PennState

PHASES PSU

Introduction to thermodynamic modeling

MatSE 501 Recitation

2017-11-27

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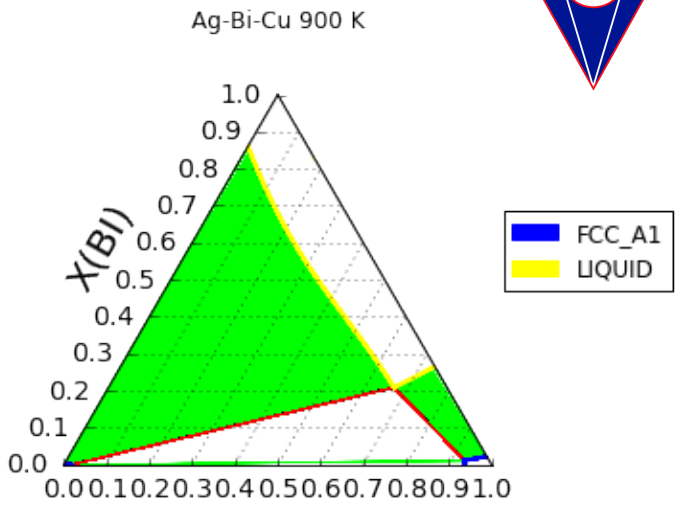
The CALPHAD Method

- **CAL**culation of **PH**ase **D**iagrams
- Pioneered by Larry Kaufman in the early 1970s



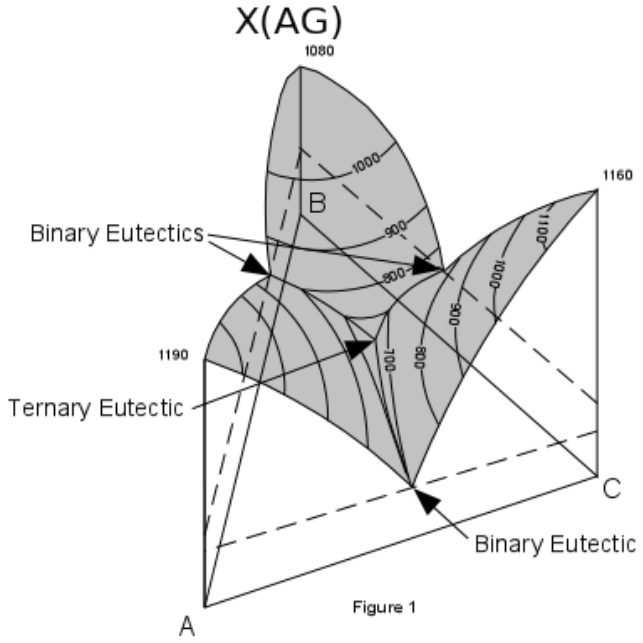
Thermochemical data: heat capacity, enthalpy, entropy, activity

Phase equilibrium data: phase stability, phase boundary

Gibbs Energy of Individual Phases

$$G^{\phi}(T,P,N_i,\xi)$$

Applications: Equilibrium, driving force, physical/chemical properties (1st, 2nd derivatives)



Read more: Spencer A brief history of CALPHAD. Calphad 32, 1–8 (2008)

http://www.tulane.edu/~sanelson/eens212/ternaryphdiag.htm

Parameterizing Gibbs free energies

- Each phase (α, ice, water, liquid, fcc) is assigned a Gibbs free energy

$$G^{\alpha} = \sum_i x_i {}^{\circ}G_i^{\alpha} + RT \sum_i x_i \ln x_i + {}^{E}G^{\alpha}$$

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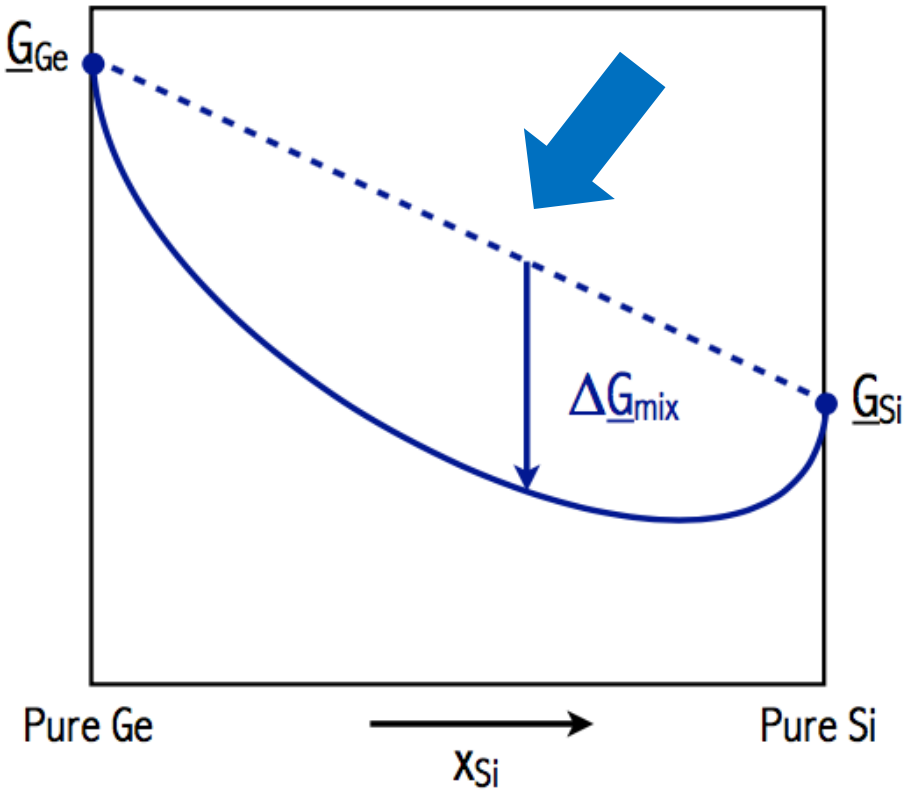
Parameterizing Gibbs free energies



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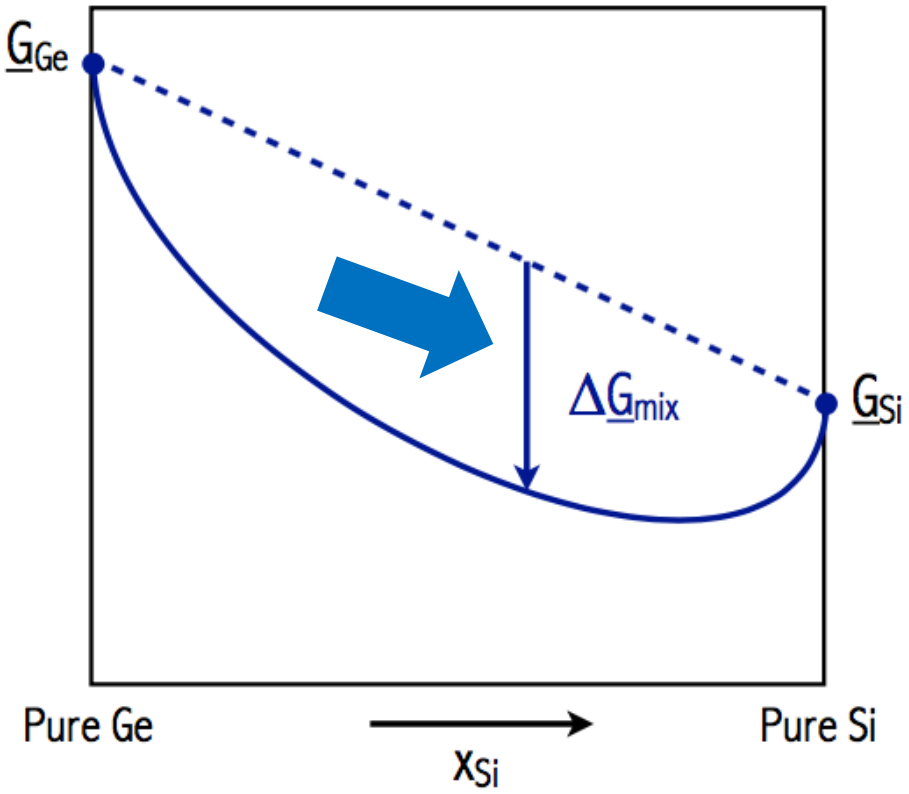
Ideal mixing

Parameterizing Gibbs free energies



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Excess mixing

Parameterizing Gibbs free energies

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Ene ure

pha mixing

- *Excess* mixing is somewhat nebulous
- Defined as any non-ideal mixing behavior
- We have seen it as: $^{E}G^{\alpha} = x_a x_b \Omega = x_a x_b H_{\text{mix}}$
- These are extended to multicomponent cases as *interaction parameters*

+ G Excess mixing

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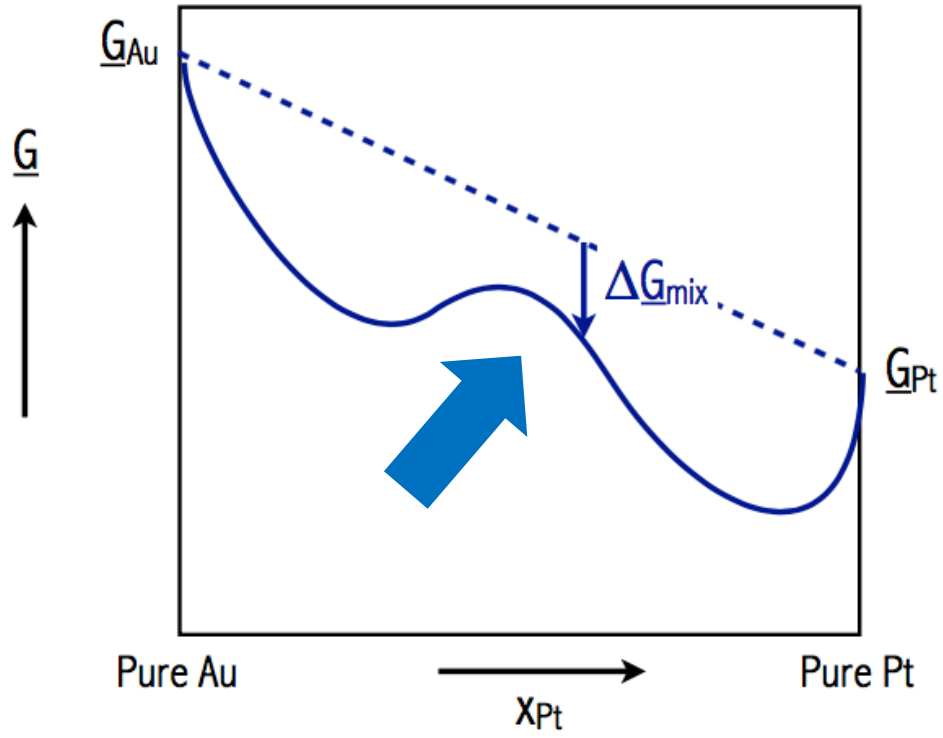

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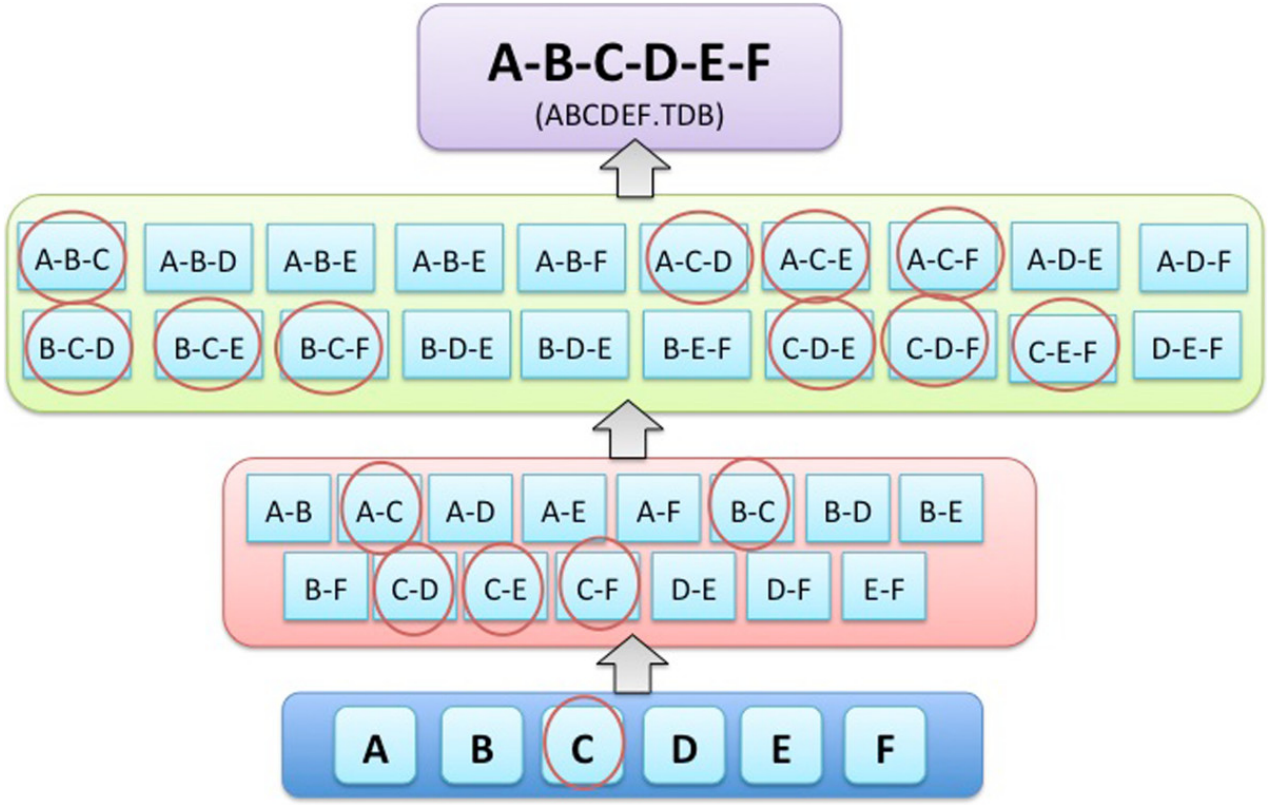
$$+ {}^{E}G^{\alpha}$$ ← Excess mixing

Lattice stability

- Pure W is stable in a bcc crystal, but often alloyed into fcc solutions
- CALPHAD descriptions must define the energy of fcc W, or the stability of W in the fcc lattice
- Determining lattice stabilities
  - Estimating with values that give correct phase diagrams
  - Extrapolate from experimental data
  - Calculate with first-principles

Building multicomponent databases



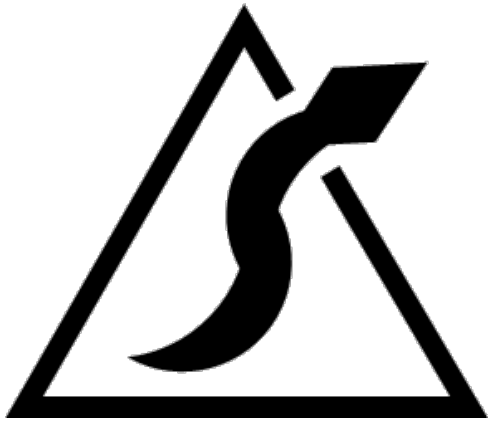
Campbell (2014).

- Databases are available in literature and commercially
- For practical calculations, modeling details are not required
- Active research areas:
  - Model development
  - (Automated) Database development

$$C_n^2 = \frac{n(n-1)}{2} \qquad C_n^3 = \frac{n(n-1)(n-2)}{6}$$

CALPHAD Software

- Most common CALPHAD software:
  - Commercial: Thermo-Calc, Pandat
  - Non-commercial: OpenCalphad, pycalphad
- pycalphad is a Python-based CALPHAD software developed by Dr. Liu's group at PSU
  - Initially released in April 2015
  - Developed in the open on GitHub: https://github.com/pycalphad/pycalphad
  - Development lead by Richard Otis at NASA JPL



pycalphad

https://pycalphad.org

Installing pycalphad

1. Install Anaconda (already done on the PSU computers)
   - Download from https://anaconda.com/downloads
2. Start -> Anaconda -> Anaconda Prompt
3. Run the commands:
   1. conda config –add channels conda-forge
   2. conda config –add channels msys2
   3. conda config –add channels pycalphad
4. Run the command: conda install pycalphad

Running pycalphad

- Any way you can run Python code, you can run pycalphad
- Recommended to use Jupyter Notebooks, which run in the browser
- Start -> Anaconda -> Jupyter Notebook
- A browser window should open

- Download notebook files with examples from Canvas or https://github.com/bocklund/notebooks/tree/master/MatSE501