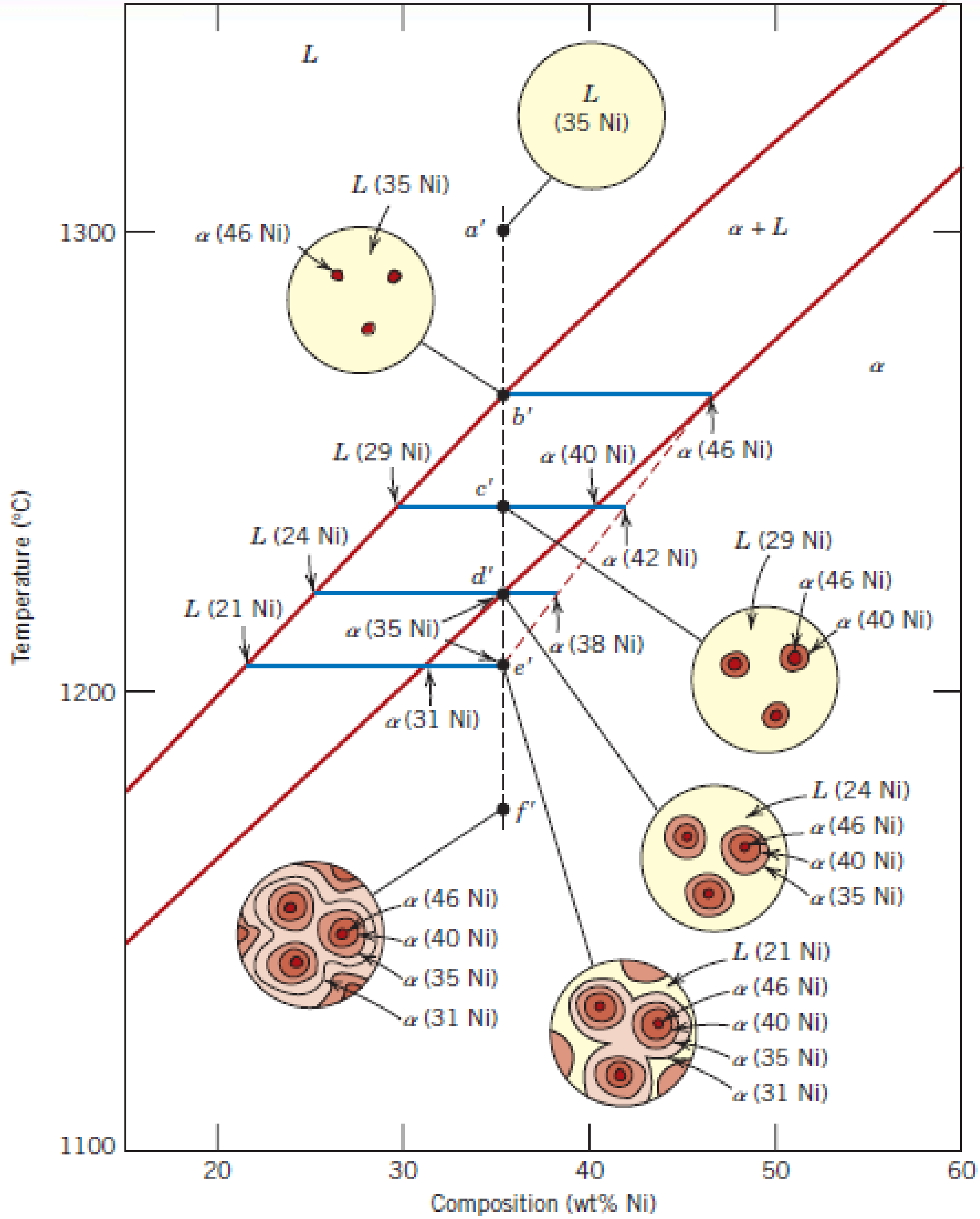
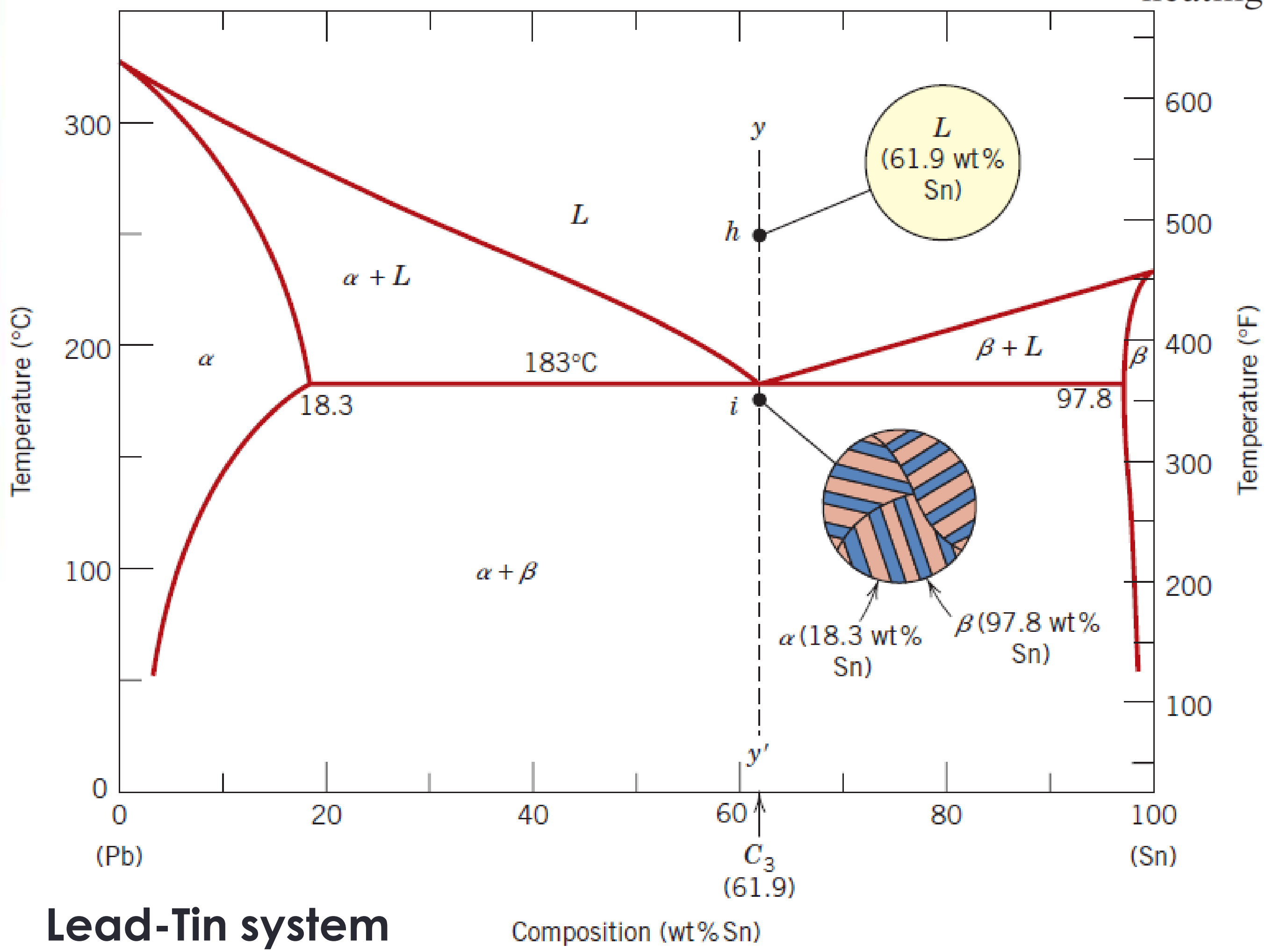


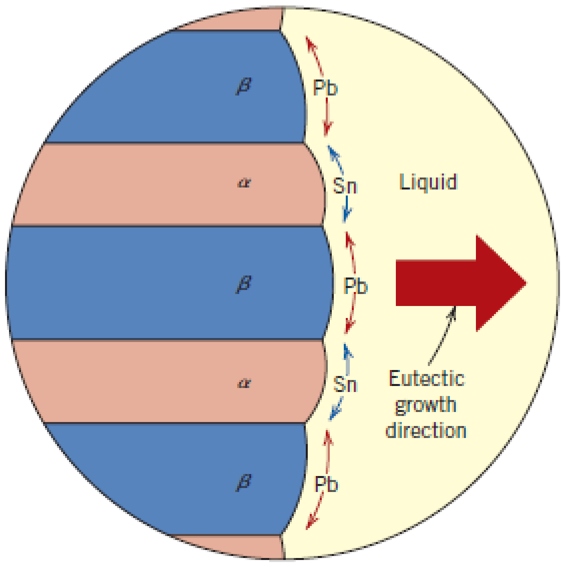
Figure from Callister, Mat. Sci. and Eng. An Introduction, 8th edition

Phase Diagrams

Eutectic reaction

Liquid phase $\underset{\text{heating}}{\overset{\text{cooling}}{\rightleftharpoons}}$ *α + β (solid phases)*

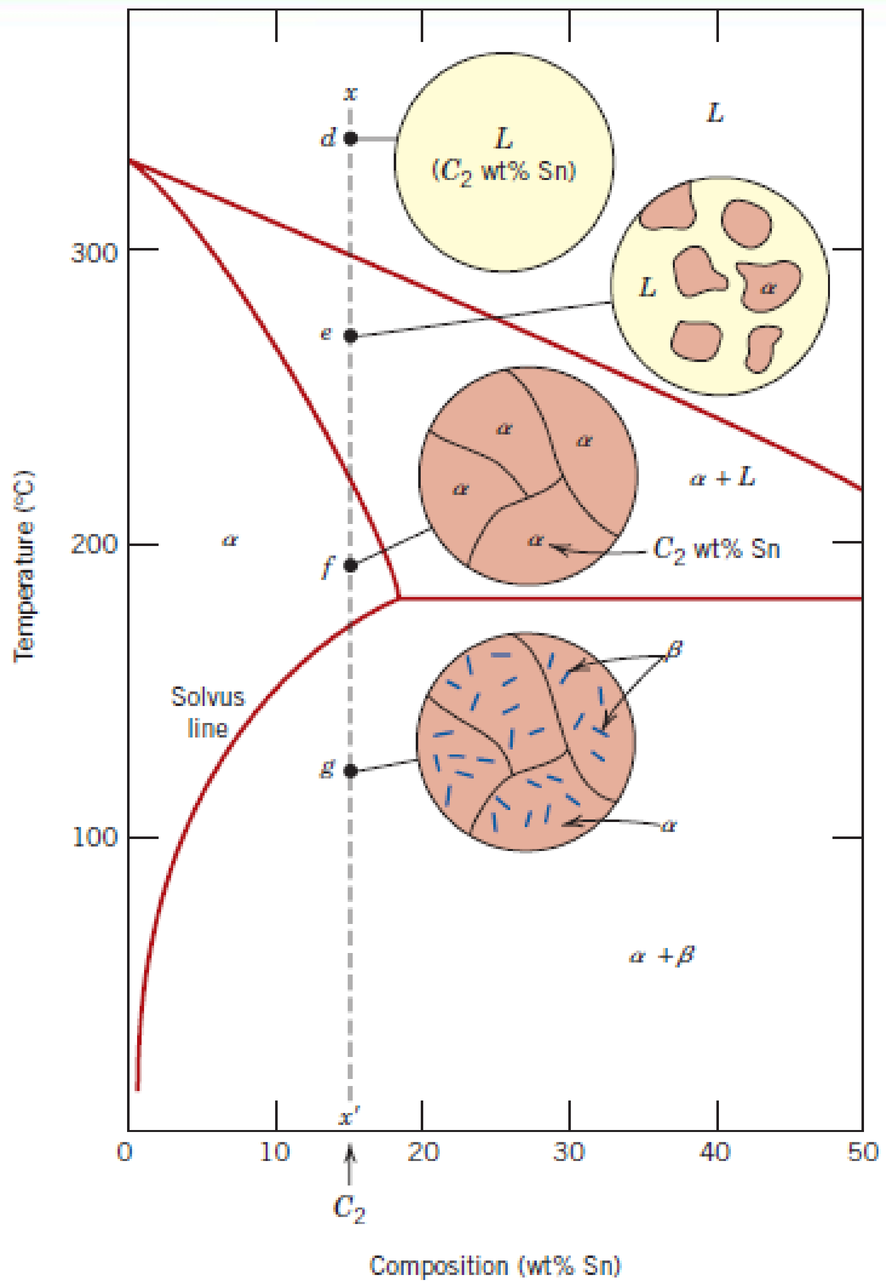




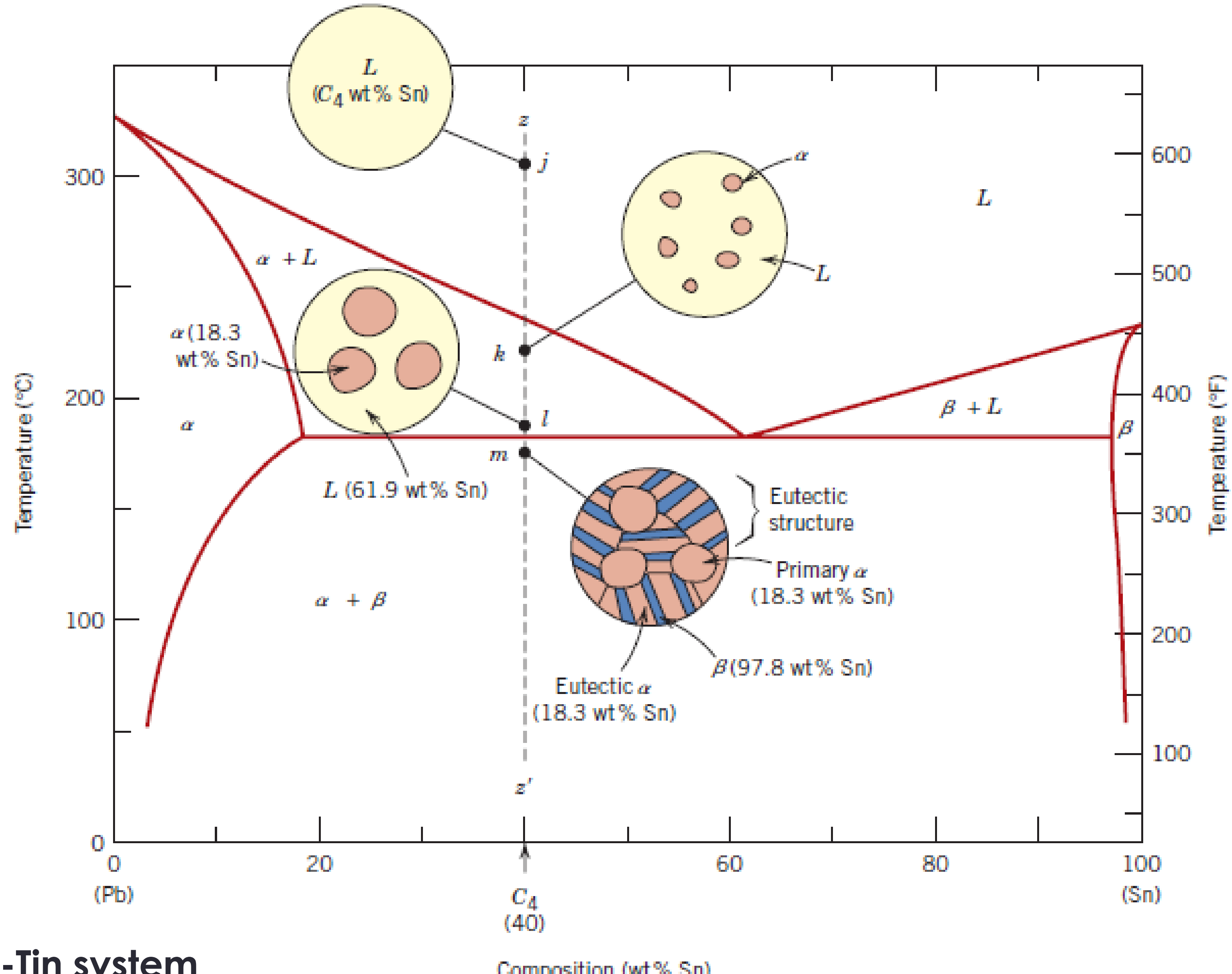
Lead-Tin system

Phase Diagrams

Lead-Tin system



Phase Diagrams

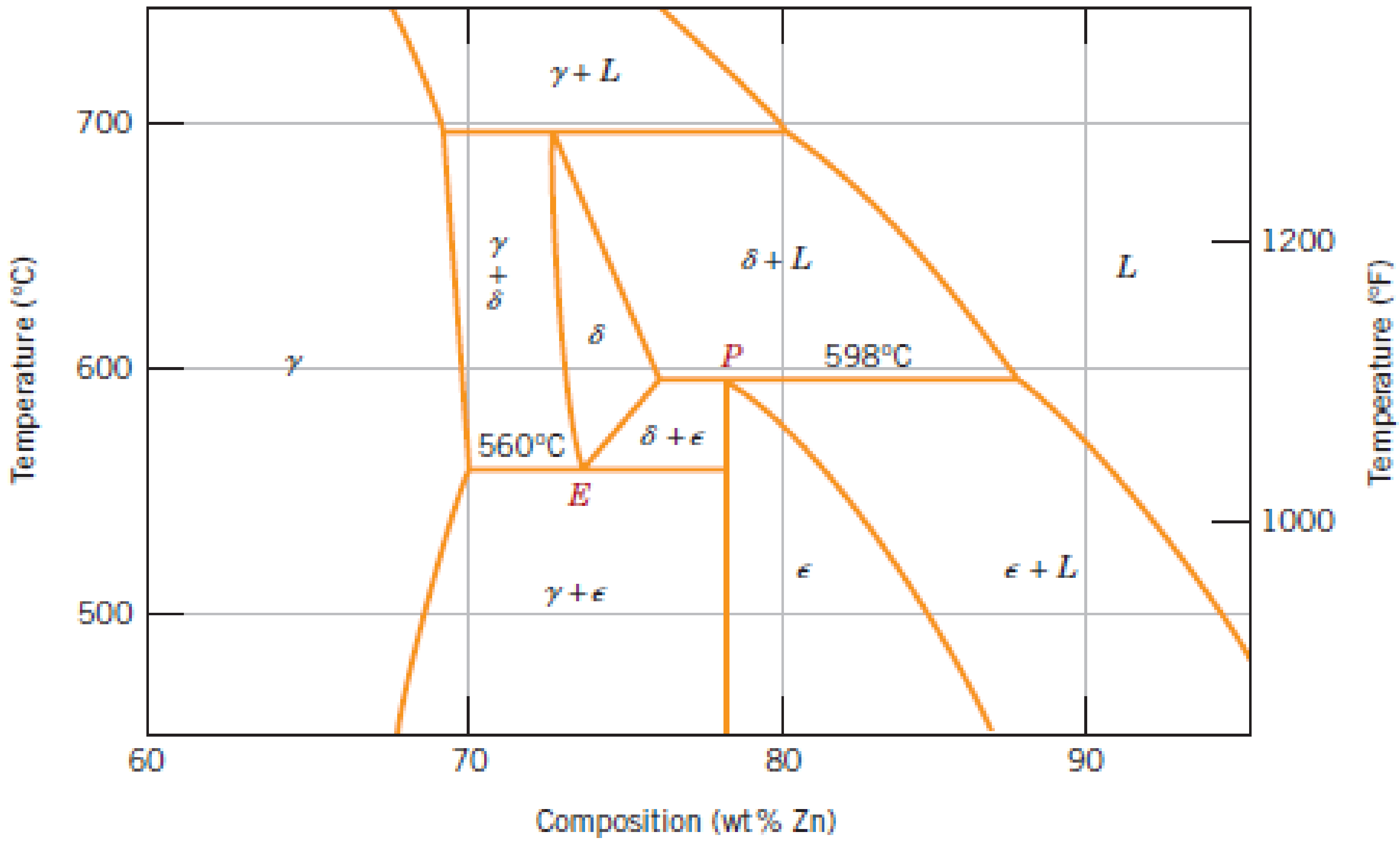


Lead-Tin system

Phase Diagrams

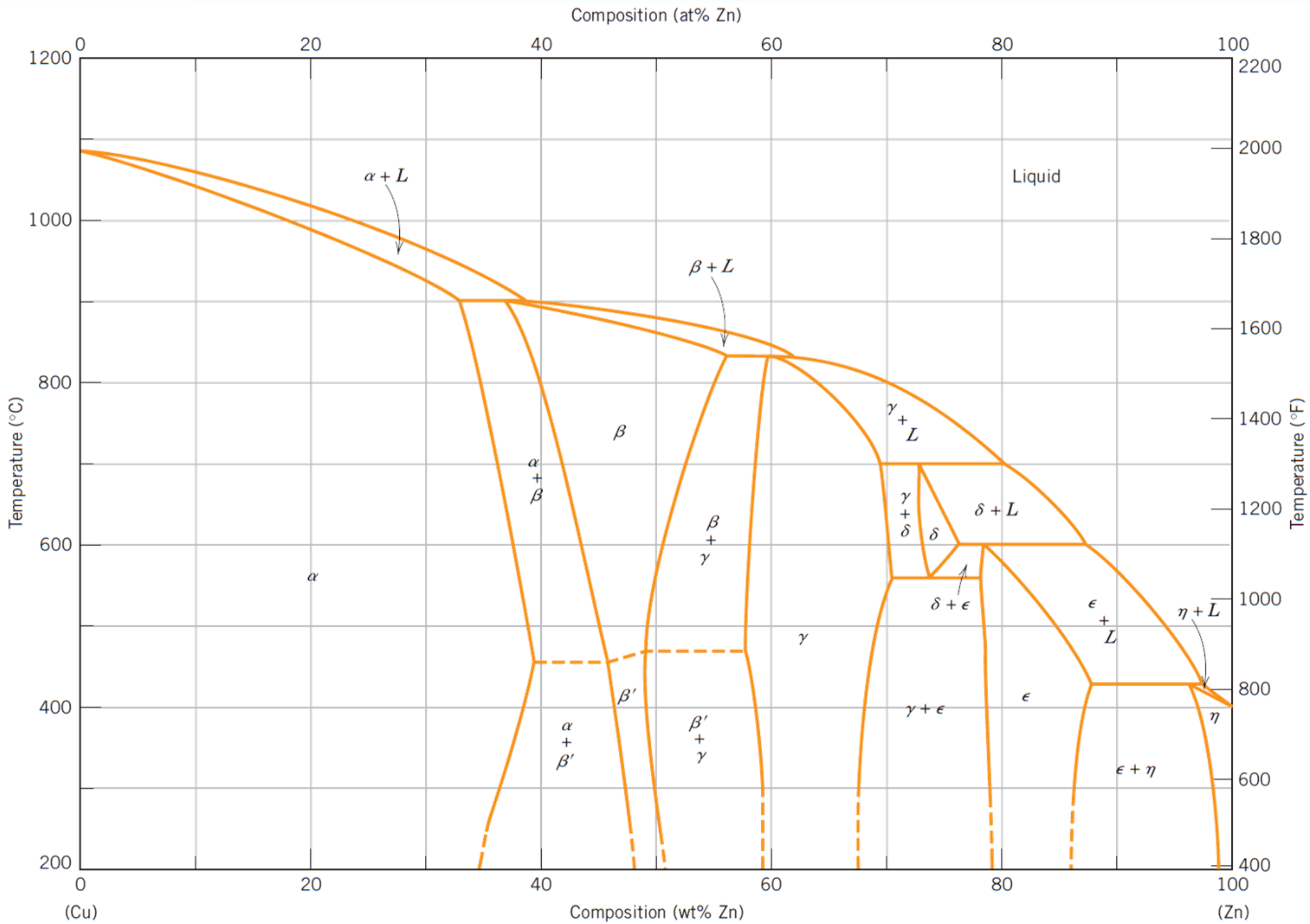
Eutectoid reaction γ *(solid phase)* $\underset{\text{heating}}{\overset{\text{cooling}}{\rightleftharpoons}}$ α + β *(solid phases)*

Peritectic reaction α *(solid phase)* + *liquid phase* $\underset{\text{heating}}{\overset{\text{cooling}}{\rightleftharpoons}}$ γ *(solid phases)*



Copper–zinc phase diagram

Phase Diagrams



Ceramic Phase Diagrams

The two components are compounds that share a common element
Similar to metal–metal systems

Al_2O_2-Cr_2O_3 phase diagram

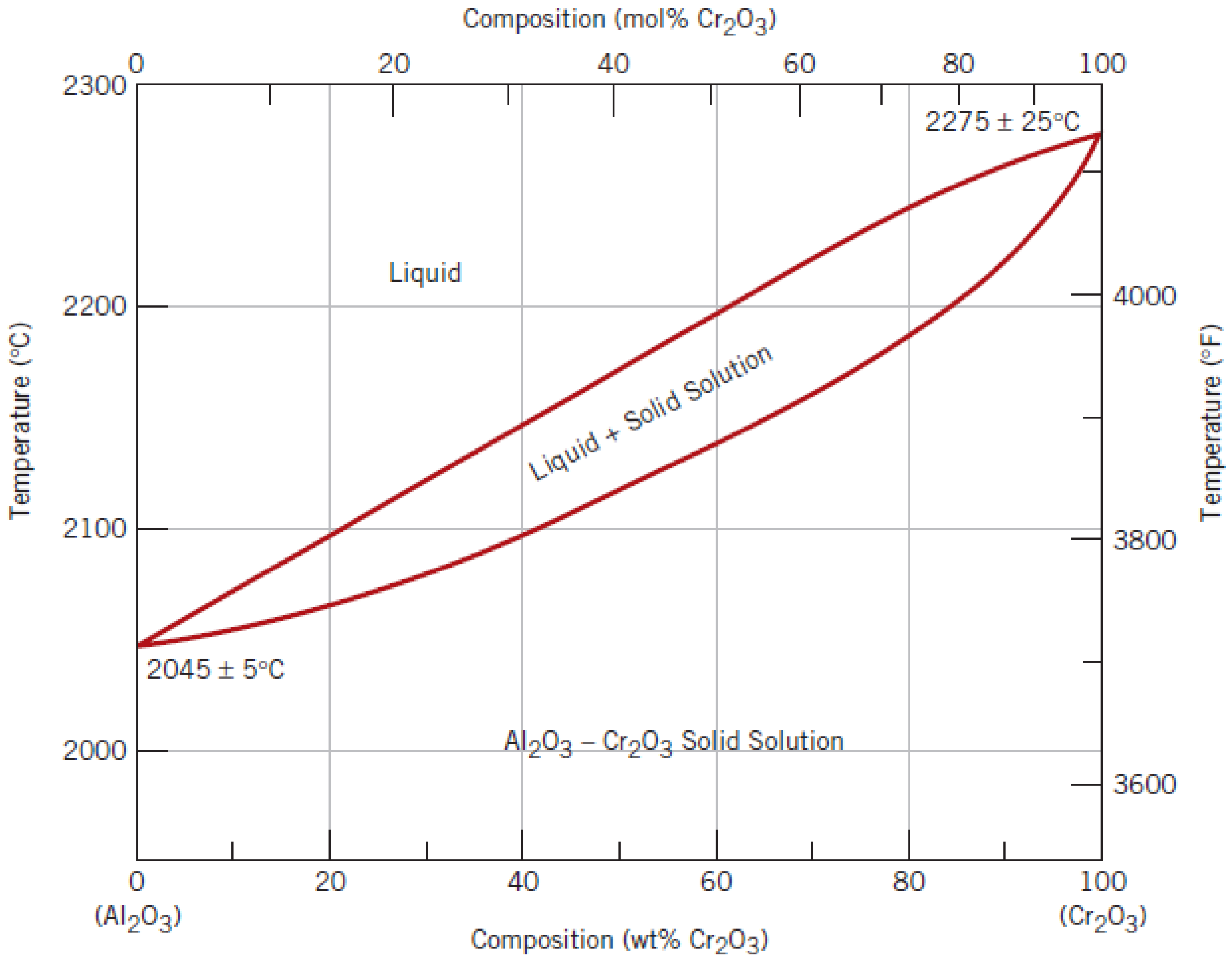
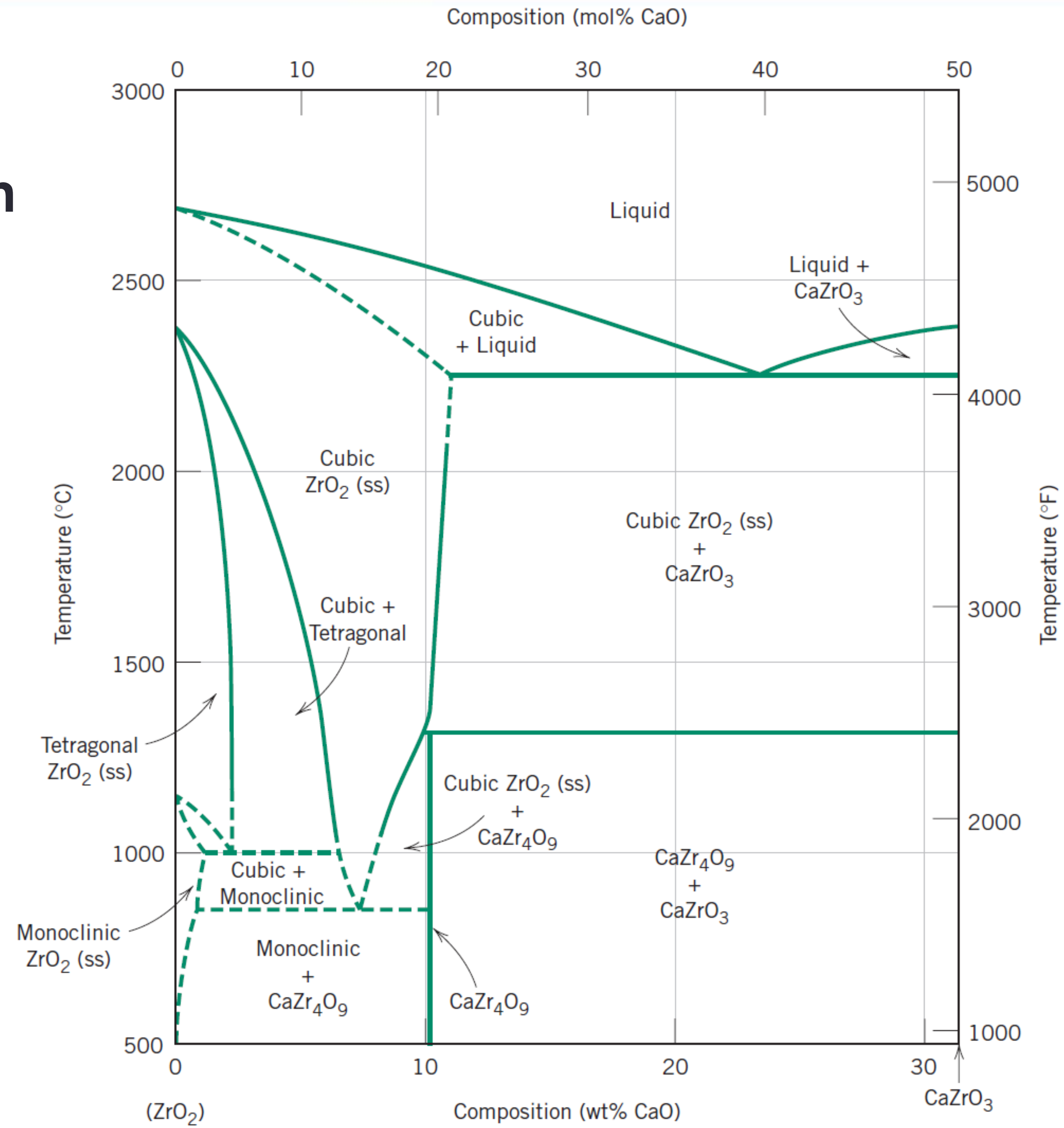


Figure from Callister, Mat. Sci. and Eng. An Introduction, 8th edition

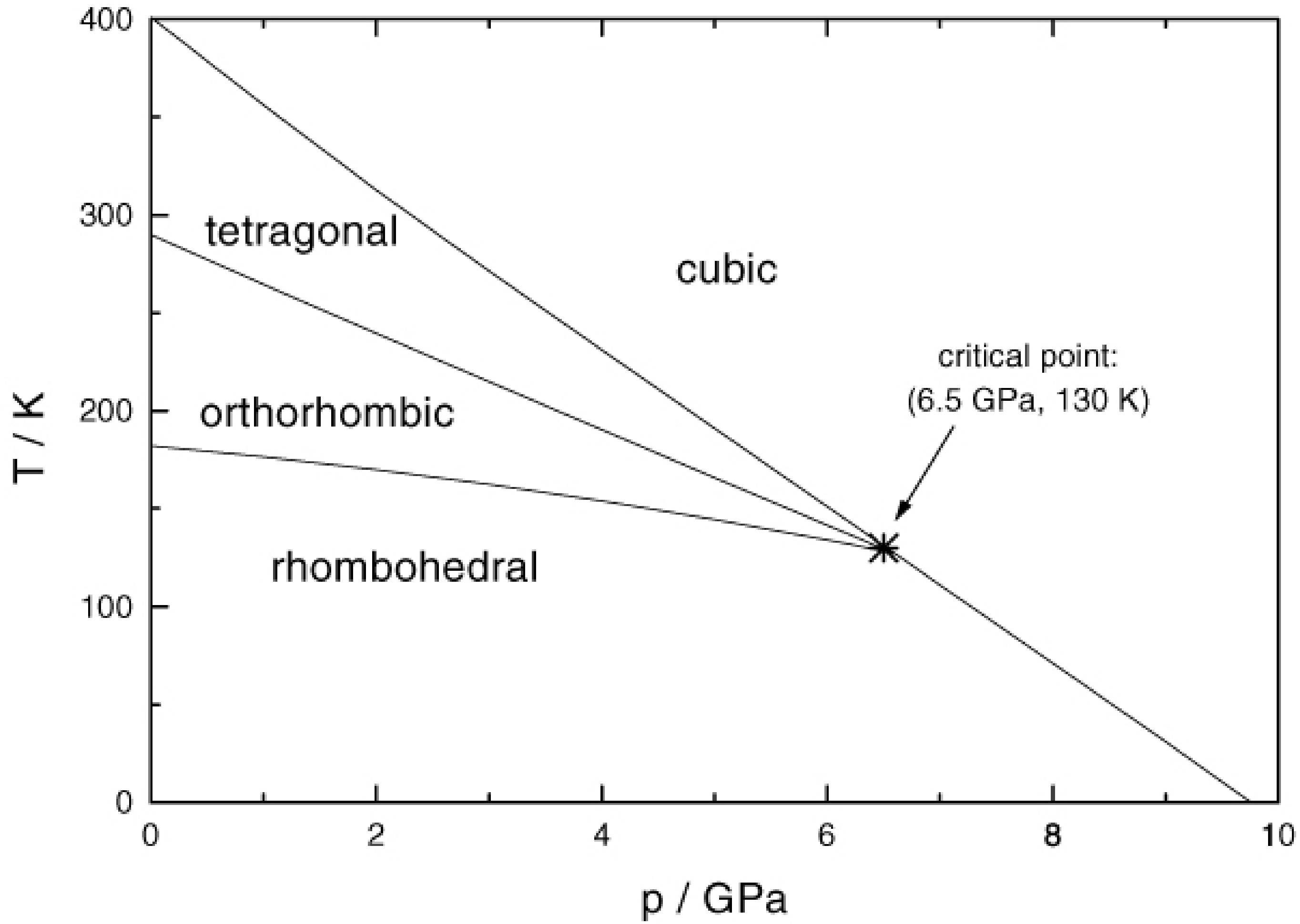
Ceramic Phase Diagrams

ZrO_2-$CaZrO_3$ phase diagram



Ceramic Phase Diagrams

$BaTiO_3$ p-T phase diagram



S A Hayward and E K H Salje ,J. Phys.: Condens. Matter 14 No 36 2002 p 599-604