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E82

Introduction to Multiphase Systems

E82 – Intro to Phase Equilibria

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Moonshiners

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https://commons.wikimedia.org/wiki/File:Confiscated_moonshine_still_photographed_by_Internal_Revenue_Bureau.jpg

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Oil Producers

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https://commons.wikimedia.org/wiki/File:Distillation_Columns_at_Saltend_-_geograph.org.uk_-_1384125.jpg

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Makers of High-Strength Alloys

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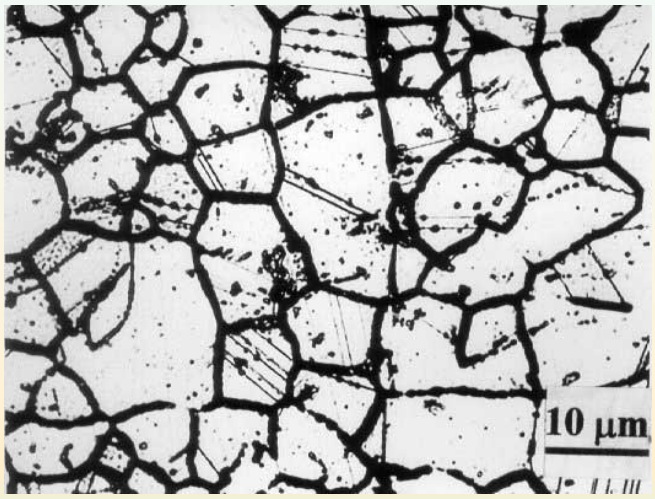

https://commons.wikimedia.org/wiki/File:Microstructure_of_a_sensitized_type_304_stainless_steel.jpg

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Gibbs Phase Rule

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$$DF = 2 + c - \Pi$$

A *Degree of Freedom*, *DF*, is a coordinate or variable.

A *Component*, *c*, is a chemical species, e.g. Al_2O_3.

A *Phase*, $\prod$, is a physical entity with a uniform composition, temperature, pressure and specific volume. In a given container, you can have multiple solid phases and multiple liquid phases, but only one vapor or gas phase.

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How do you calculate phase equilibria?
What does phase equilibrium mean?

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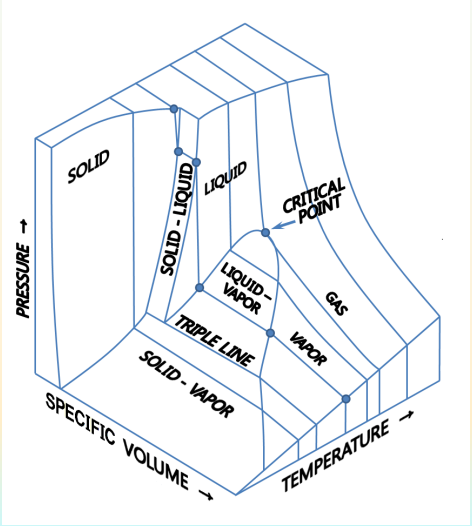
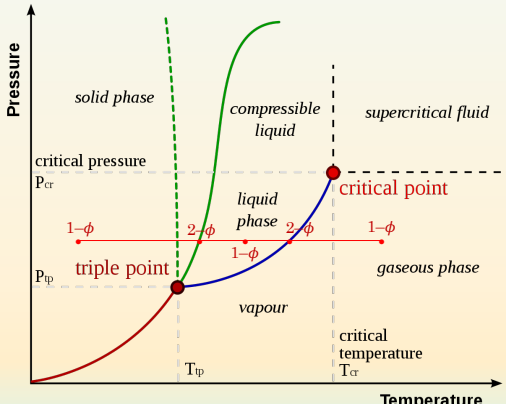
https://commons.wikimedia.org/wiki/File:PVT_3D_diagram.png



https://commons.wikimedia.org/wiki/File:Phase-diag2.svg



$$DF = 2 + c - \Pi = 3 - \Pi$$

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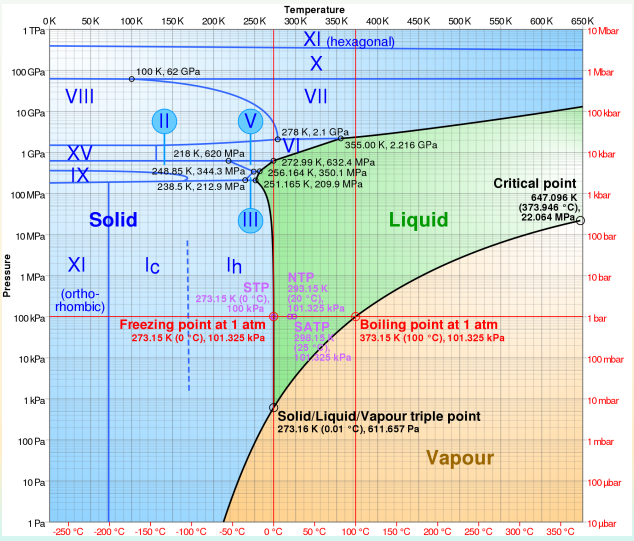
How do you calculate phase equilibria? What does phase equilibrium mean?

https://commons.wikimedia.org/wiki/File:Phase_diagram_of_water.svg



$$DF = 2(-1, P = \text{ const.}) + c - \Pi$$
$$= 3 - \Pi$$

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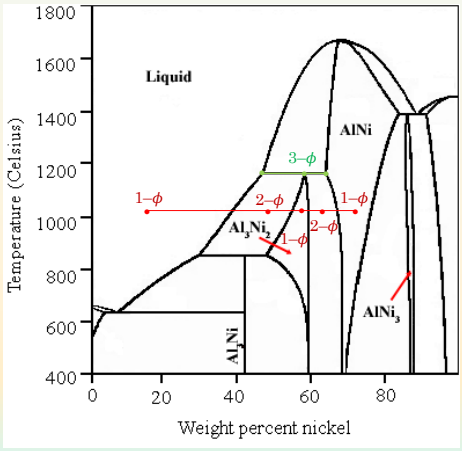
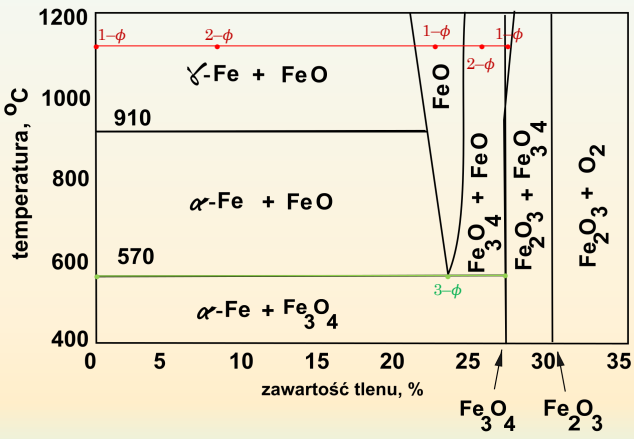
https://commons.wikimedia.org/wiki/File:Raney_nickel_phase_diagram.png



How do you calculate phase equilibria? What does phase equilibrium mean?

https://commons.wikimedia.org/wiki/File:Fe-O_phase_diagr.svg



$$DF = 2(-1, P = \text{ const.}) + c - \Pi$$
$$= 3 - \Pi$$

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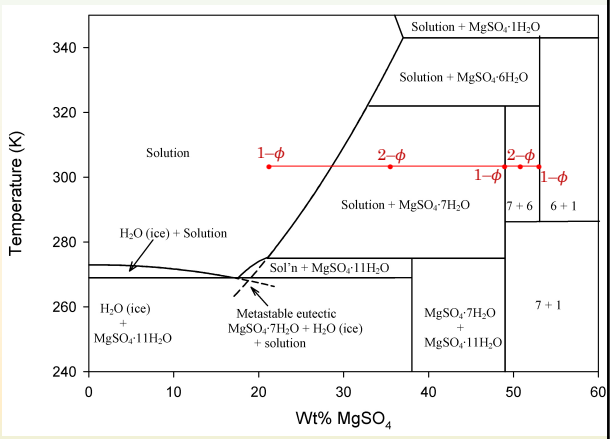
https://commons.wikimedia.org/wiki/File:Meridianiite6.jpg



How do you calculate phase equilibria?
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https://www.scielo.br/scielo.php?script=sci_arttext&pid=S0104-66322006000300010

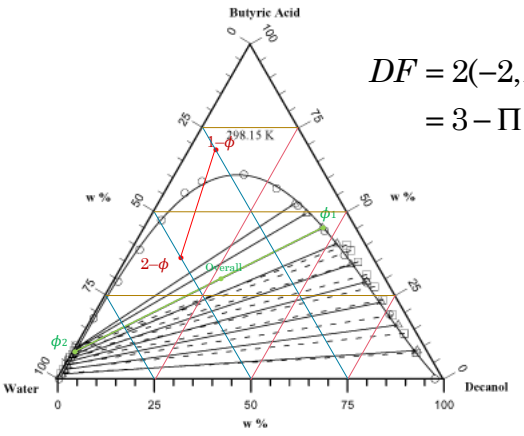

Figure 2: Ternary diagram for LLE of water (1) + butyric acid (2) + decanol (3) at 298.15 K; –o– experimental solubility curve; –Δ– experimental tie lines; --□-- calculated (UNIFAC method) tie lines.

$$DF = 2(-2, P, T = \text{ const.}) + c - \Pi$$
$$= 3 - \Pi$$

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Pxy and *Txy* Binary Phase Diagrams

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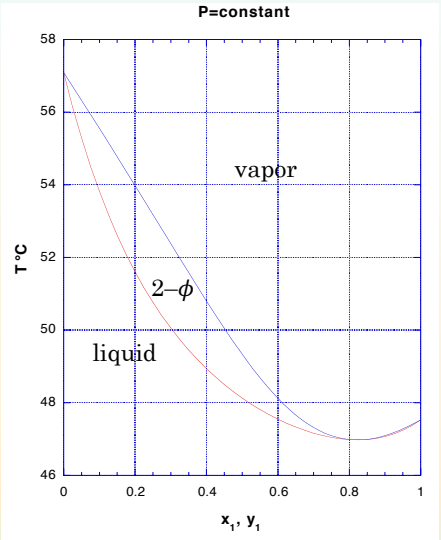

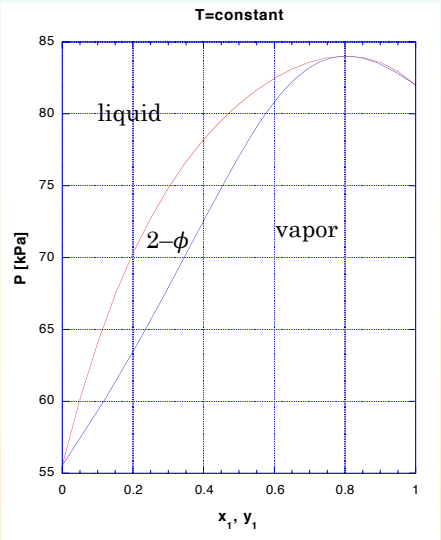

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The Lever Rule

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If

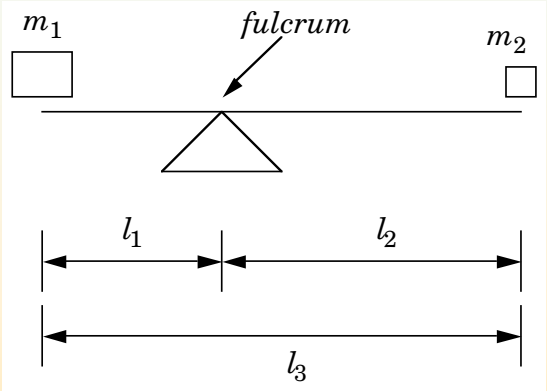
$$m_3 = m_1 + m_2$$

then

$$m_1 l_1 = m_2 l_2$$

and

$$\frac{m_1}{m_3} = \frac{l_2}{l_3} \quad \text{and} \quad \frac{m_2}{m_3} = \frac{l_1}{l_3}$$



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The Lever Rule for Phase Diagrams

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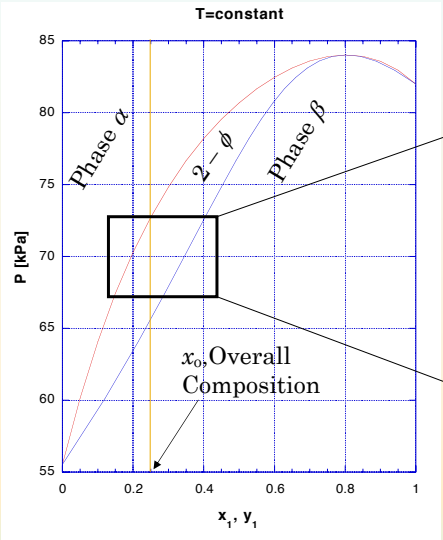

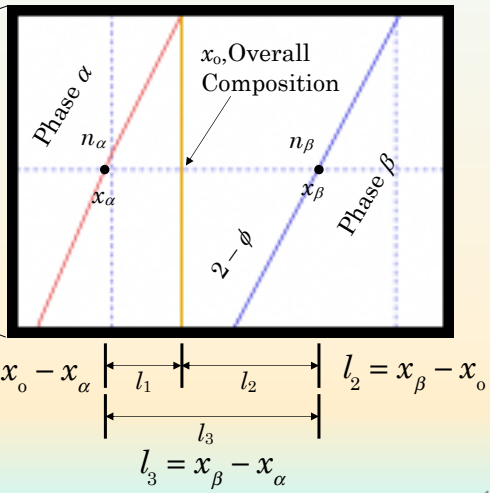

$$l_1 = x_o - x_\alpha \qquad l_2 = x_\beta - x_o$$

$$l_3 = x_\beta - x_\alpha$$

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The Lever Rule for Phase Diagrams

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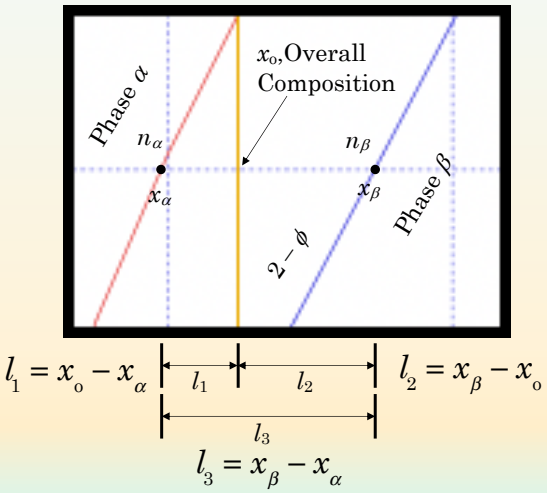

If

$$n_o = n_\alpha + n_\beta$$

Then

$$n_\alpha l_1 = n_\beta l_2$$

$$\frac{n_\alpha}{n_o} = \frac{l_2}{l_3}$$

$$\frac{n_\beta}{n_o} = \frac{l_1}{l_3}$$

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Example

We have an equilibrium mixture of aluminum and nickel at 1000°C. 50% of the overall mixture is nickel. Give the compositions and relative amounts of all phases present.

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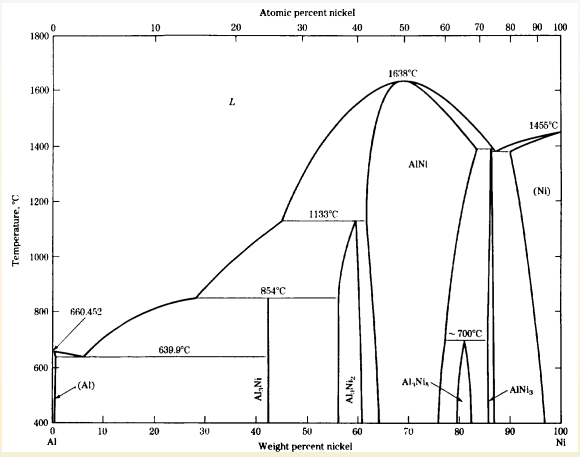

If we don't have a phase diagram, or if we wish to automate the calculation procedure, what do we do?

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Example Solution

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Example doesn't specify atomic or weight percent.

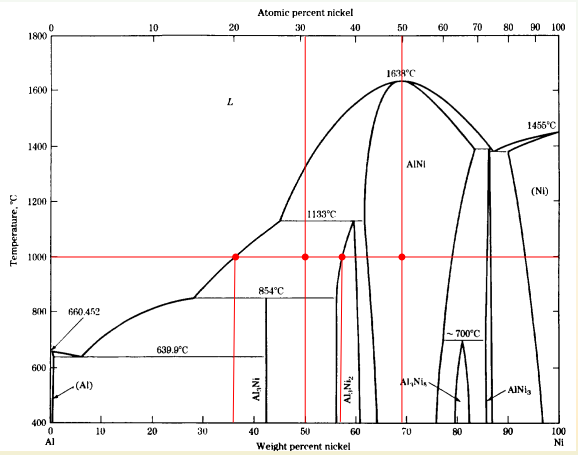
Atomic percent: 100% AlNi

Weight percent: In 2-ϕ between L and Al_3Ni_2

$$x_L = 36\%, \quad x_{Al_3Ni_2} = 57\%$$

$$\frac{n_{Al_3Ni_2}}{n_o} = \frac{x_{Al_3Ni_2} - x_o}{x_{Al_3Ni_2} - x_L} = \frac{57-50}{57-36} = 33.3\%$$

$$\frac{n_L}{n_o} = 1 - \frac{n_{Al_3Ni_2}}{n_o} = 100\% - 33.3\% = 66.7\%$$



If we don't have a phase diagram, or if we wish to automate the calculation procedure, what do we do?

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