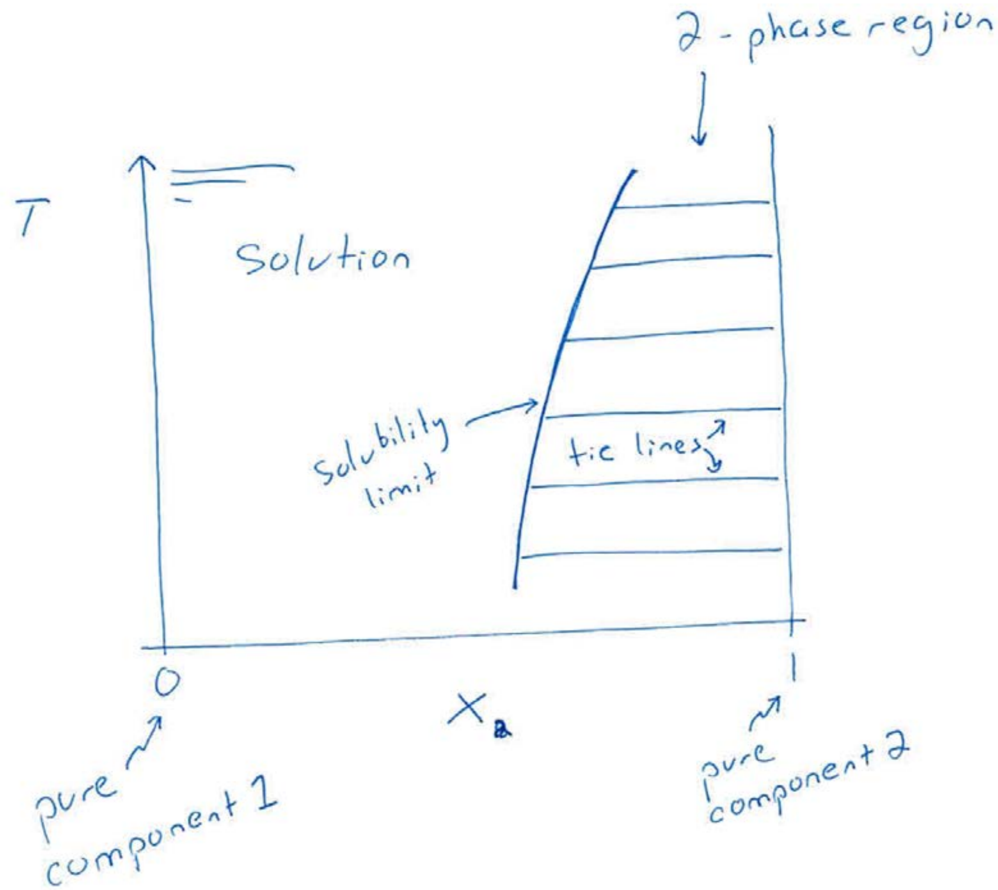
3.020 Lecture 15

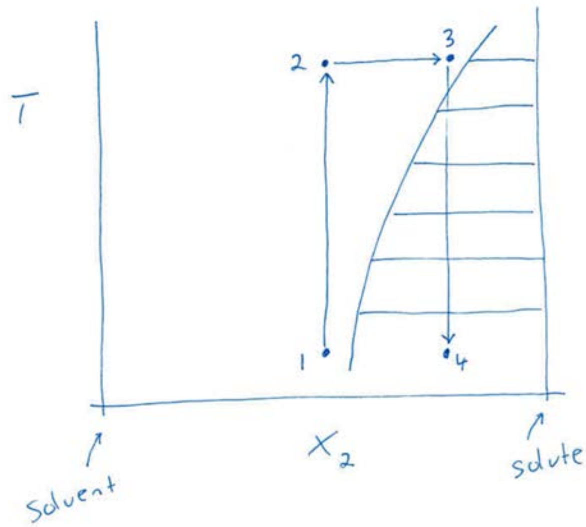
Prof. Rafael Jaramillo

1 Binary phase diagrams



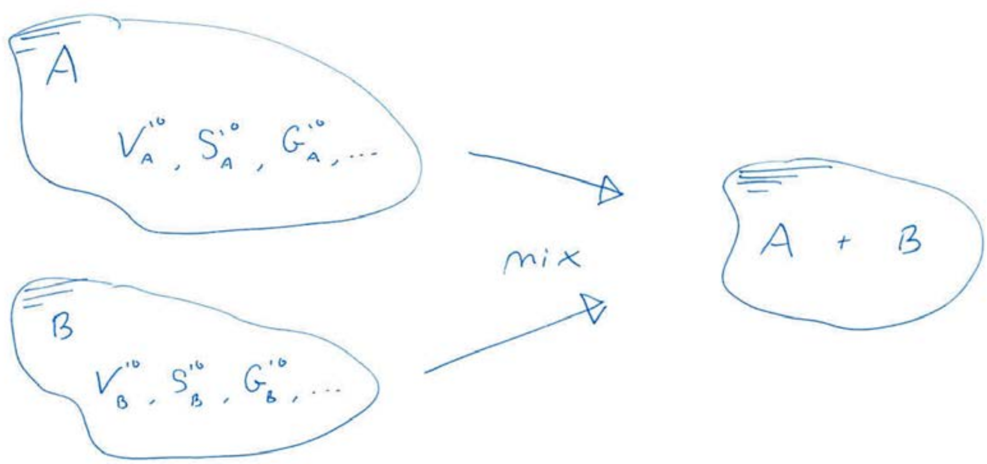
ex. Crystal growth by supersaturation.

rock candy



1. Start with room-T solution
2. Heat up
3. Add more solute
4. Cool down to create supersaturated condition
   Crystal growth is spontaneous

2 Process of making solutions



- Quantities of mixing

$$
\begin{aligned}
V' &= V_A'^0 + V_B'^0 + \Delta V'_{mix} \\
S' &= S_A'^0 + S_B'^0 + \Delta S'_{mix} \\
G' &= \underbrace{G_A'^0 + G_B'^0}_{} + \Delta G'_{mix}
\end{aligned}
\quad \Longrightarrow
$$

When making solutions, the whole is not simply the sum of the pants

reference states of pure components

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3 Solutions all around us

- Gas phase: air
- Liquid phase: ocean water, sweet drinks, gasoline
- Solid phase: Steel, brass, superalloys (e.g. jet turbine blades), lithium ion battery electrodes, semiconductors

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4 Solutions and reactions

Reactions: A + B = C

- A discrete process, with fixed reactants and products
- Individual chemical components (A, B, C) undergo substantial atomic-scale change

Solutions: $A_x + B_{1-x} = A_x B_{1-x}$

- A continuous process, with composition variable x
- Individual chemical components (A, B) remain recognizable on atomic scale

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5 Solution modeling

- To make predictions we need thermodynamic data
- Every material is different $\longrightarrow$ Do we need to measure infinite data to understand a system like Si:Ge ?

$$\text{Si}, \quad \text{Si}_{0.9999}\text{Ge}_{0.0001}, \quad \text{Si}_{0.9998}\text{Ge}_{0.0002}, \quad \ldots$$

We hope not !!!

- Model trends in thermodynamics with composition

modeling in the sciences

- Solution models:
  - Understand underlying atomic-scale phenomena
  - Make useful predictions

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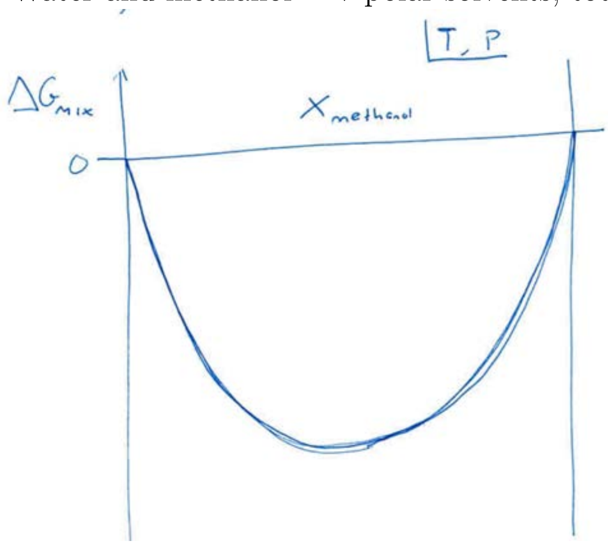
e.g. Water and methanol $\longrightarrow$ polar solvents, totally miscible



$$\textbf{Unmixed } G = \mu^0_{H_2O} X_{H_2O} + \mu^0_{meth} X_{meth}$$
$$= G^0$$
$$\textbf{Mixed } G = G^0 + \Delta G_{mix}$$
$$G_{mixed} < G^0 = G_{unmixed}$$

System mixes spontaneously to achieve equilibrium

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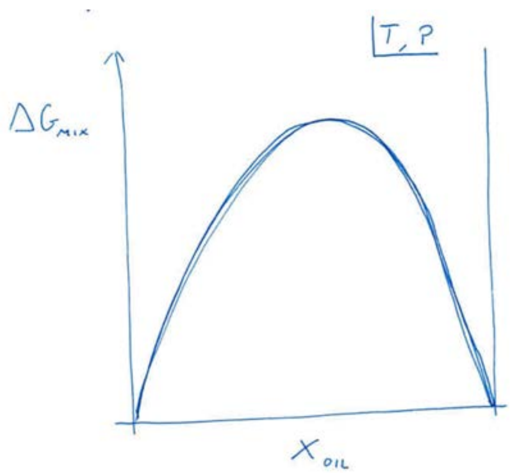
e.g. Water and oil



$$G_{unmixed} = G^0 < G_{mixed}$$

$\Longrightarrow$ System will remain unmixed. If initially mixed, it will spontaneously unmix to reach equilibrium

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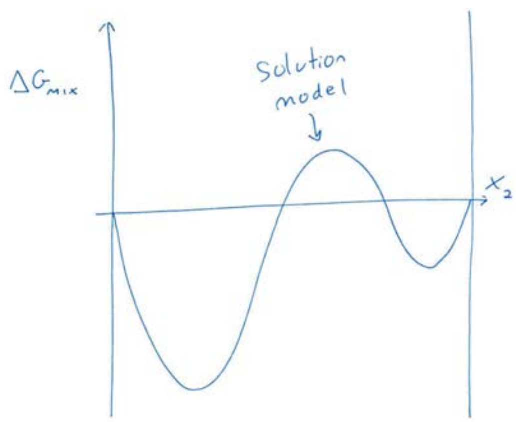
- Free energy-composition diagrams



- Solution models represent particular phases
- Models are derived from
  - experimental data
  - empirical modeling
  - atomistic modeling