Lecture slides are available under:

www.gtt-technologies.de/mc2lecture

Materials Chemistry II
-Applications 2-

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Outline

1. Understanding processes&materials based on G(x,T,p)

QUALITATIVE APPLICATION OF MC II

2. Modelling G(x,T,p) based on theory&experiment

QUALITATIVE → QUANTITATIVE

3. Modelling processes&materials based on G(x,T,p)

QUANTITATIVE APPLICATION OF MC II

Outline

1. Understanding processes&materials based on G(x,T,p)
QUALITATIVE APPLICATION OF MC II

2. **CalPhaD method**
Calculation of **Pha**se **D**iagrams

3. Modelling processes&materials based on G(x,T,p)
QUANTITATIVE APPLICATION OF MC II

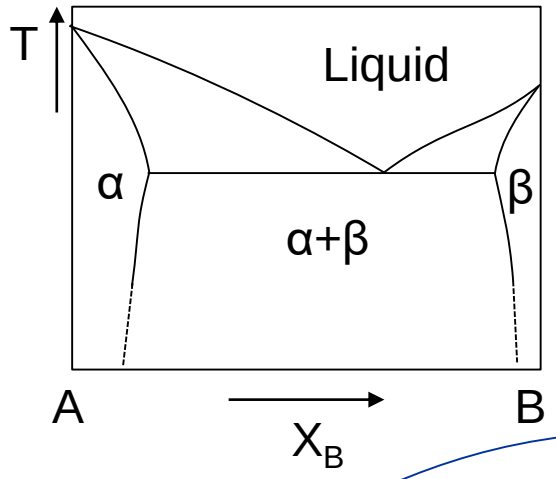
CalPhaD

(Calculation of Phase Diagrams)

System B-C

System A-C

System A-B



Phase Liquid

Phase β

Phase α

$G = f(X_A, X_B, X_C, T, p)$

usually extrapolated from high temperatures

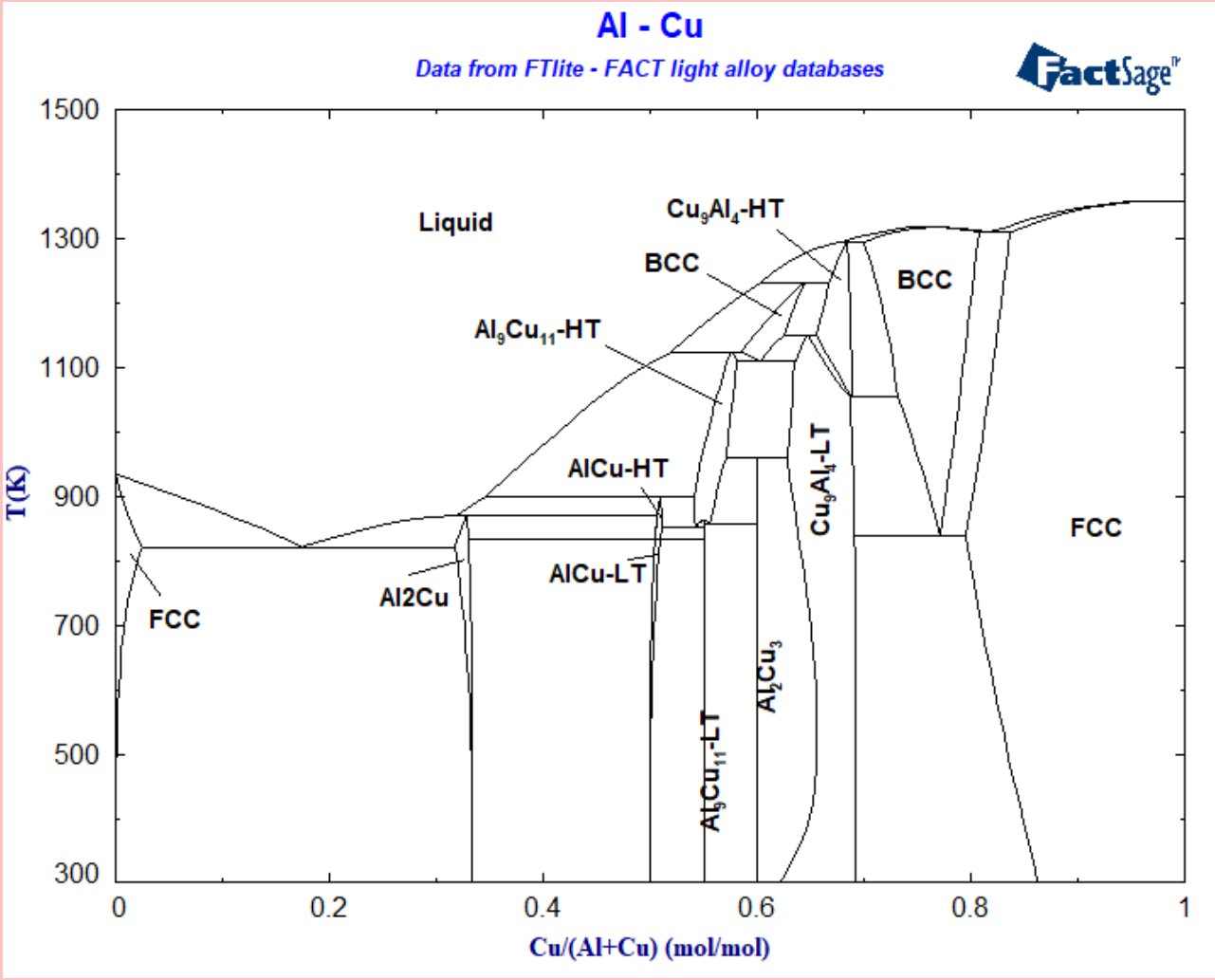
Phase diagram database

Gibbs energy database

What information can be extracted from the Al-Cu phase diagram?

A) $\Omega_{fcc} < \Omega_{bcc}$

B) $\Omega_{fcc} > \Omega_{bcc}$



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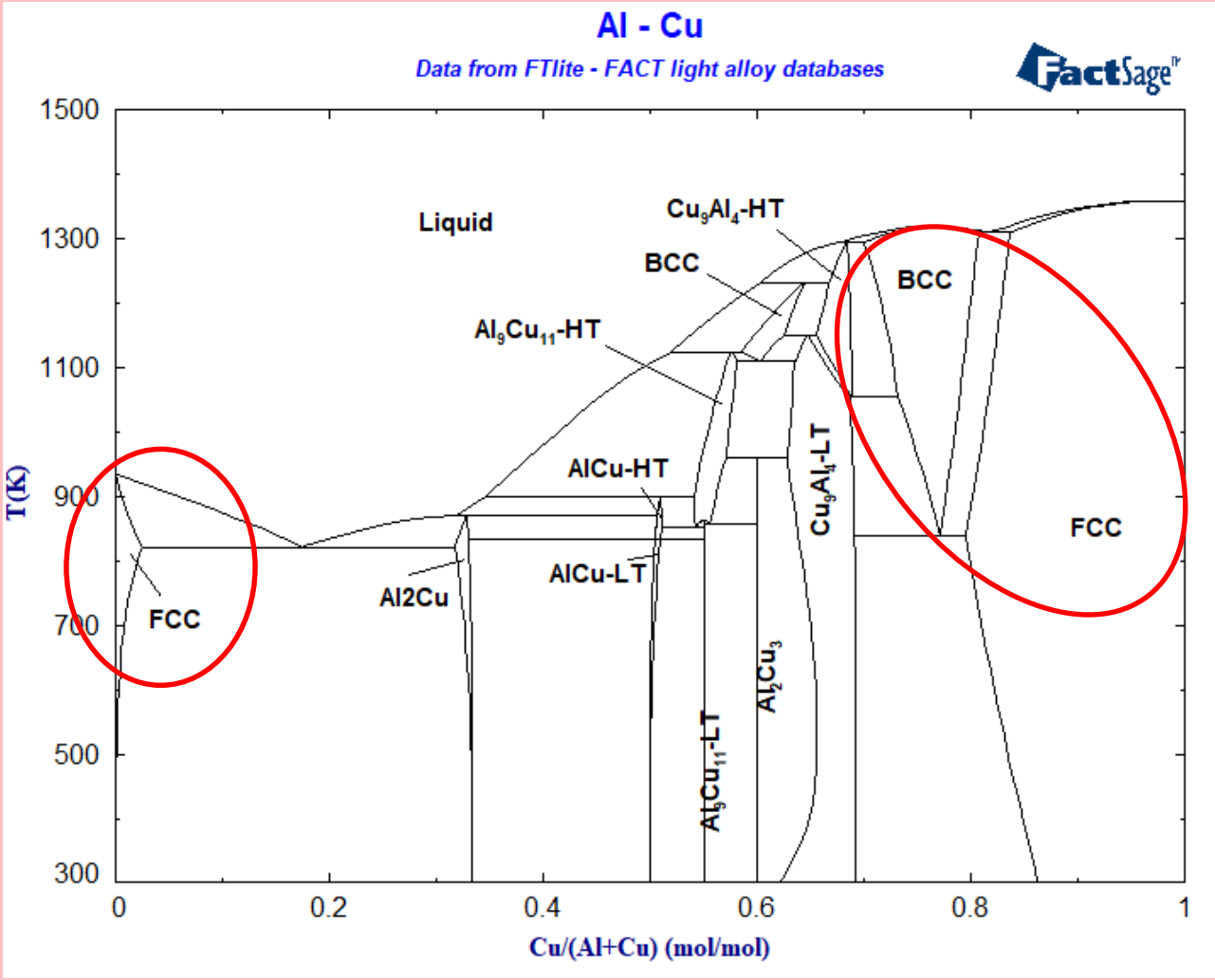

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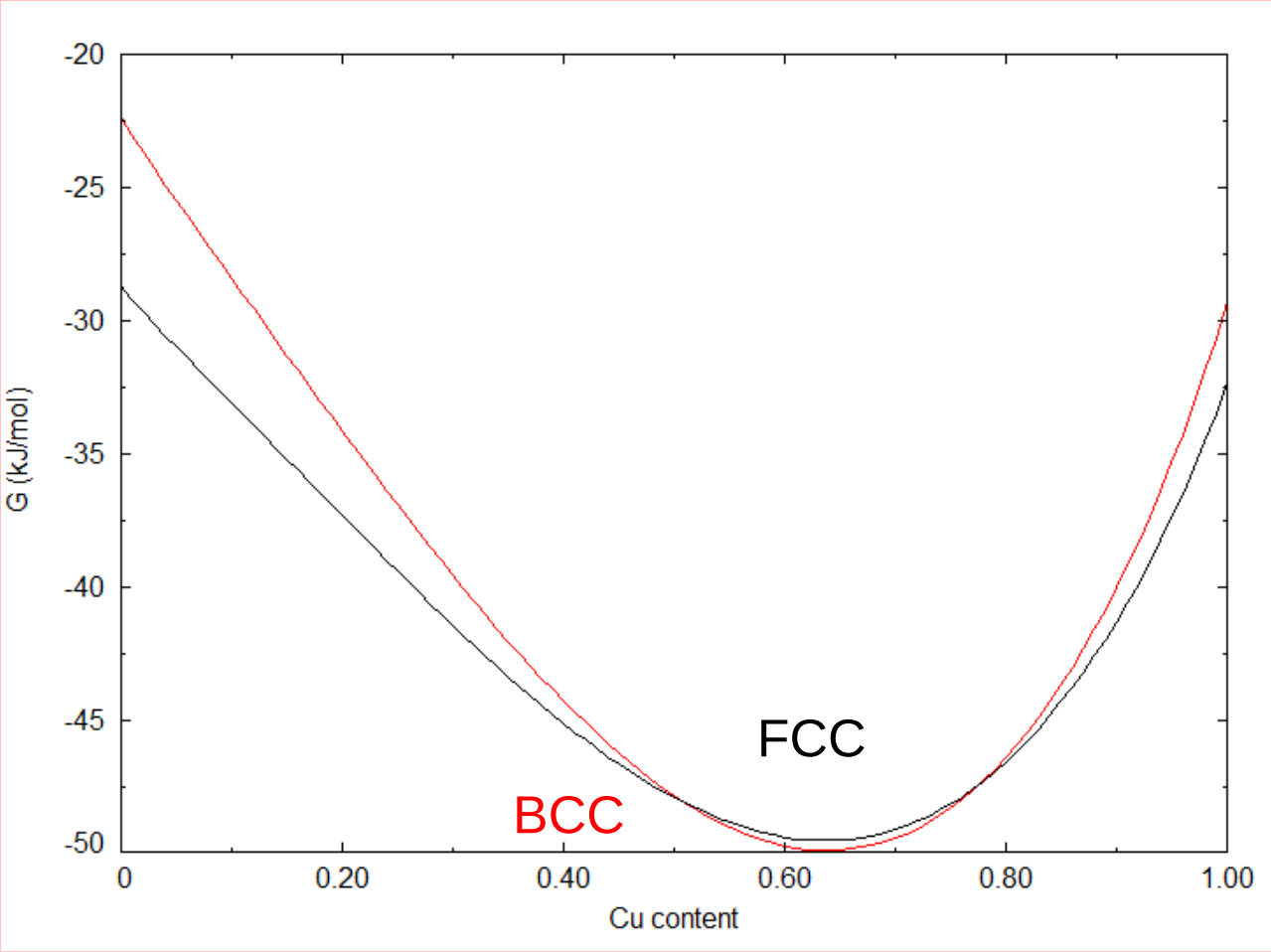

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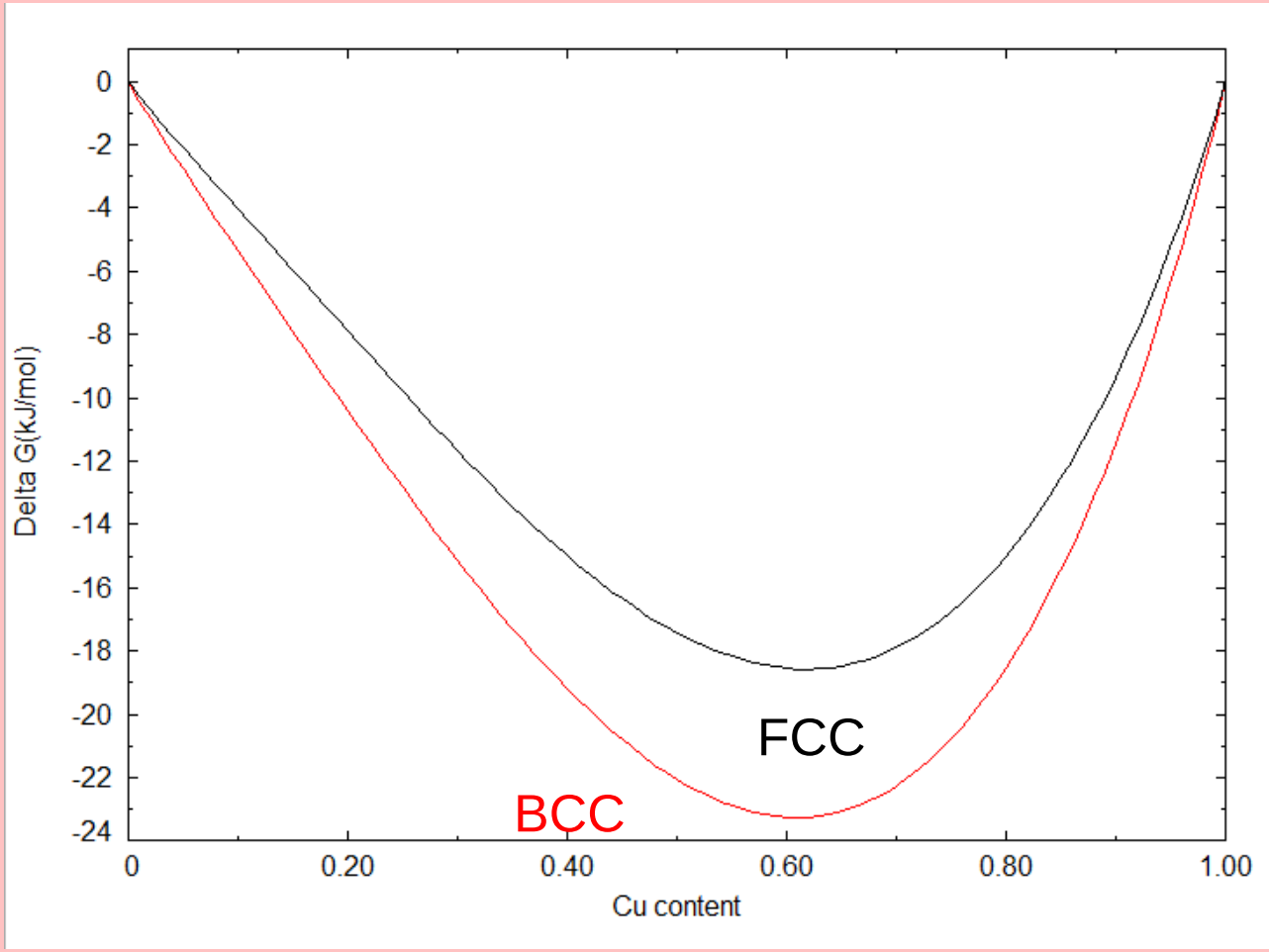
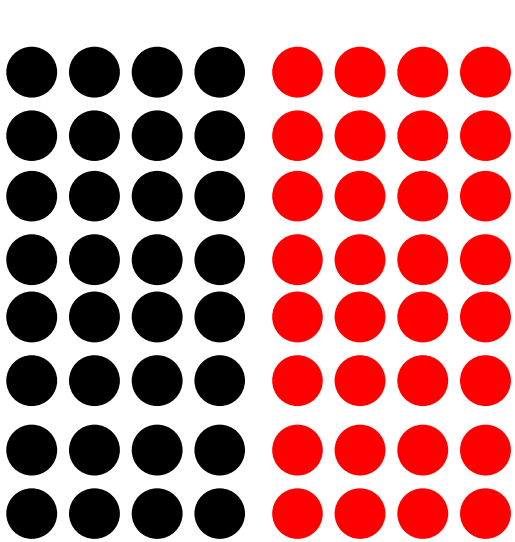
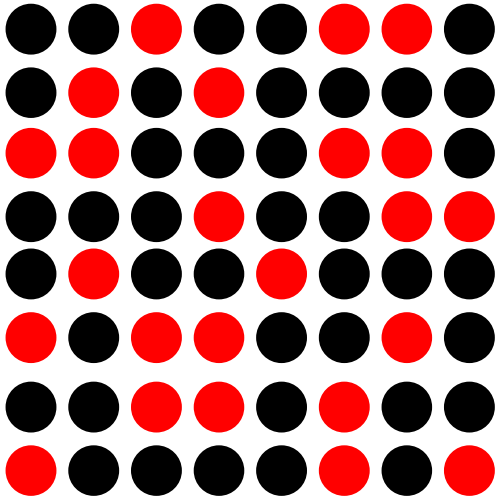


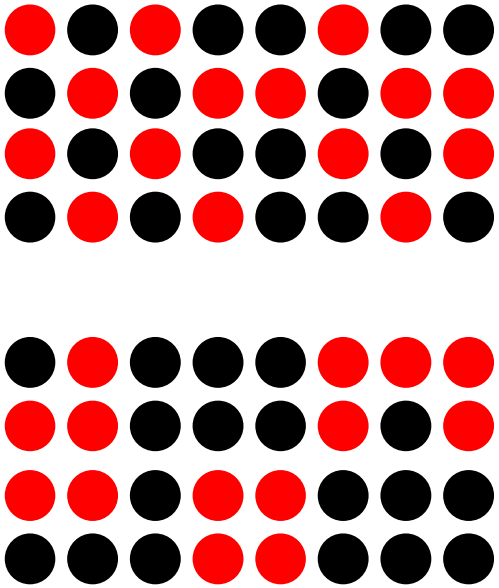
Strategy:

$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$

Think about bonds & configurations







mechanical mixture (two powders) → ideal/regular solution mixed → **real solution ordering/clustering**

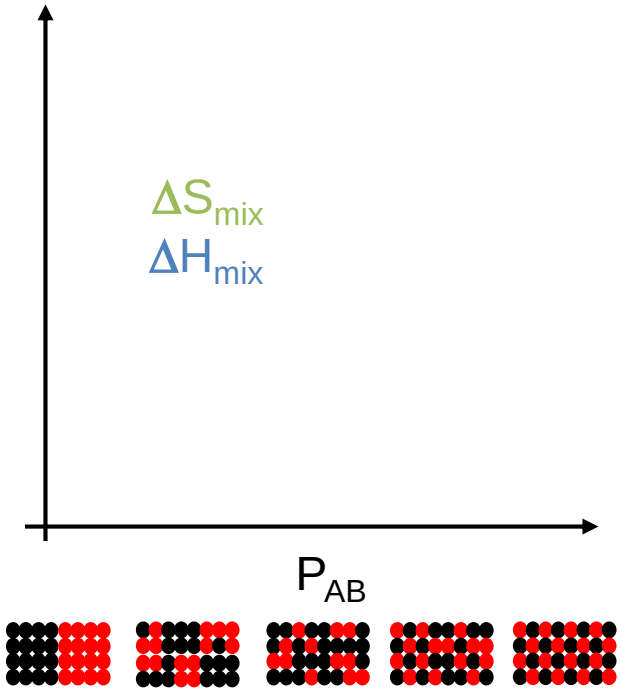
What happens if Ω is significantly different from 0?

$\Omega < 0$

Example: Solution of 50% A and 50% B

$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$

- ΔG_{mix} minimizes with minimum ΔH_{mix} and maximum ΔS_{mix}



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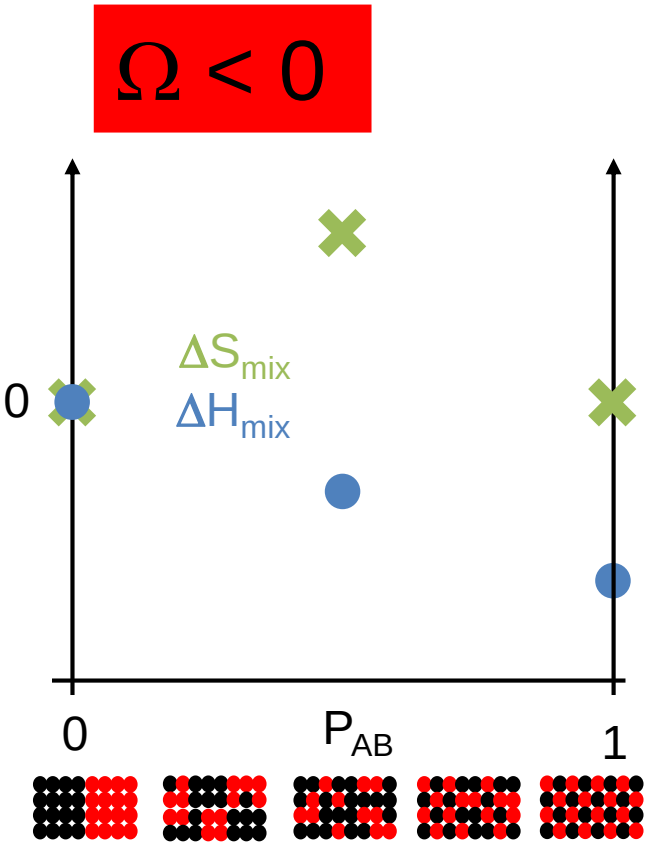

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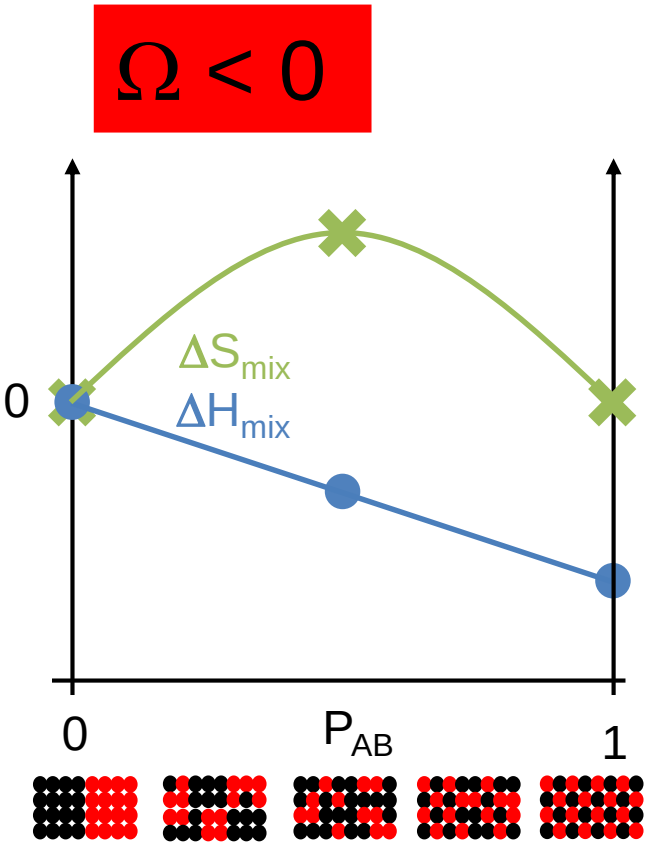

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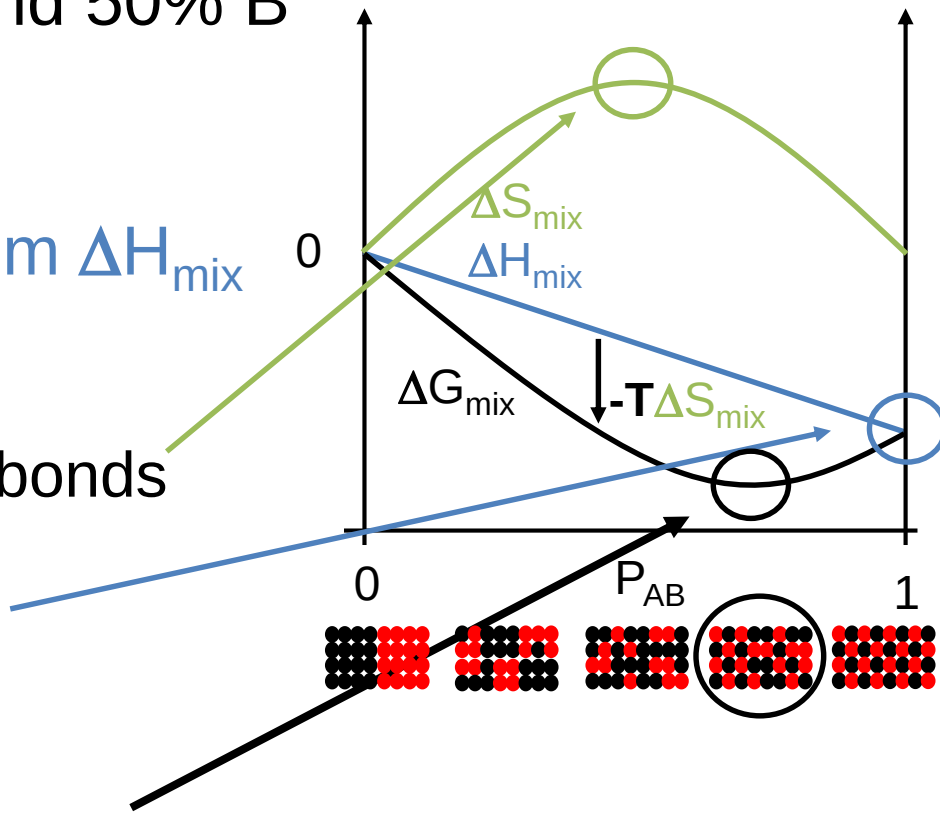
Example: Solution of 50% A and 50% B

$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$

- ΔG_{mix} minimizes with minimum ΔH_{mix} and maximum ΔS_{mix}

ΔS_{mix} maximizes when # of A-B bonds $= 2*X_A*X_B$

ΔH_{mix} minimizes with maximum number of A-B bonds



ΔG_{mix} minimizes between 0.5 and 1!

What happens if Ω is significantly different from 0?

$\Omega < 0$

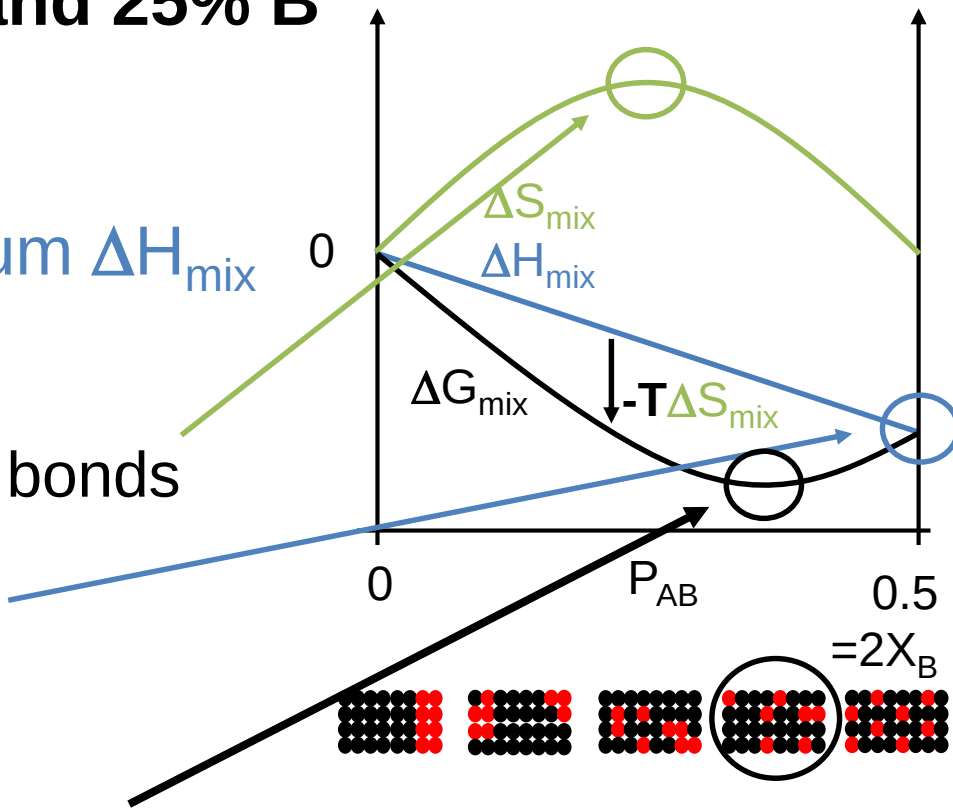
Example: Solution of **75% A and 25% B**

$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$

- ΔG_{mix} minimizes with minimum ΔH_{mix} and maximum ΔS_{mix}

ΔS_{mix} maximizes when # of A-B bonds $= 2*X_A*X_B$

ΔH_{mix} minimizes with maximum number of A-B bonds



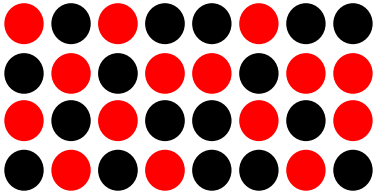
ΔG_{mix} minimizes between $P_{AB,random}$ and $P_{AB,max}$!

Strategy:

$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$

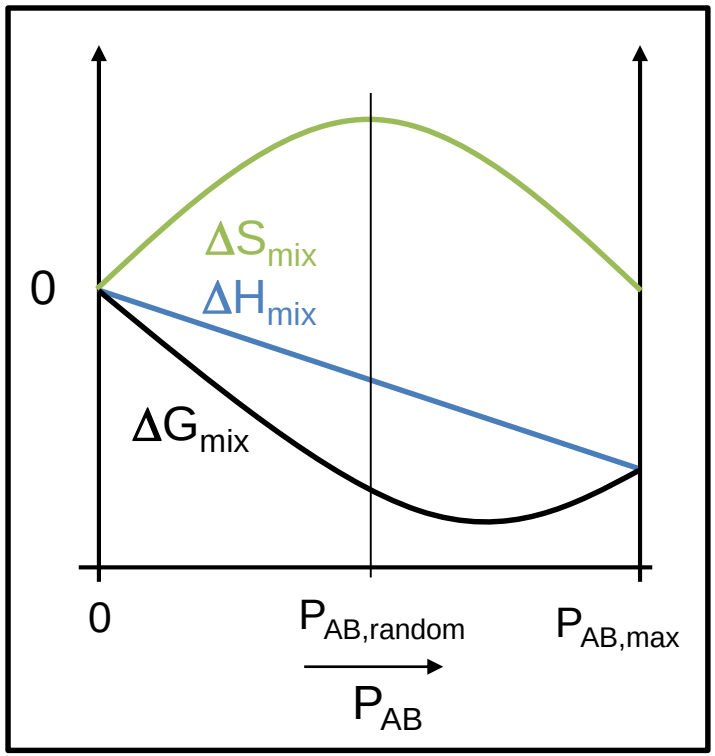
Think about bonds & configurations

REAL SOLUTIONS



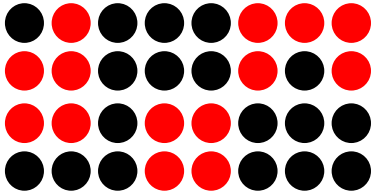
Ω<0

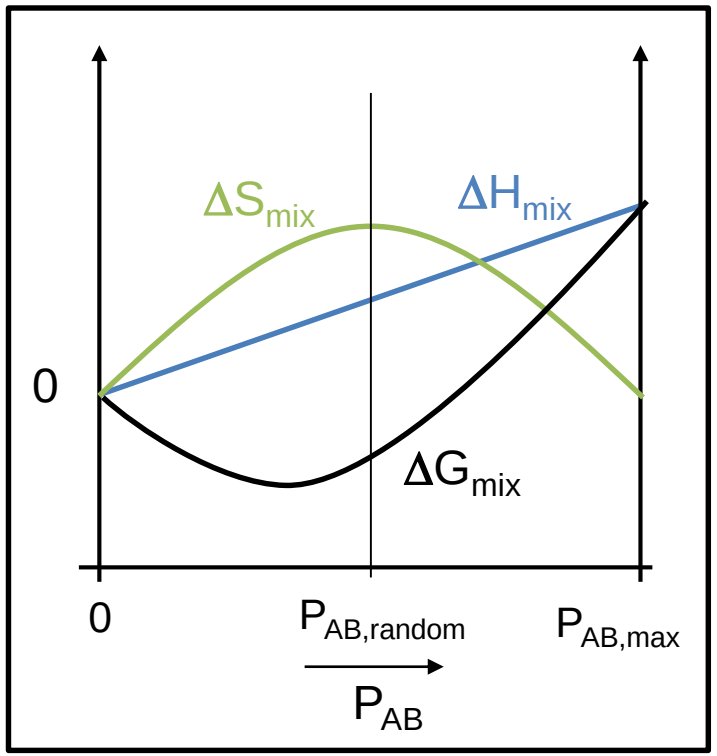
Ordering



Ω>0

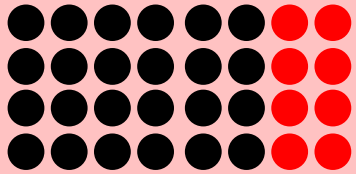
Clustering



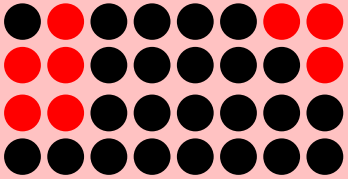


What could be a sensible atomic arrangement for BCC-$Ti_{0.75}Al_{0.25}$ at 1800K?

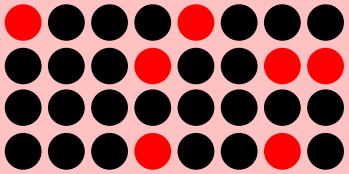
A)



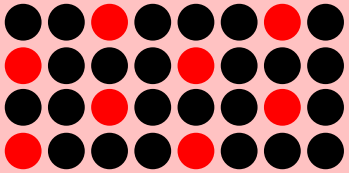
B)

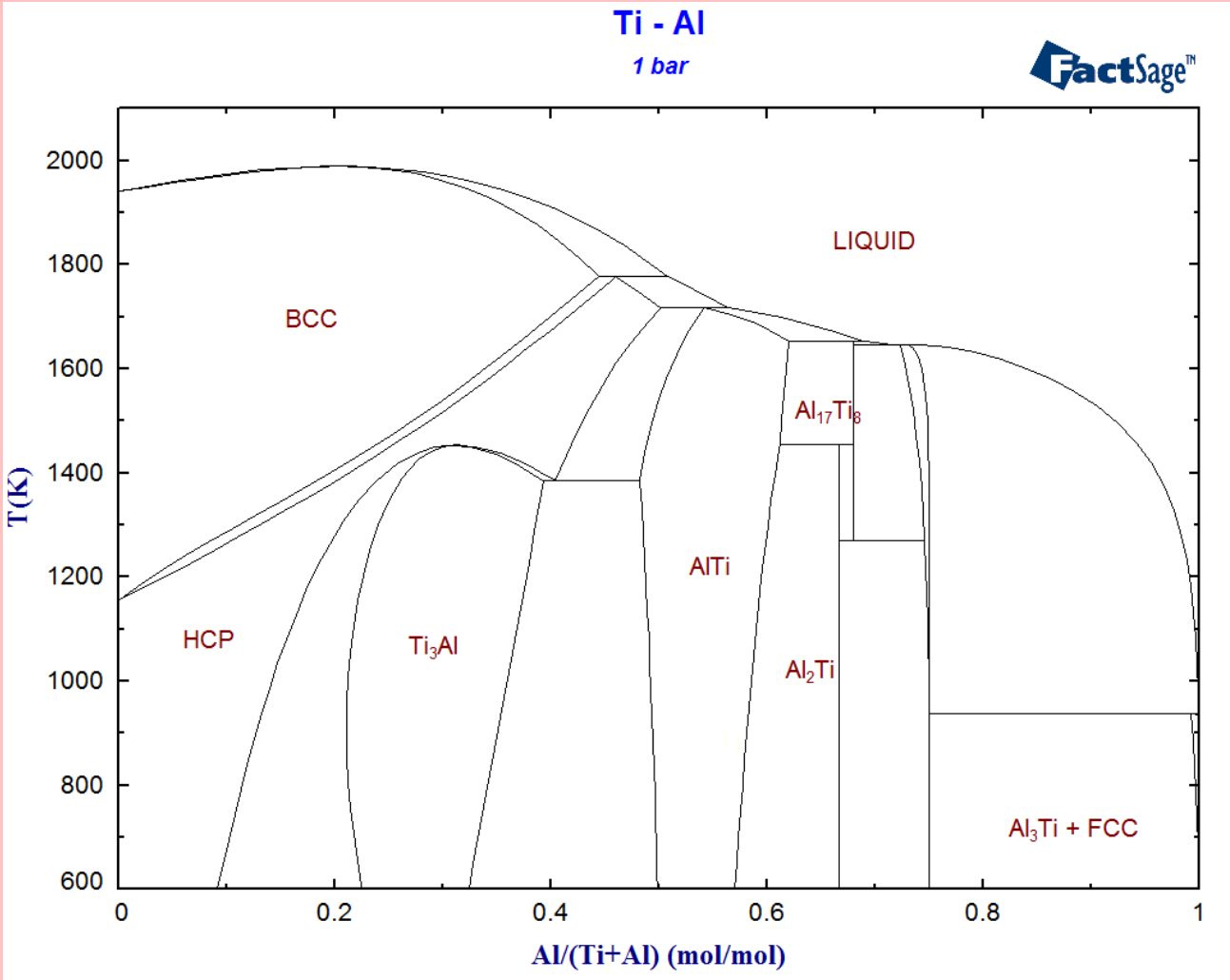


C)



D)





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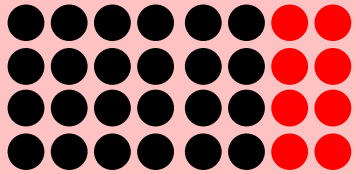

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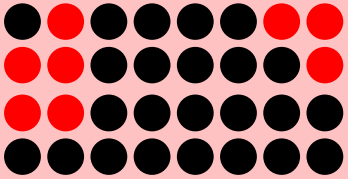

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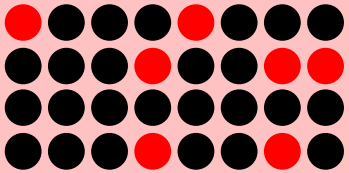

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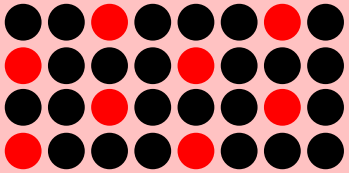
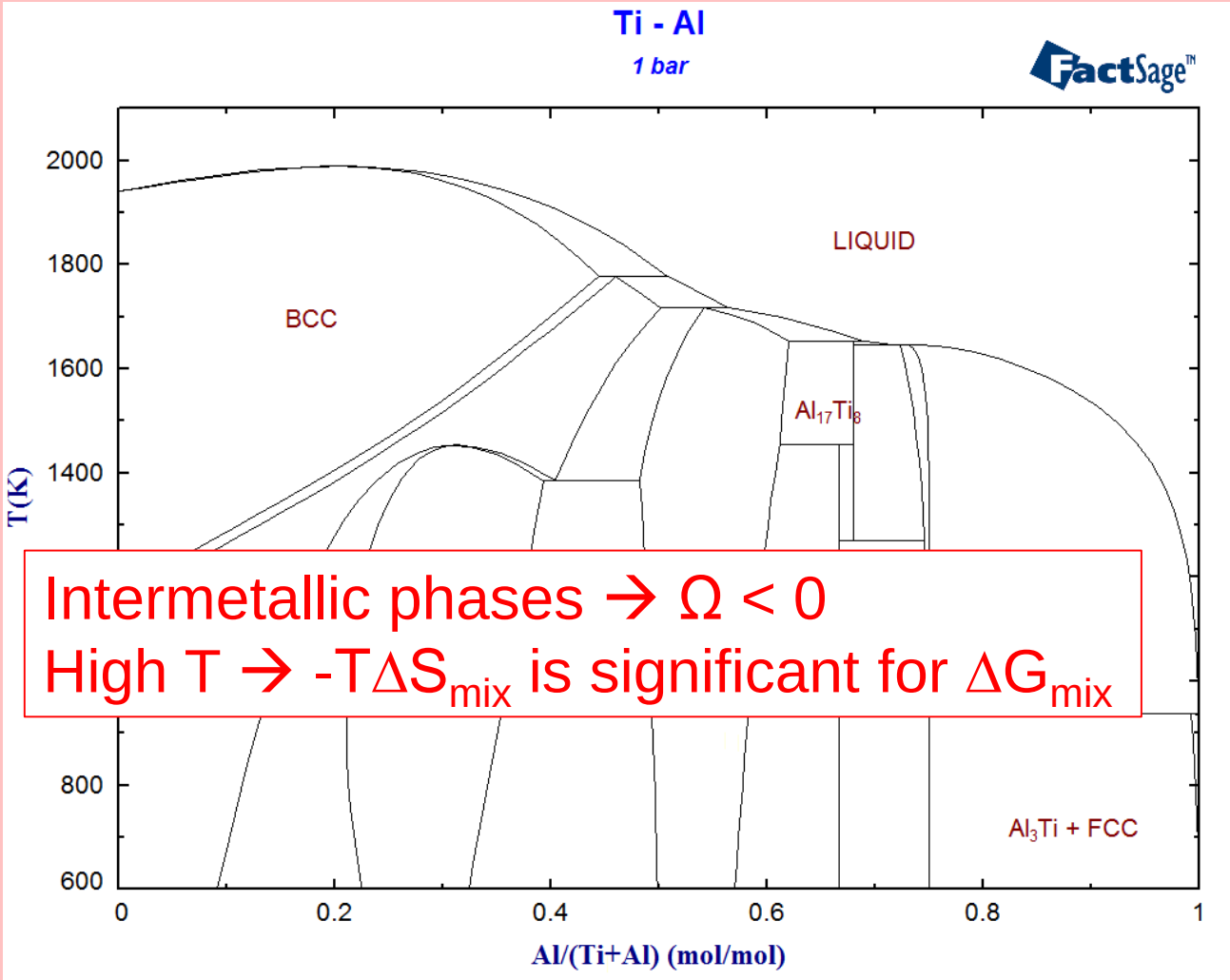
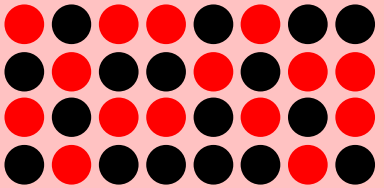




Intermetallic phases → $\Omega < 0$

High T → $-T\Delta S_{mix}$ is significant for ΔG_{mix}

The following atomic arrangement is observed for an alloy at 1500K. What could be a sensible atomic arrangement at 300K?



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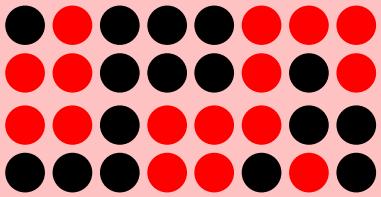

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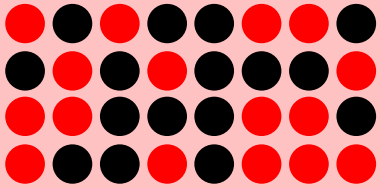

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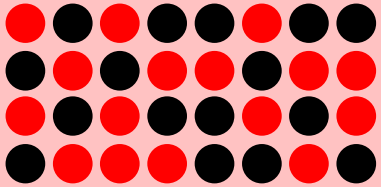

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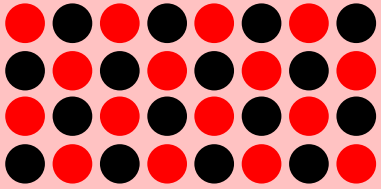

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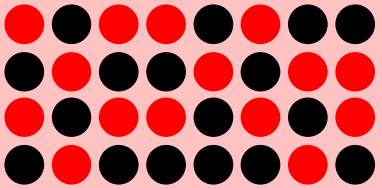

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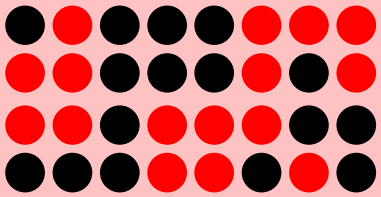
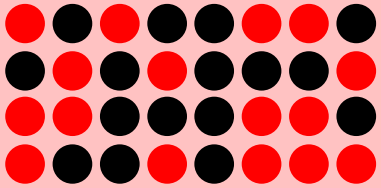


B)



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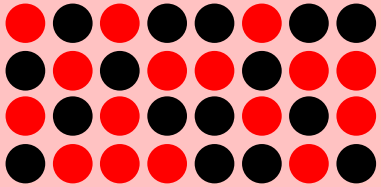

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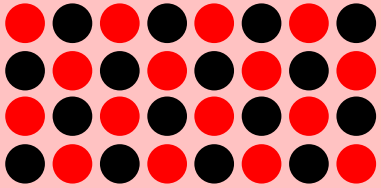


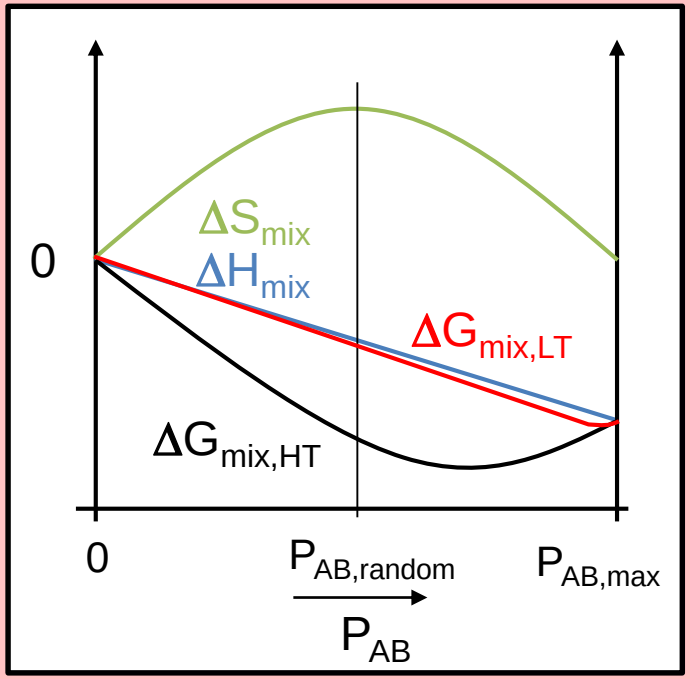
Ordering ($P_{AB} > P_{AB,random}$)

→ $\Omega < 0$

Lower T

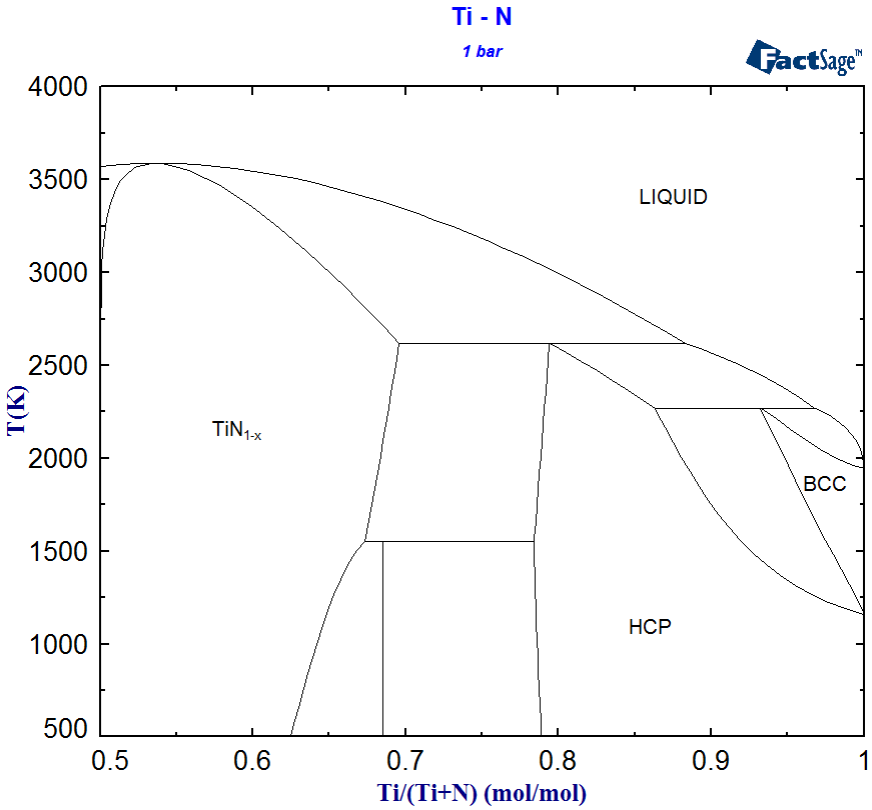
→ $-T\Delta S_{mix}$ less significant for ΔG_{mix}

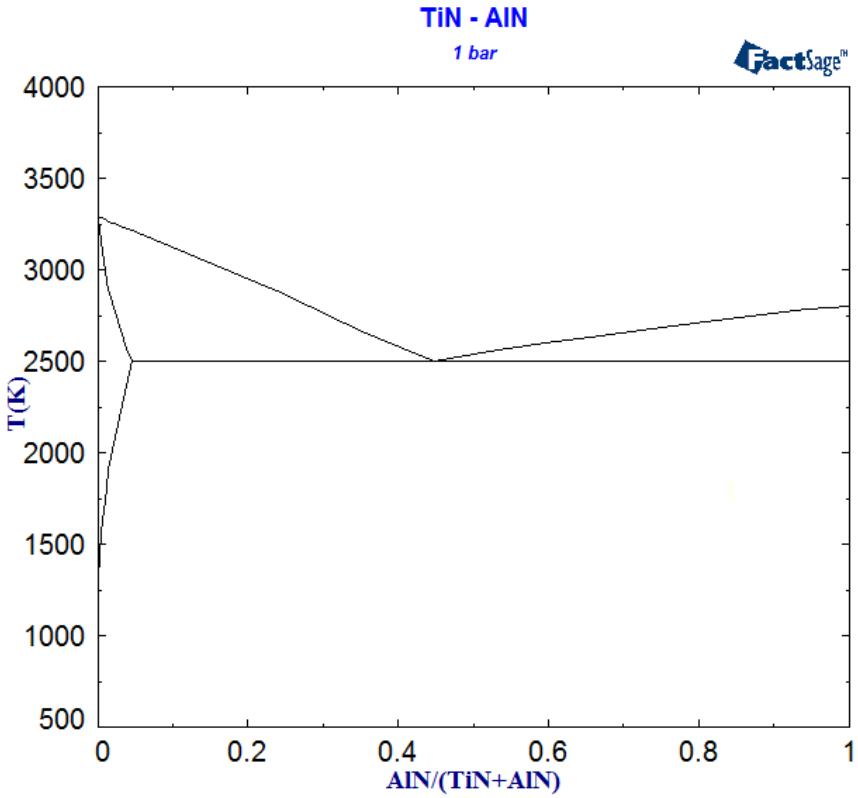
→ ΔH_{mix} minimization!



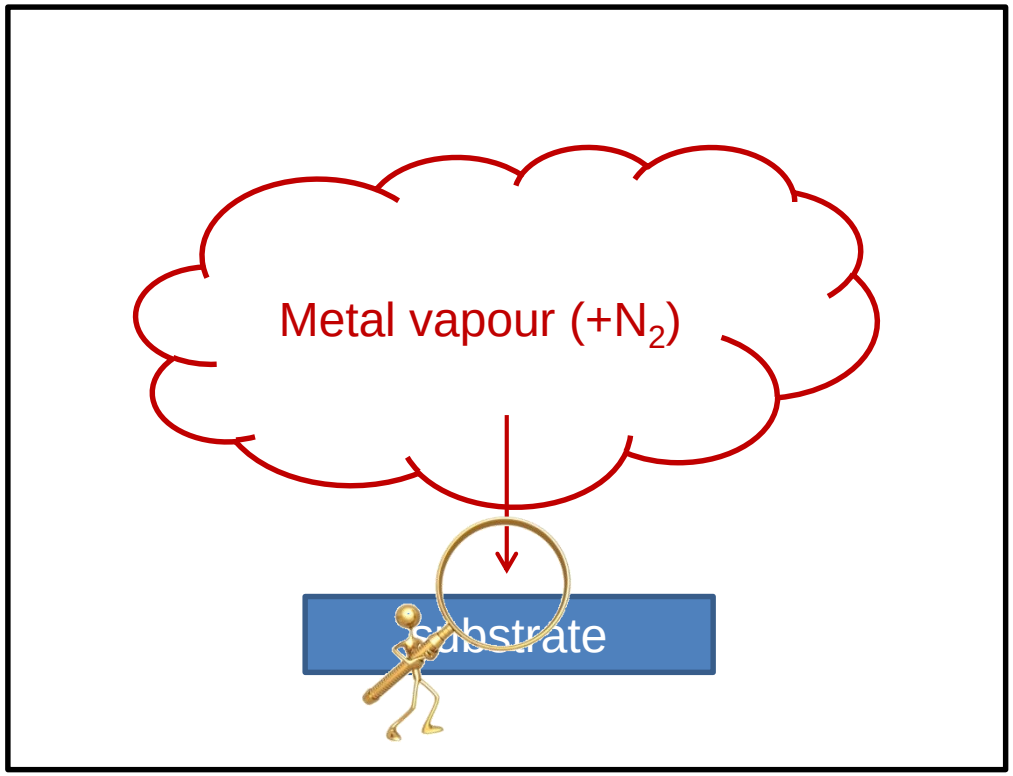
Application: (Ti,Al)N coatings for cutting tools

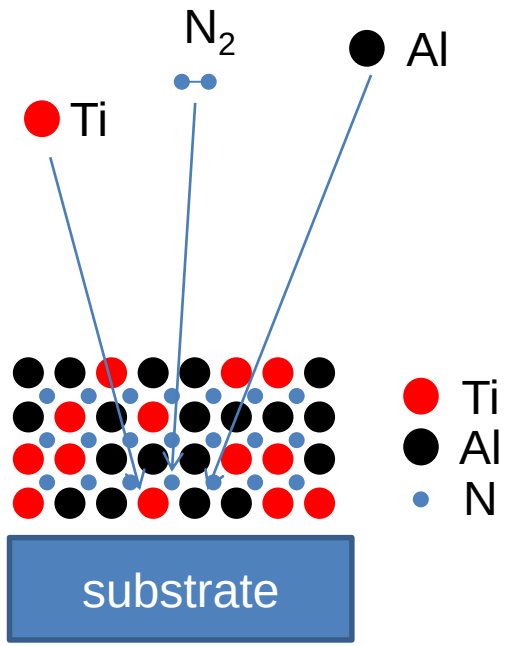
State of the art for protective coatings on cutting tools :
1980 - 2000 TiN
Since ~2000 (Ti,Al)N coatings WHY?





Vapour phase condensation

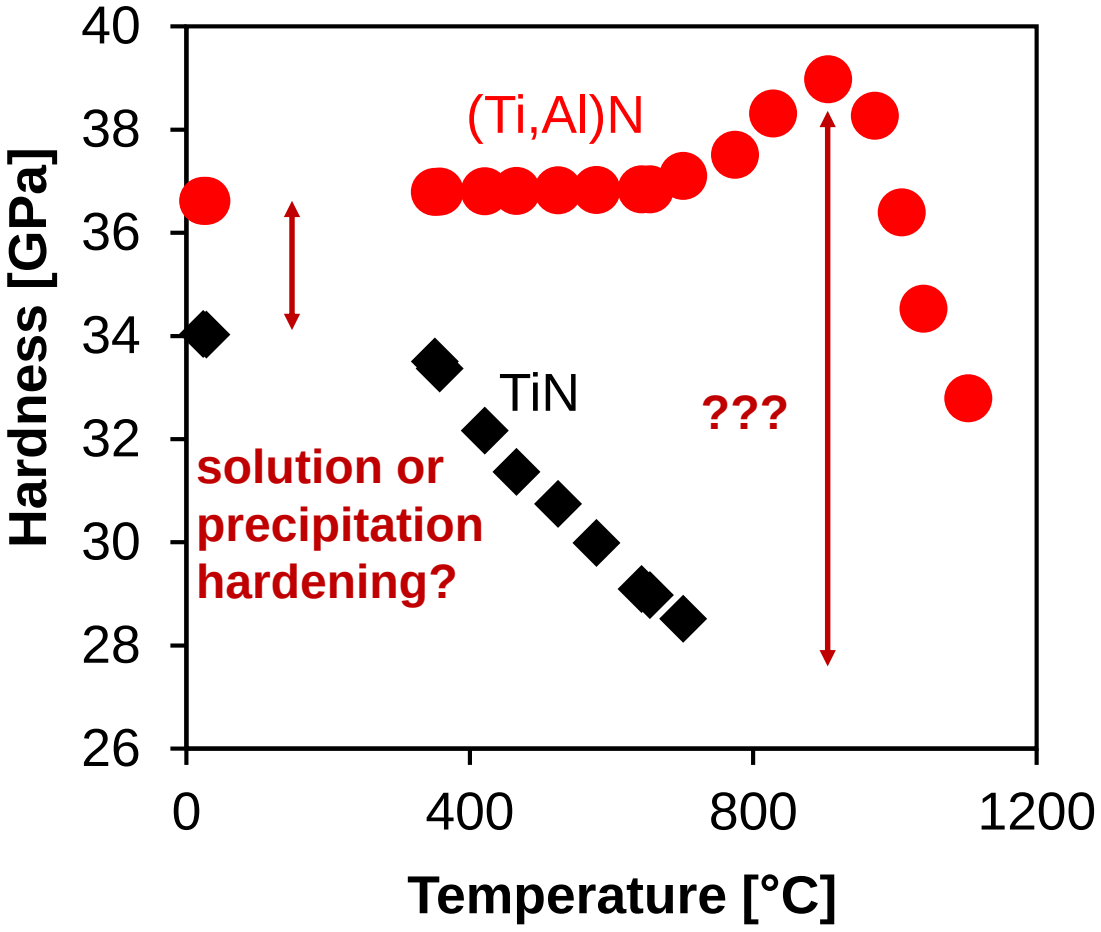




From metal vapour to solid within a fraction of 1 µs

→ Extreme quenching rates (>> 10^{10} °C/s)!

Application: (Ti,Al)N coatings for cutting tools

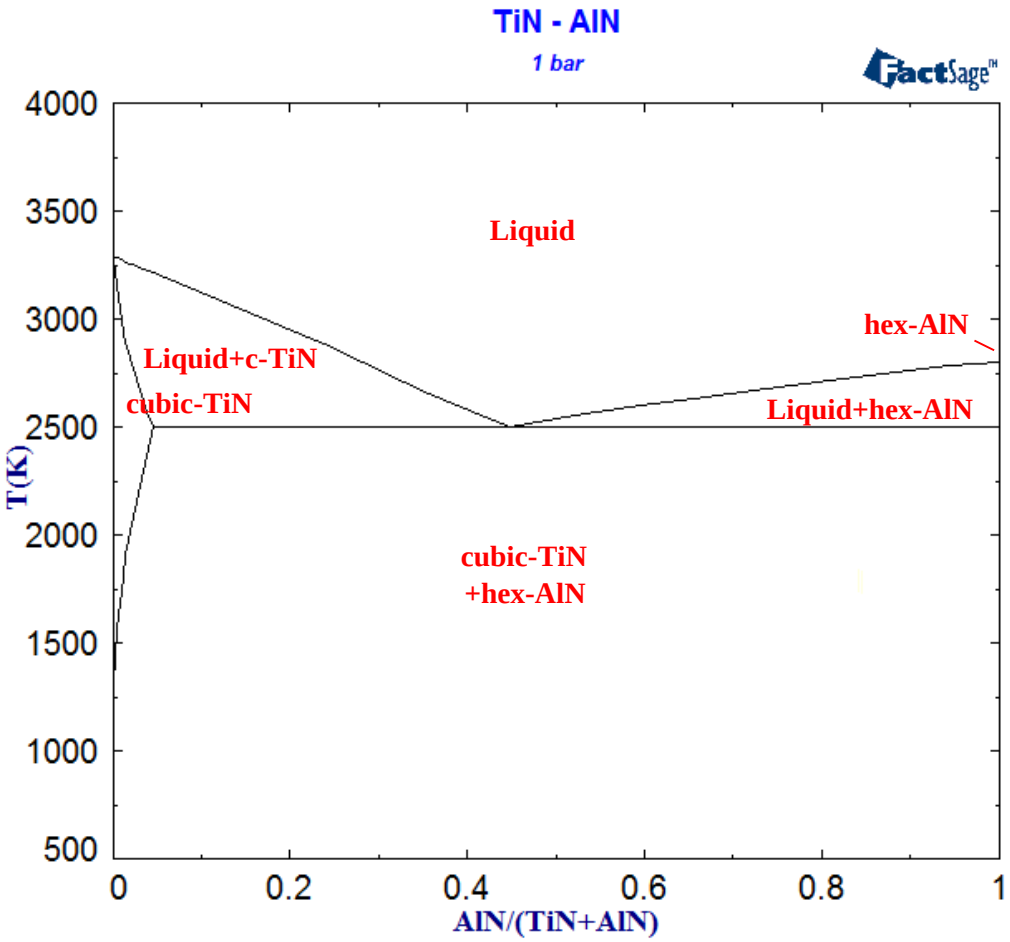


H increases by Al addition!

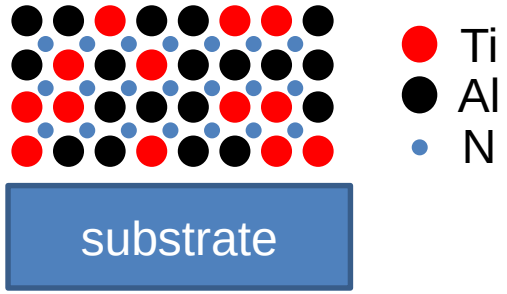
But WHY?

Mayrhofer, Rachbauer, Rovere, Schneider, *Protective Transition Metal Nitride Coatings* (2012).

Vapour phase condensation

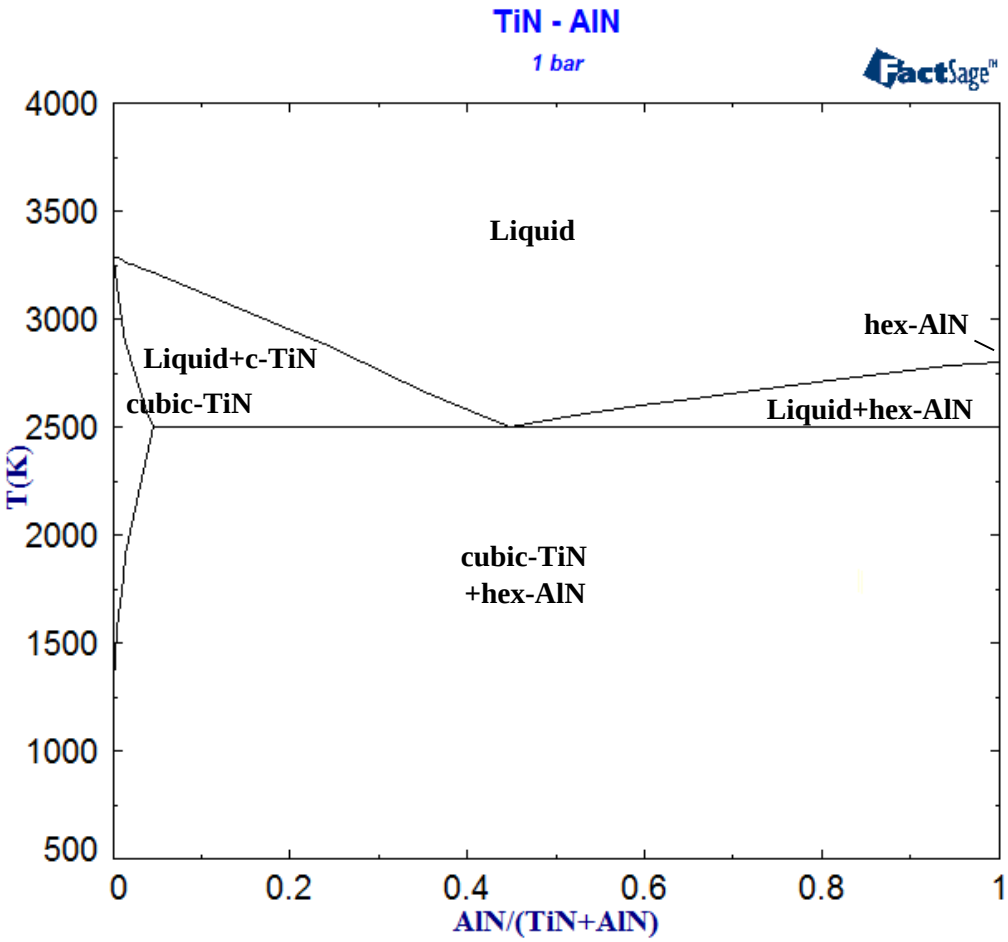


Atoms cannot form two phases TiN+AlN because of limited mobility (non-equilibrium processing).
What do we learn from the phase diagram?
NOTHING AT ALL!?
Wait: Please sketch the G(x) curves at T = 250°C.



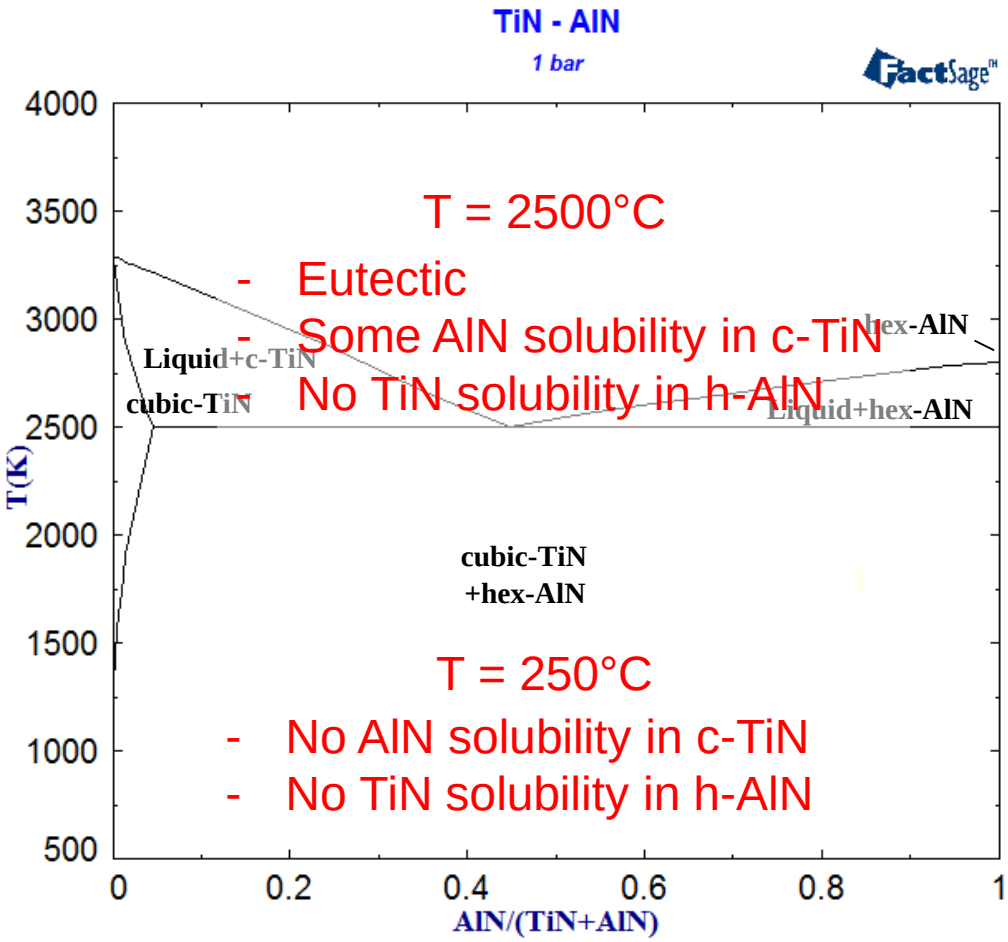
From metal vapour to solid within a fraction of 1 µs
→ Extreme quenching rates (>> 10^{10} °C/s)!

Draw G(x) @ 250°C and 2500°C



1. Choose the temperature at which you find more information in the phase diagram!
2. Order the Gibbs energy of the pure components in the different phases.
3. Think about Ω for solid phases (cubic and hex): Do you expect $\Omega_{c/h}<0$ or $\Omega_{c/h}>0$? If you cannot judge Ω for one phase, assume $\Omega_c=\Omega_h$.
4. Do you expect $|\Delta H_{mix}| < |T\Delta S_{mix}|$ or $|\Delta H_{mix}| > |T\Delta S_{mix}|$?
5. Draw ΔH_{mix}, $-T\Delta S_{mix}$ and ΔG_{mix} for all phases. Assume $\Delta H_{mix}(\text{liquid}) \approx 0$.
6. Draw G(x) for the solid phases.
7. Draw G(x) for the liquid phase, taking into account position of the eutectic. Eventually adjust G(x) for the solid phases to match solubility limits.
8. Repeat the steps for the other temperature.

Draw G(x) @ 250°C and 2500°C



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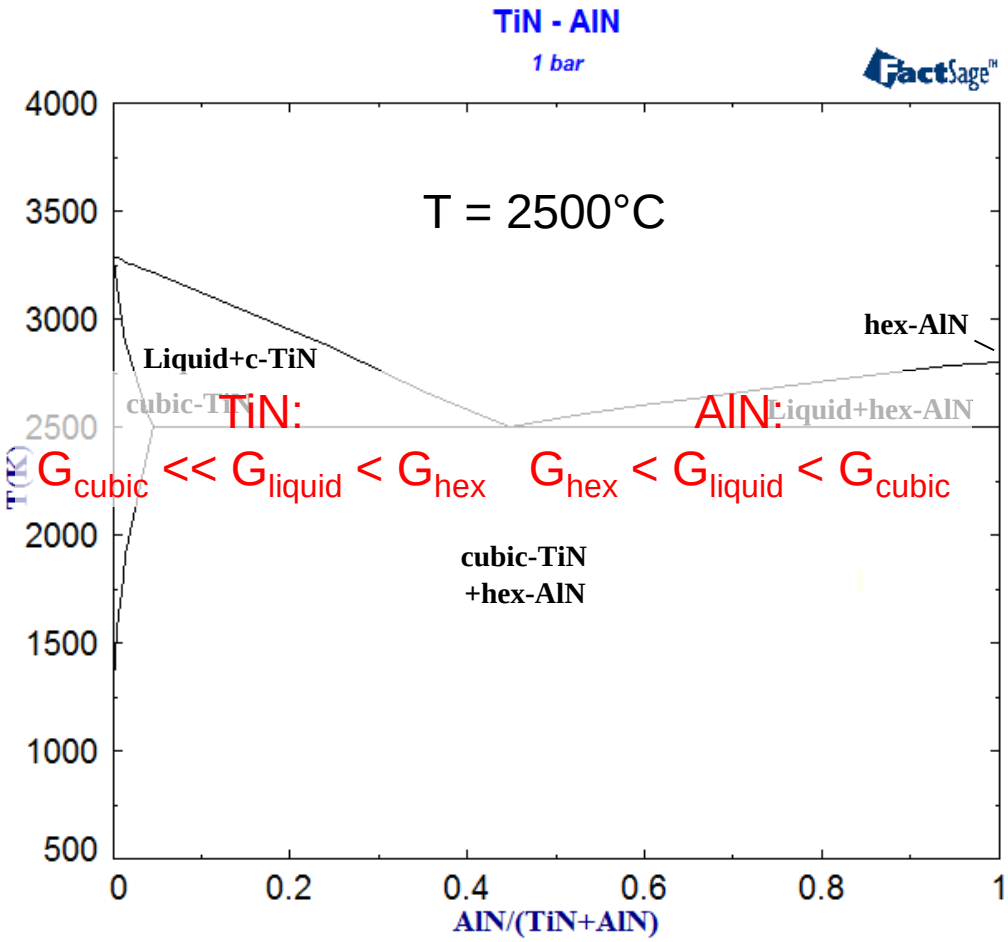
5. Draw ΔH_{mix}, $-T\Delta S_{mix}$ and ΔG_{mix} for all phases. Assume $\Delta H_{mix}(\text{liquid}) \approx 0$.
6. Draw G(x) for the solid phases.
7. Draw G(x) for the liquid phase, taking into account position of the eutectic. Eventually adjust G(x) for the solid phases to match solubility limits.
8. Repeat the steps for the other temperature.

Draw G(x) @ 250°C and 2500°C



TiN: $G_{cubic} << G_{liquid} < G_{hex}$

AlN: $G_{hex} < G_{liquid} < G_{cubic}$

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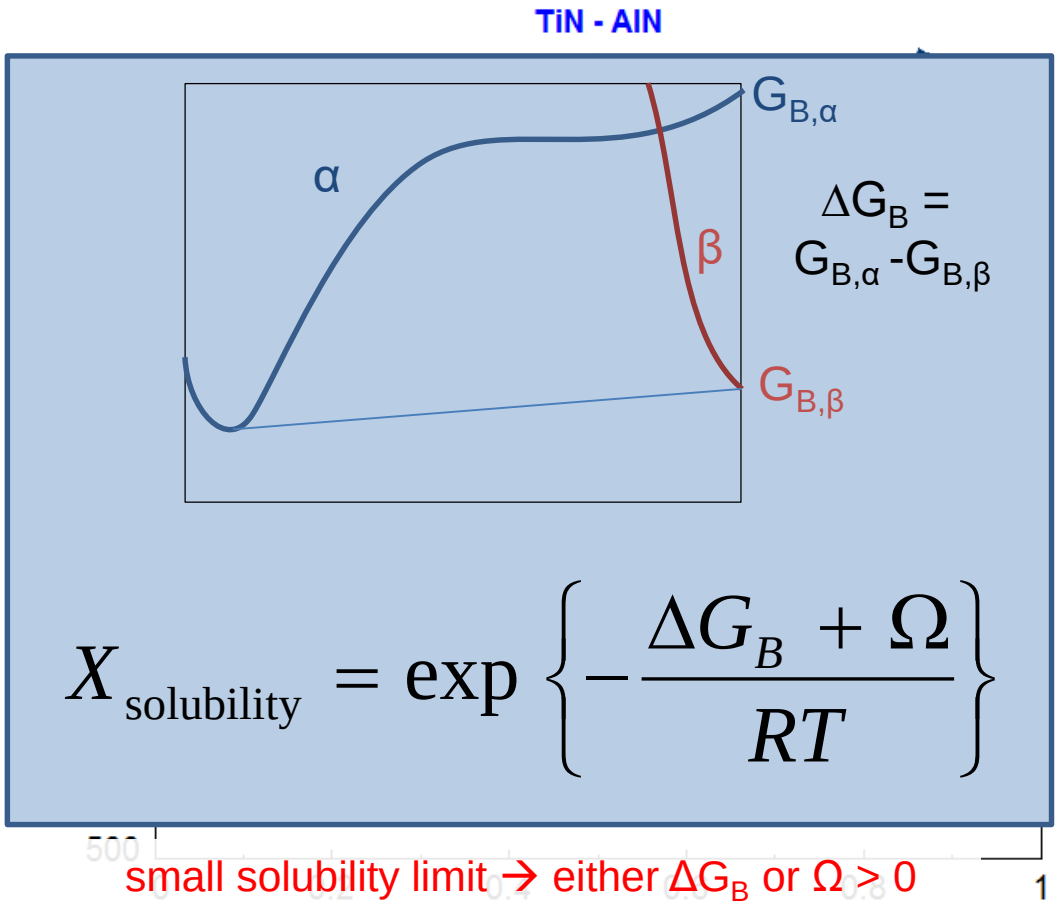

small solubility limit → either ΔG_B or $\Omega > 0$
virtually no solubility limit → both ΔG_B or $\Omega > 0$
→ Ω_{cubic} **or** $\Delta G_{AlN} > 0$
→ Ω_{hex} **and** $\Delta G_{TiN} > 0$

1. Choose the temperature at which you find more information in the phase diagram!
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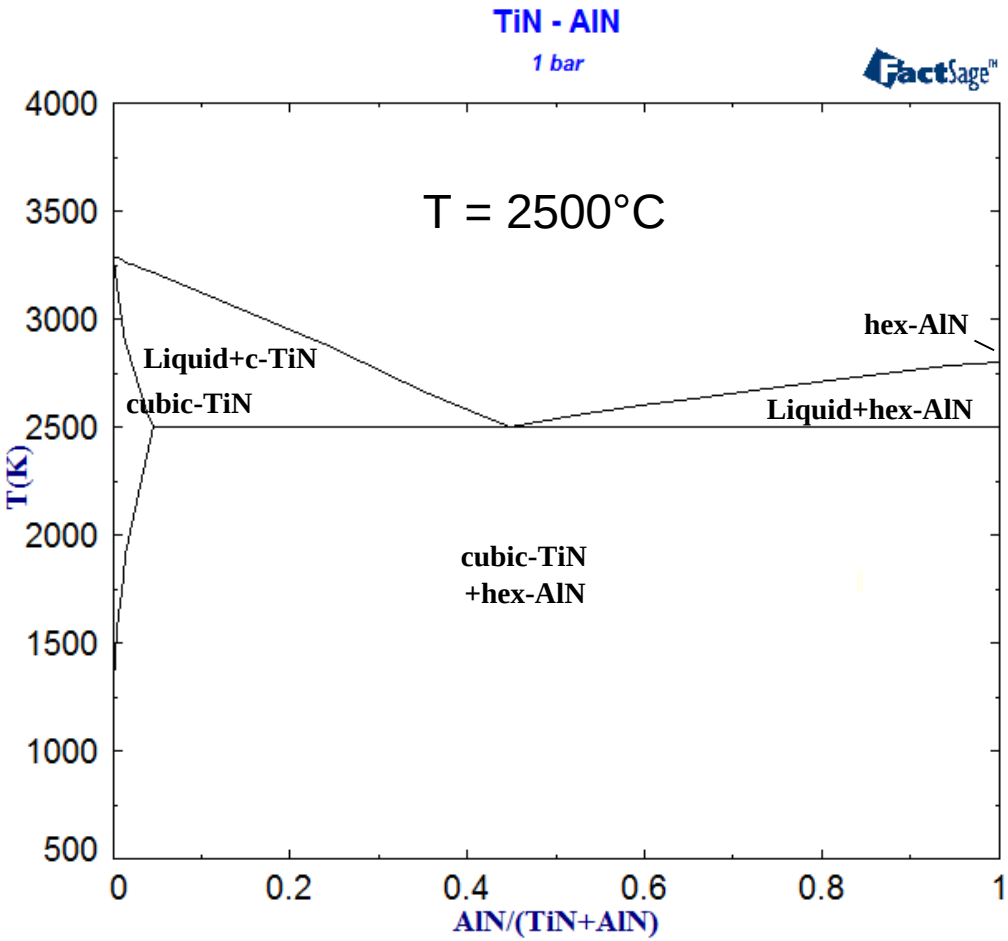
$\Omega_{cubic} = \Omega_{hex} > 0$
$\Delta G_{TiN} > \Delta G_{AlN}$

AlN: $G_{hex} < G_{liquid} < G_{cubic}$

Draw G(x) @ 250°C and 2500°C



Low/virtually no solubility → $|\Delta H_{mix}| > |T\Delta S_{mix}|$

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$\Omega_{cubic} = \Omega_{hex} > 0$ $\Delta G_{TiN} > \Delta G_{AlN}$

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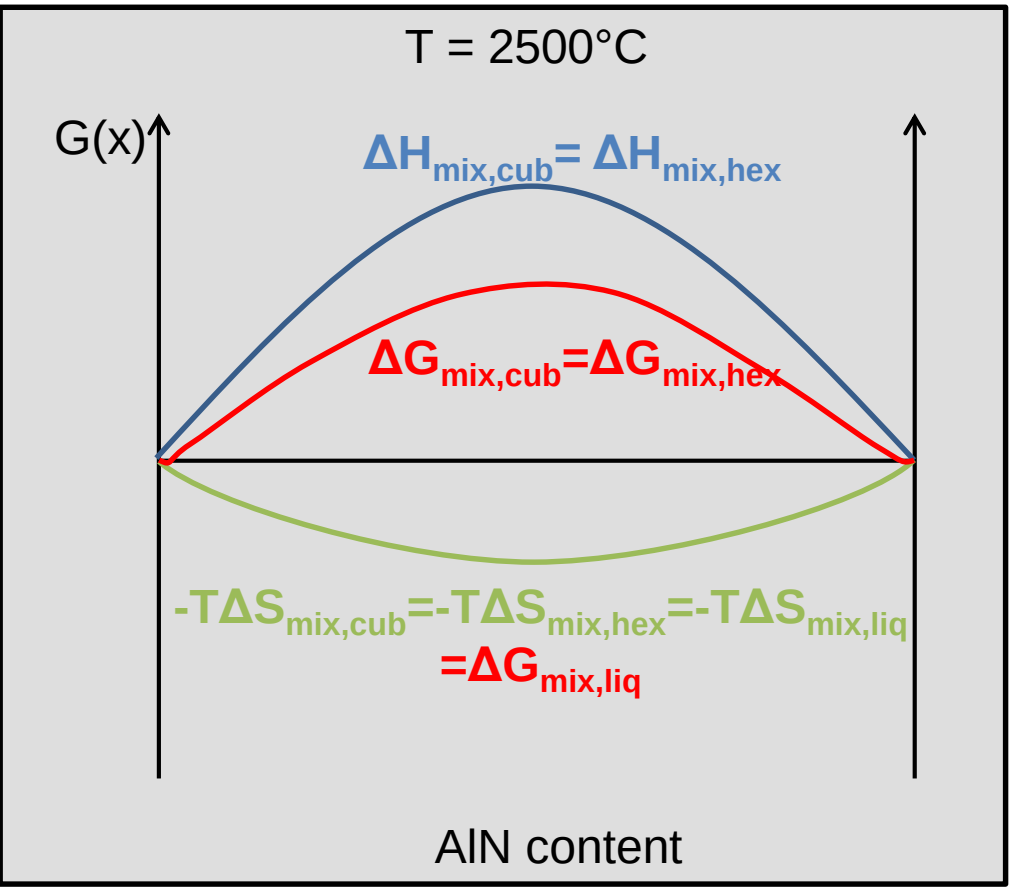
Draw G(x) @ 250°C and 2500°C



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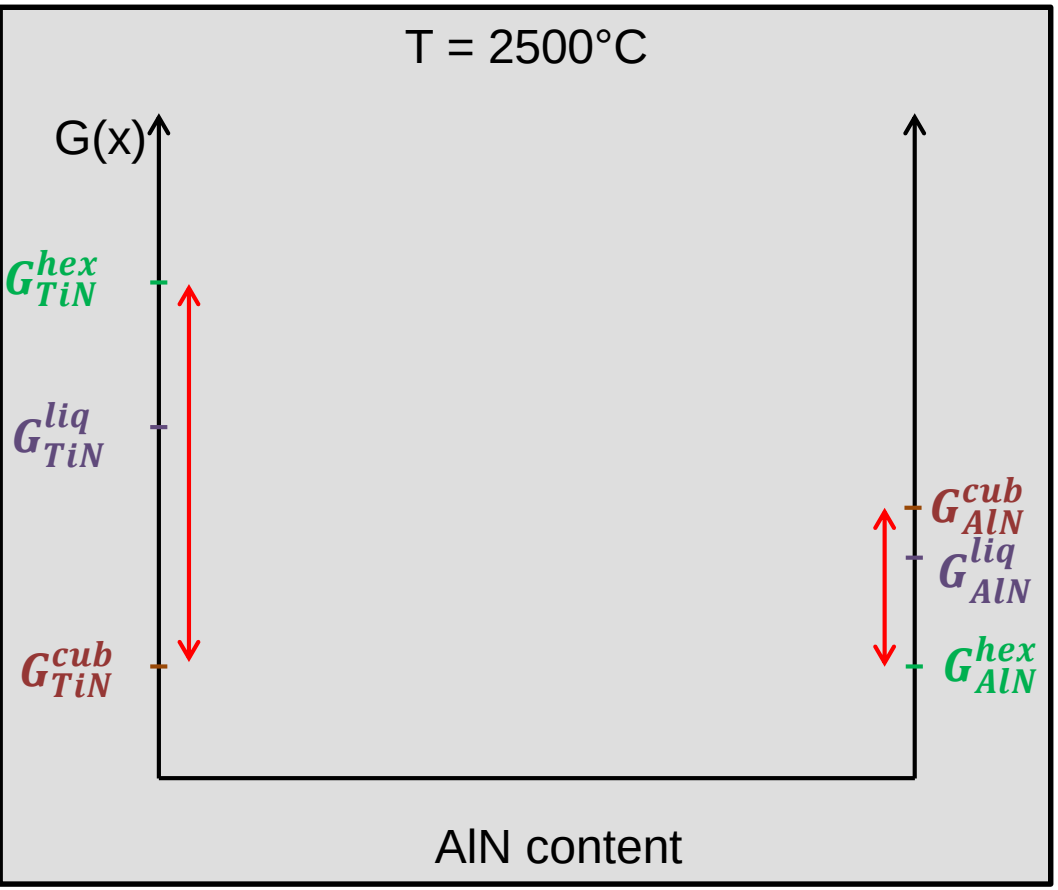
Draw G(x) @ 250°C and 2500°C



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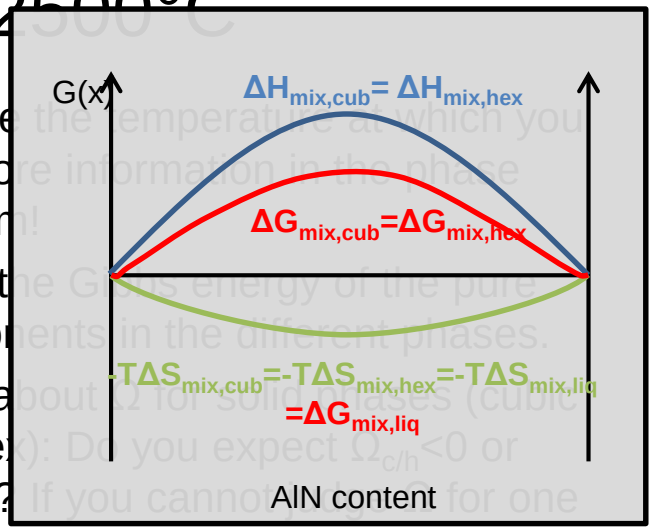
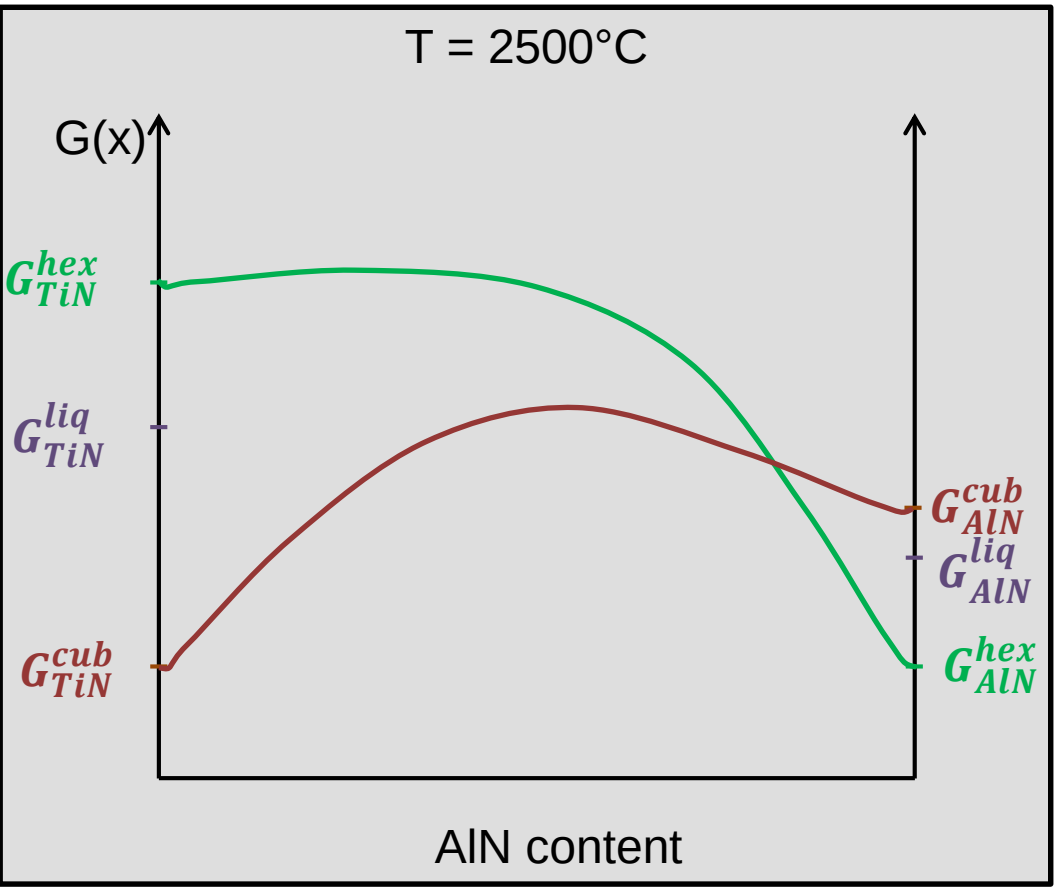


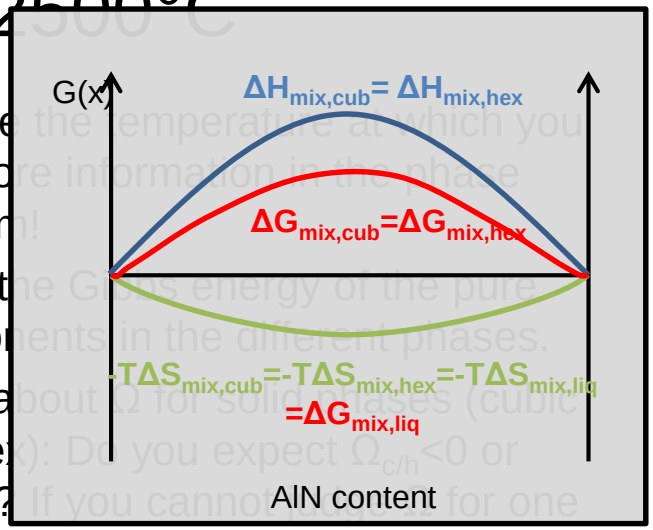
Low/virtually no solubility → $|\Delta H_{mix}| > |T\Delta S_{mix}|$

TiN: $G_{cubic} << G_{liquid} < G_{hex}$ | $\Omega_{cubic} = \Omega_{hex} > 0$ | $\Delta G_{TiN} > \Delta G_{AlN}$

AlN: $G_{hex} < G_{liquid} < G_{cubic}$

Draw G(x) @ 250°C and 2500°C





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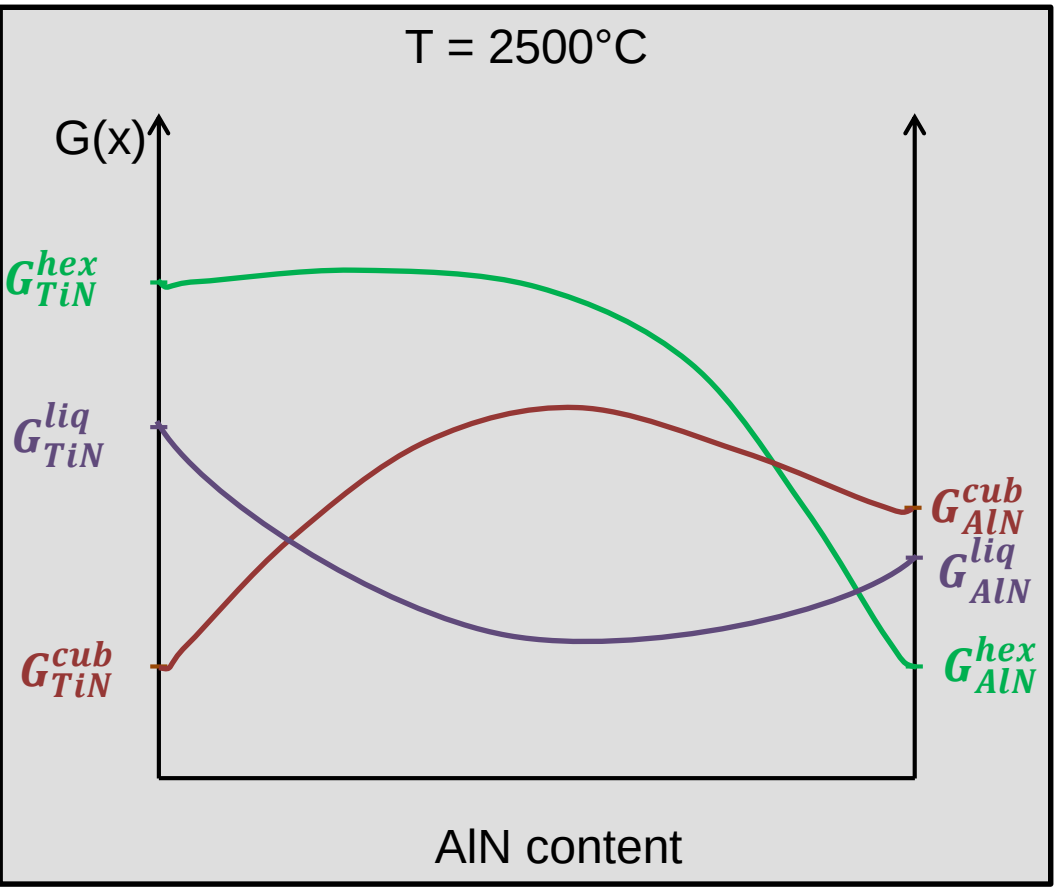
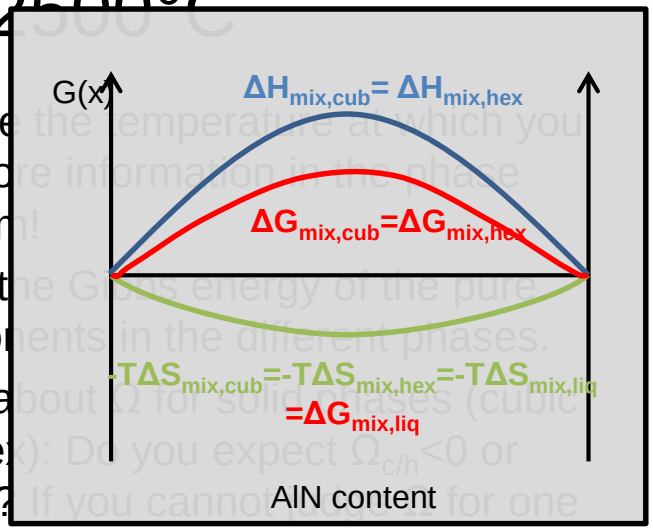
Draw G(x) @ 250°C and 2500°C





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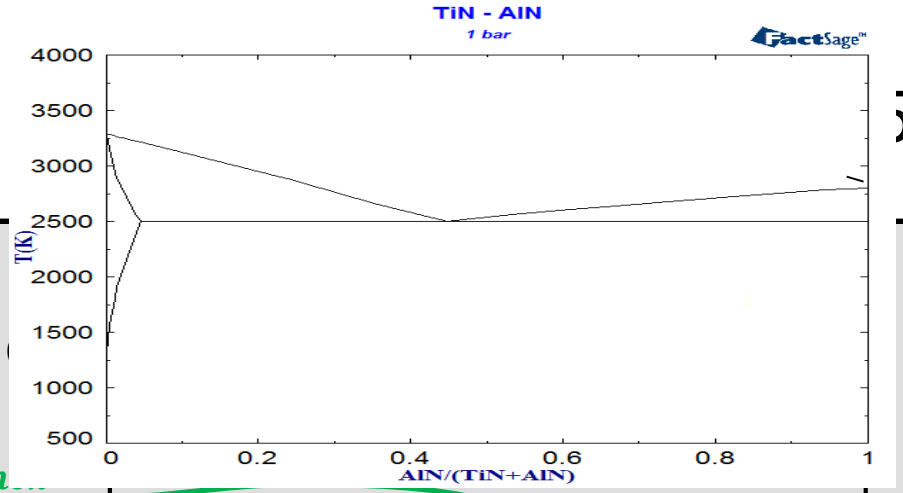
50°C and 2500°C



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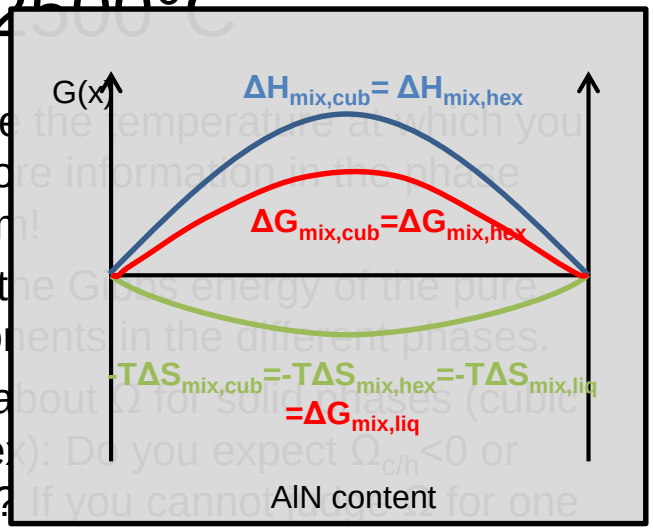

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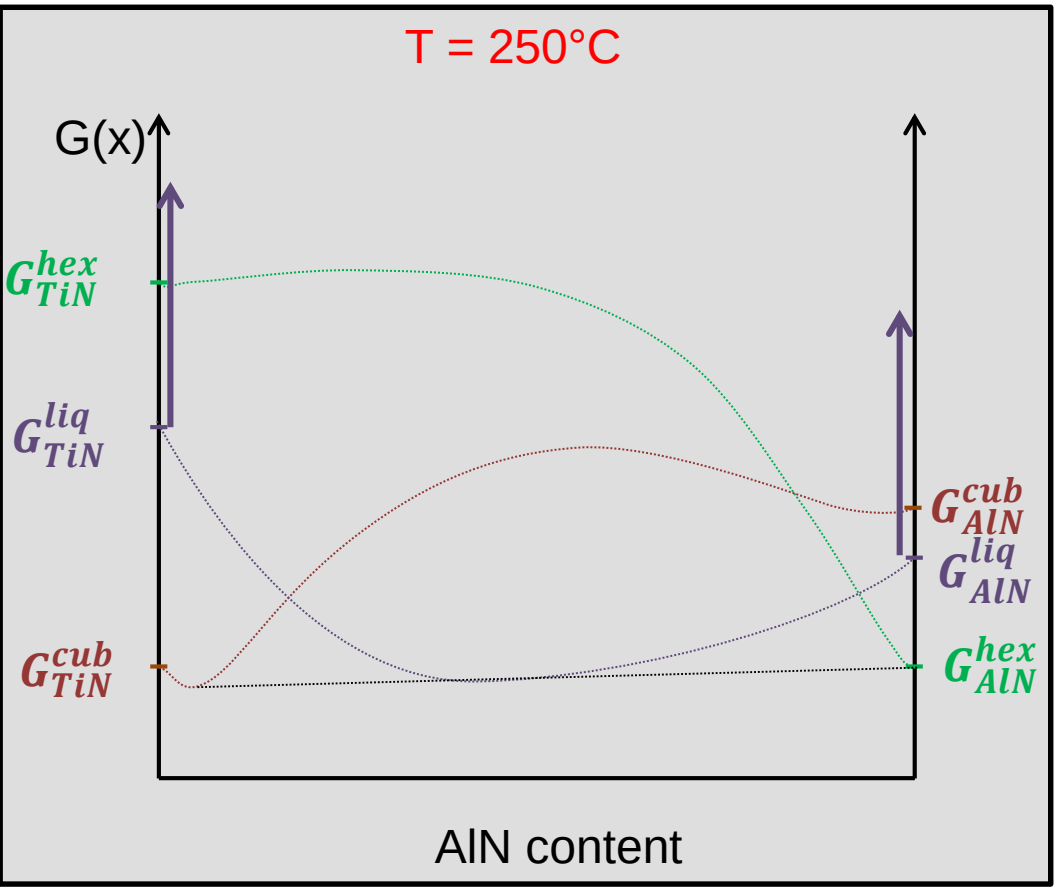
Draw G(x) @ 250°C and 2500°C



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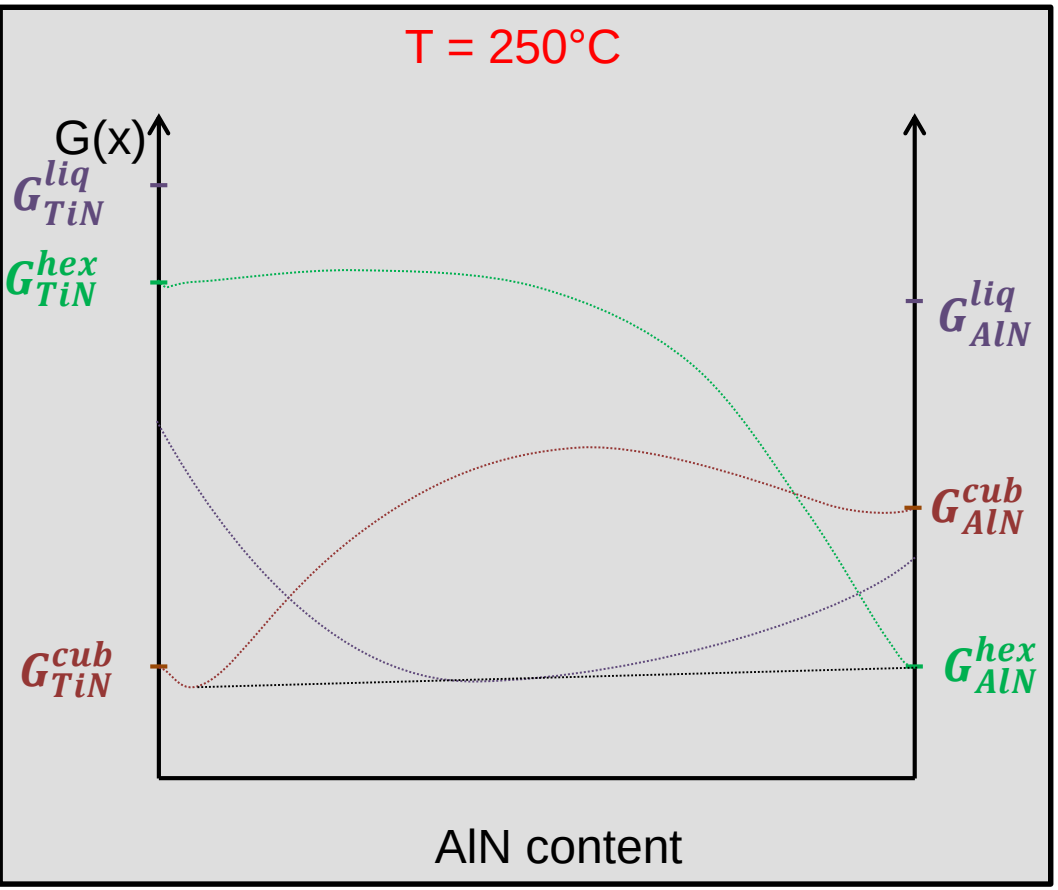

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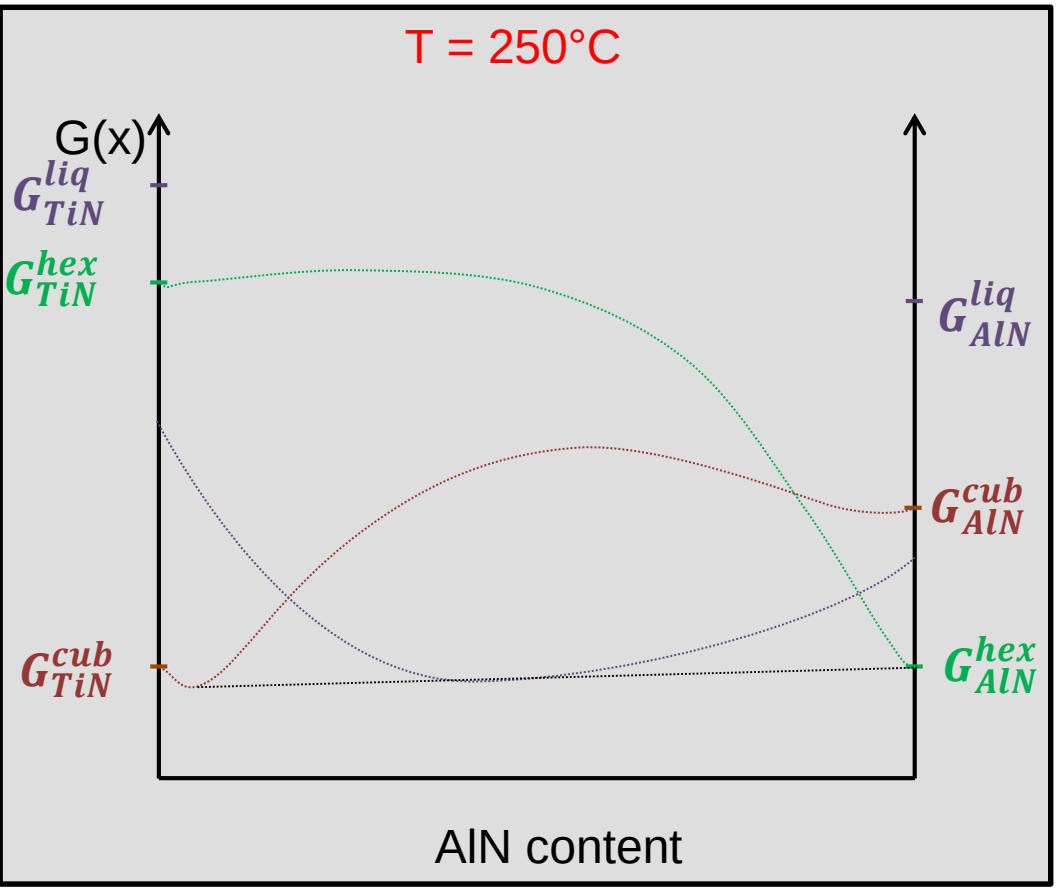

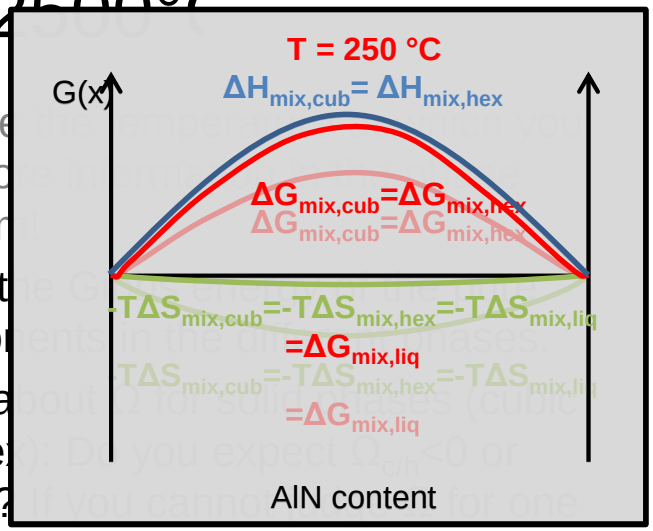

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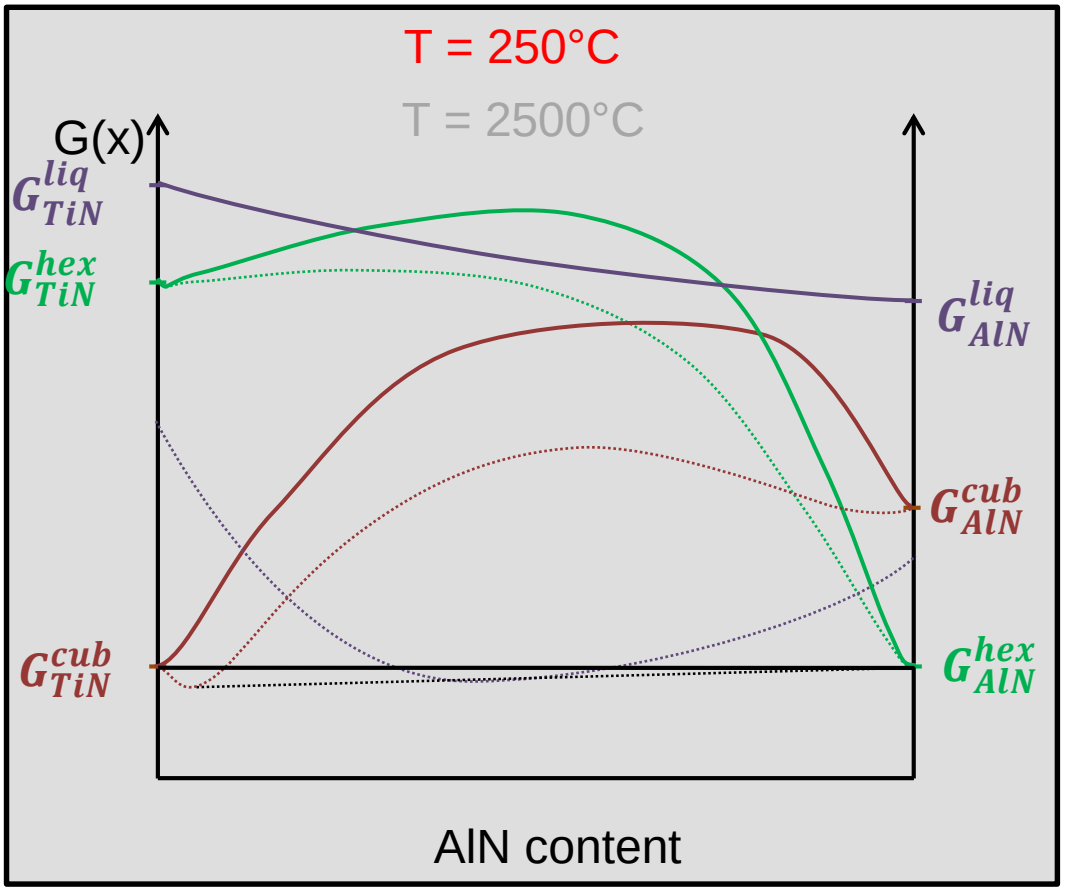
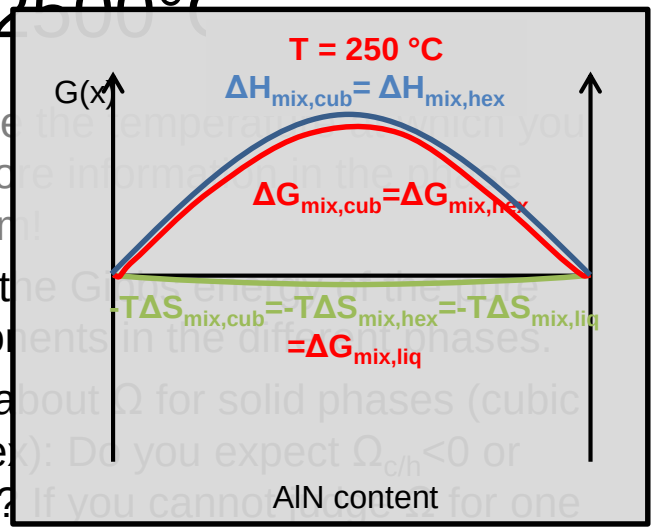
Draw G(x) @ 250°C and 2500°C





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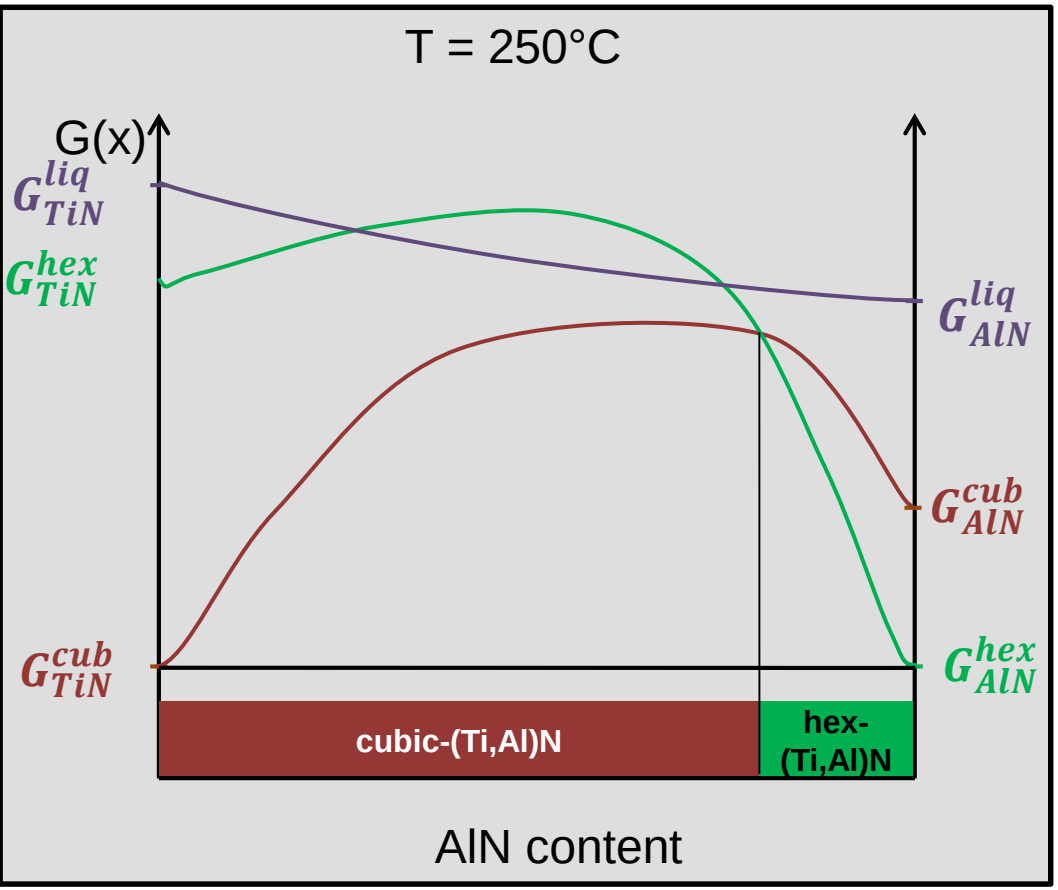
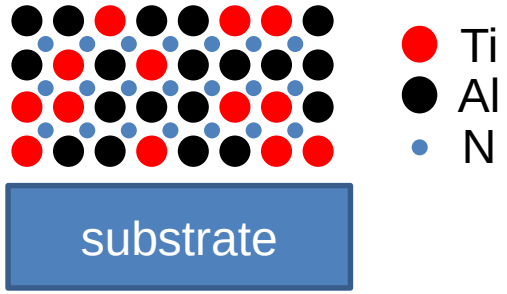
Vapour phase condensation



Atoms cannot form two phases TiN+AlN because of limited mobility (non-equilibrium processing).

Therfore, only a single (Ti,Al)N phase can form.

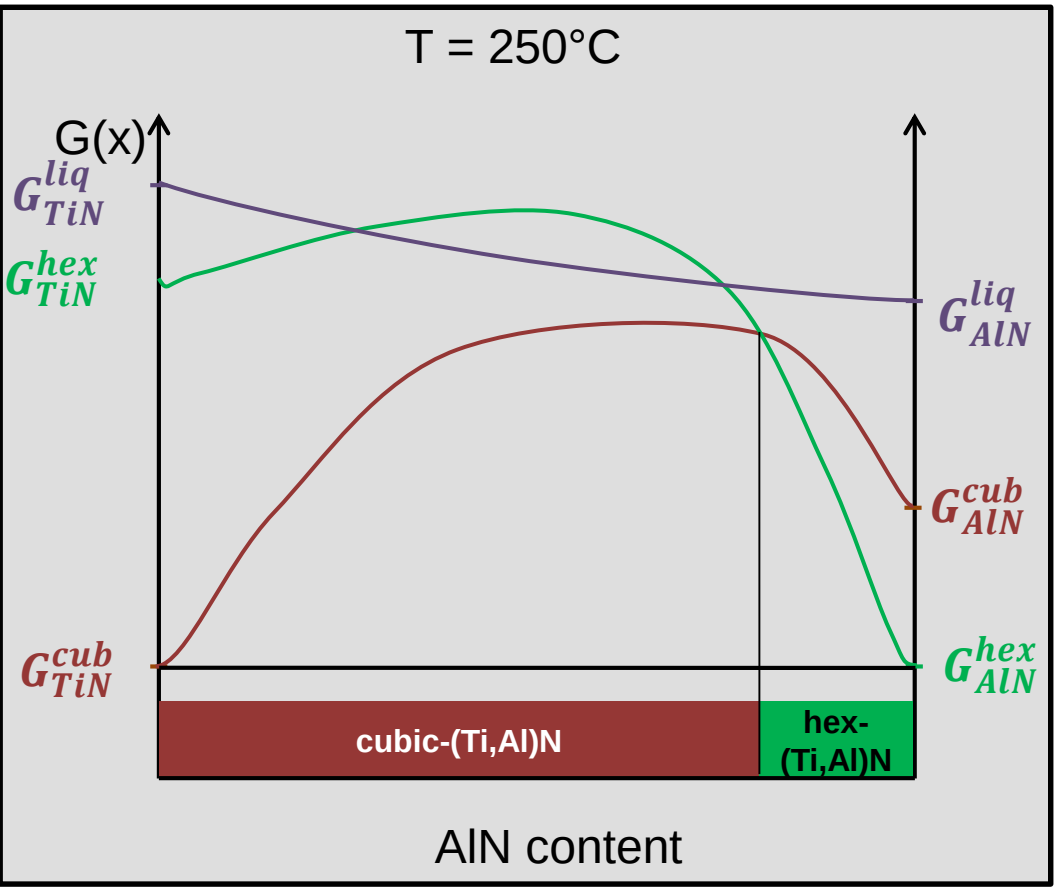
→ What is the single phase with lowest energy?

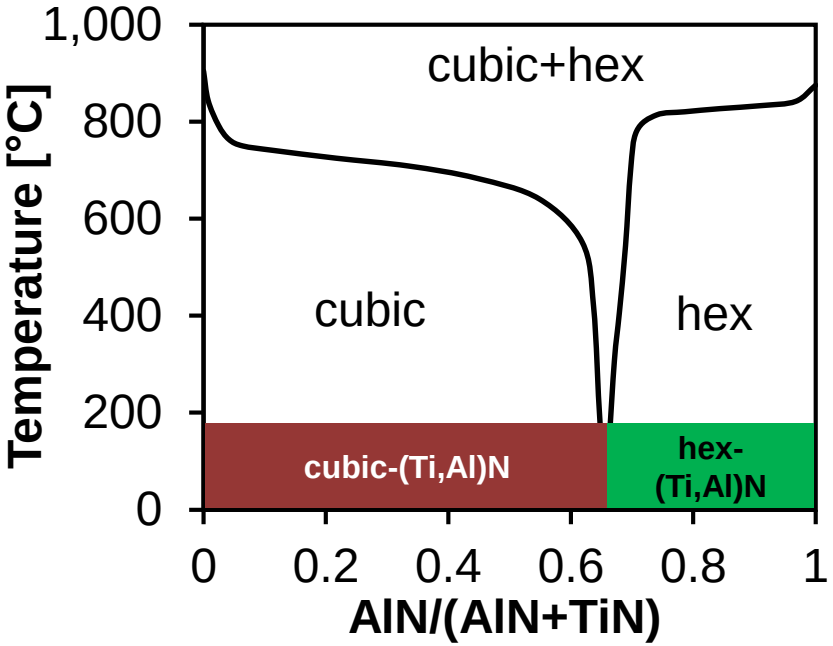


From metal vapour to solid within a fraction of 1 µs

→ Extreme quenching rates (>> 10^{10} °C/s)!

Vapour phase condensation





Experimental non-equilibrium (metastable) TiN-AlN phase diagram [Spencer, Z. Metallk. 92 (2001) 10]

→ G(x) curves can predict metastable phase formation!

From metal vapour to solid within a fraction of 1 µs

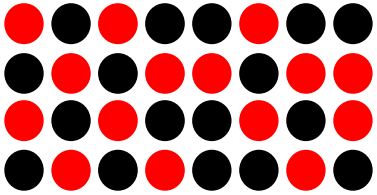
→ Extreme quenching rates (>> 10^{10} °C/s)!

$Ti_{0.5}Al_{0.5}N$: A real solution

$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$

Think about bonds & configurations

REAL SOLUTIONS

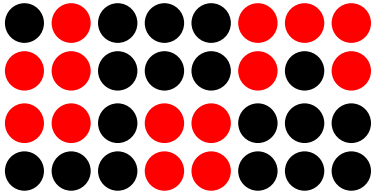


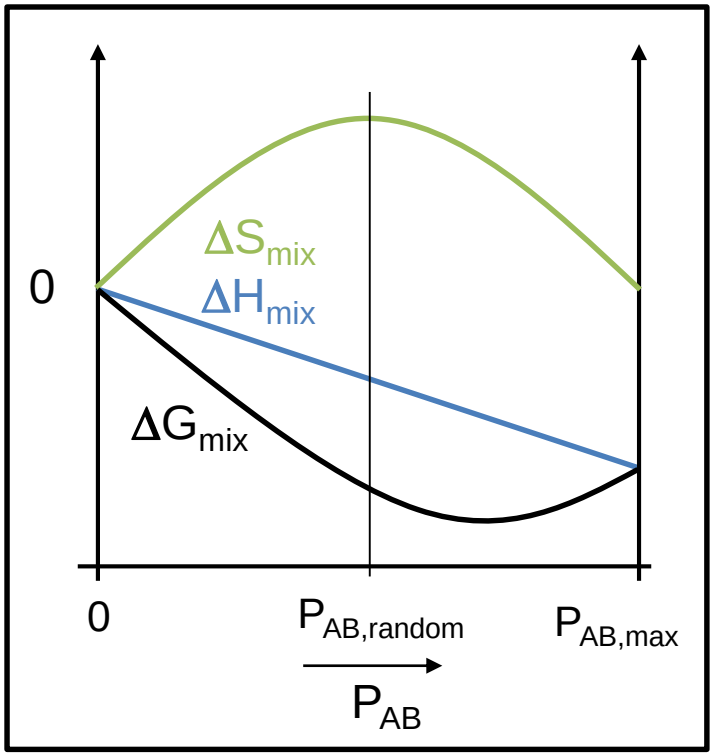
Ω<0

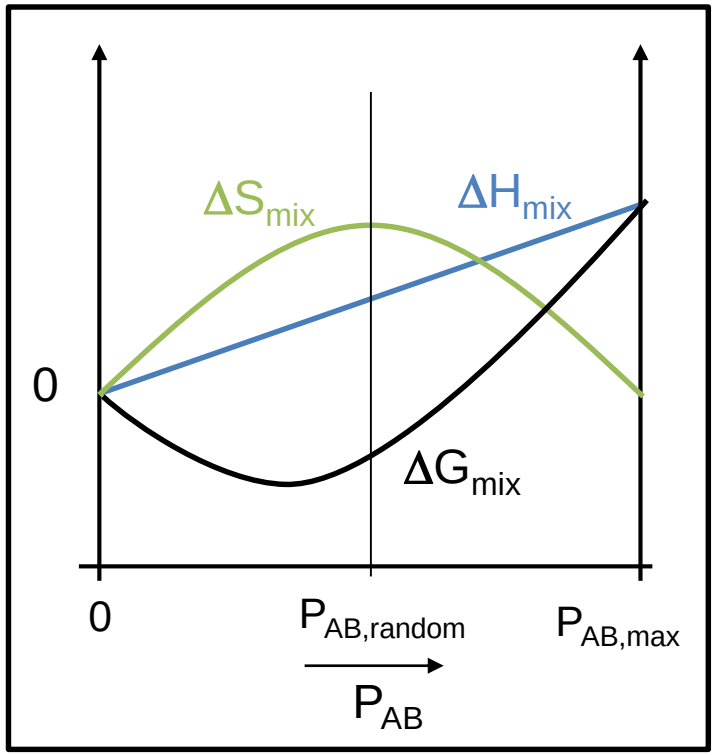
Ordering

Ω>0

Clustering





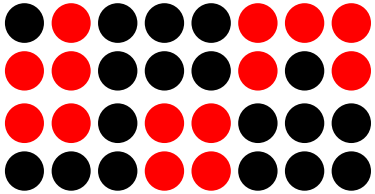


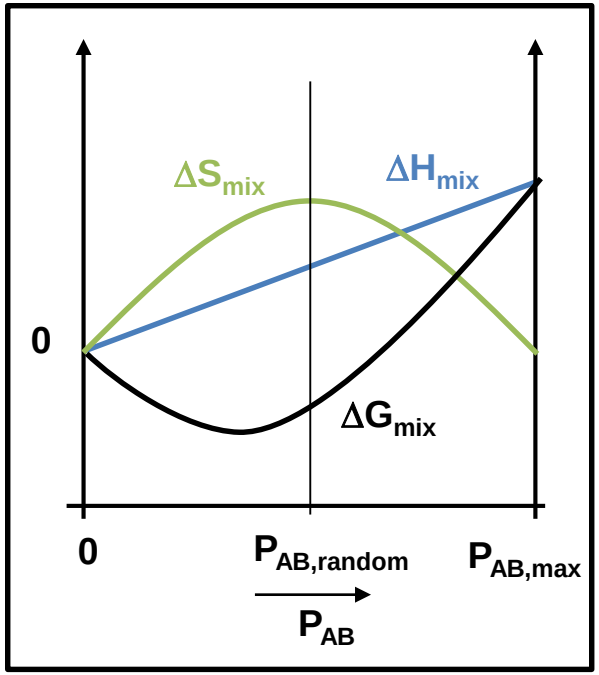
$Ti_{0.5}Al_{0.5}N$: A real solution

Visualizing atomic composition in 3D: 3D atom probe tomography

REAL SOLUTIONS

↓Clustering↓





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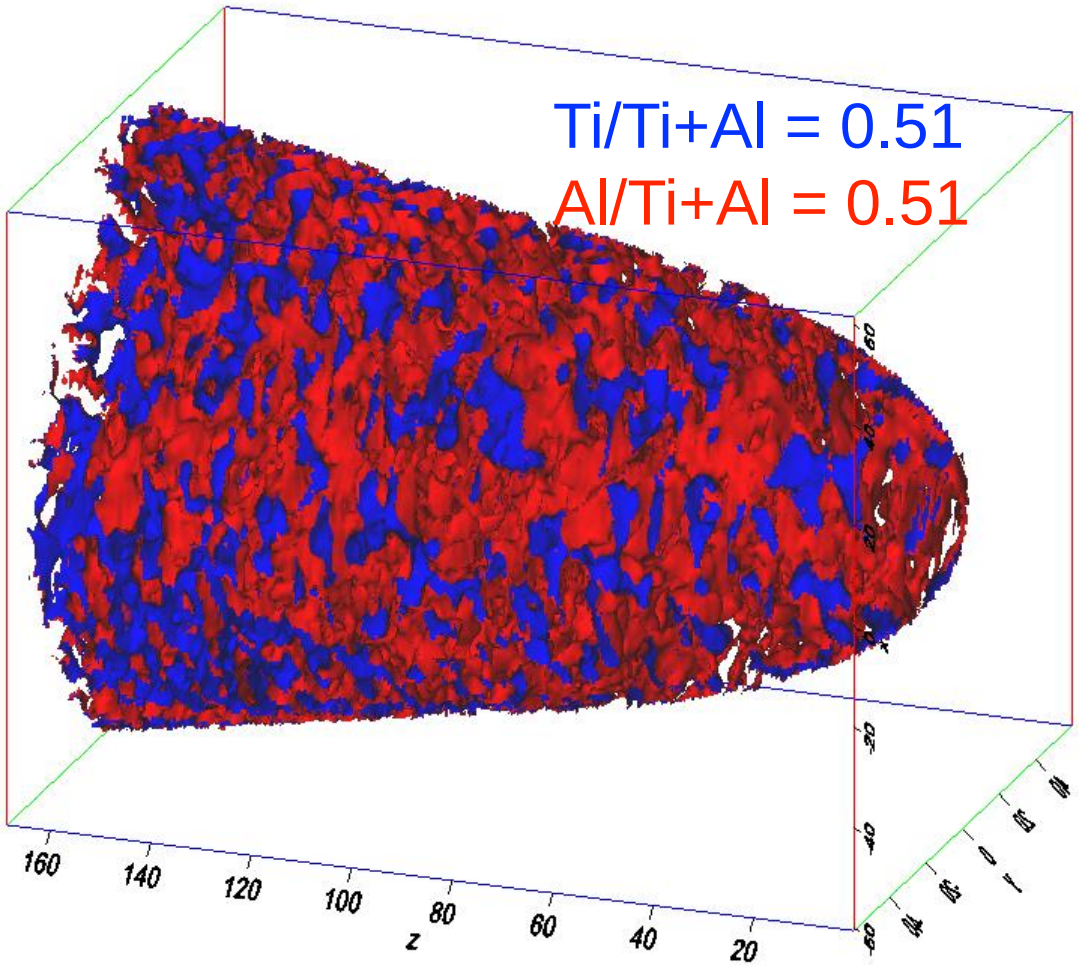

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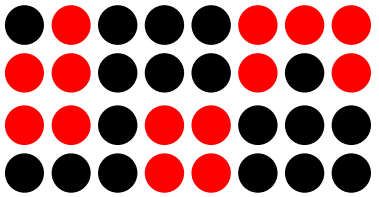
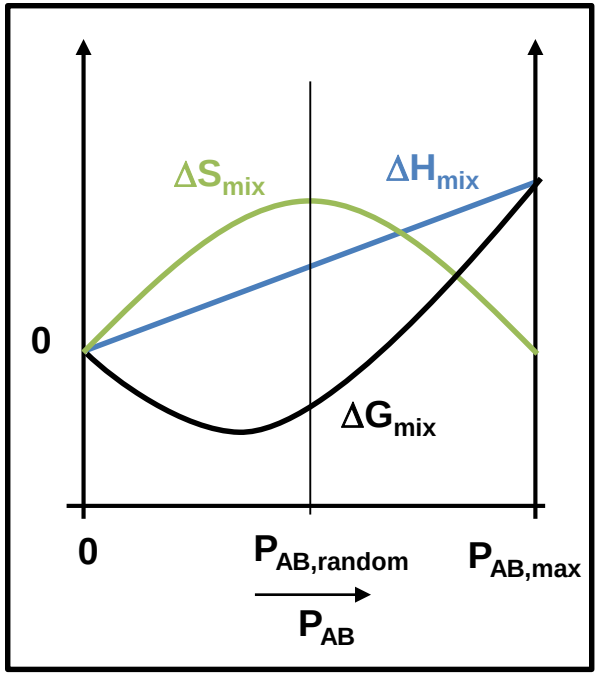




Concepts, key ideas

Strategy for predicting metastable phase formation in vapour phase condesation:
1. Derive G(x) curves from the stable phase diagram.
2. For each composition, the single phase with lowest Gibbs energy forms during vapour phase condensation.

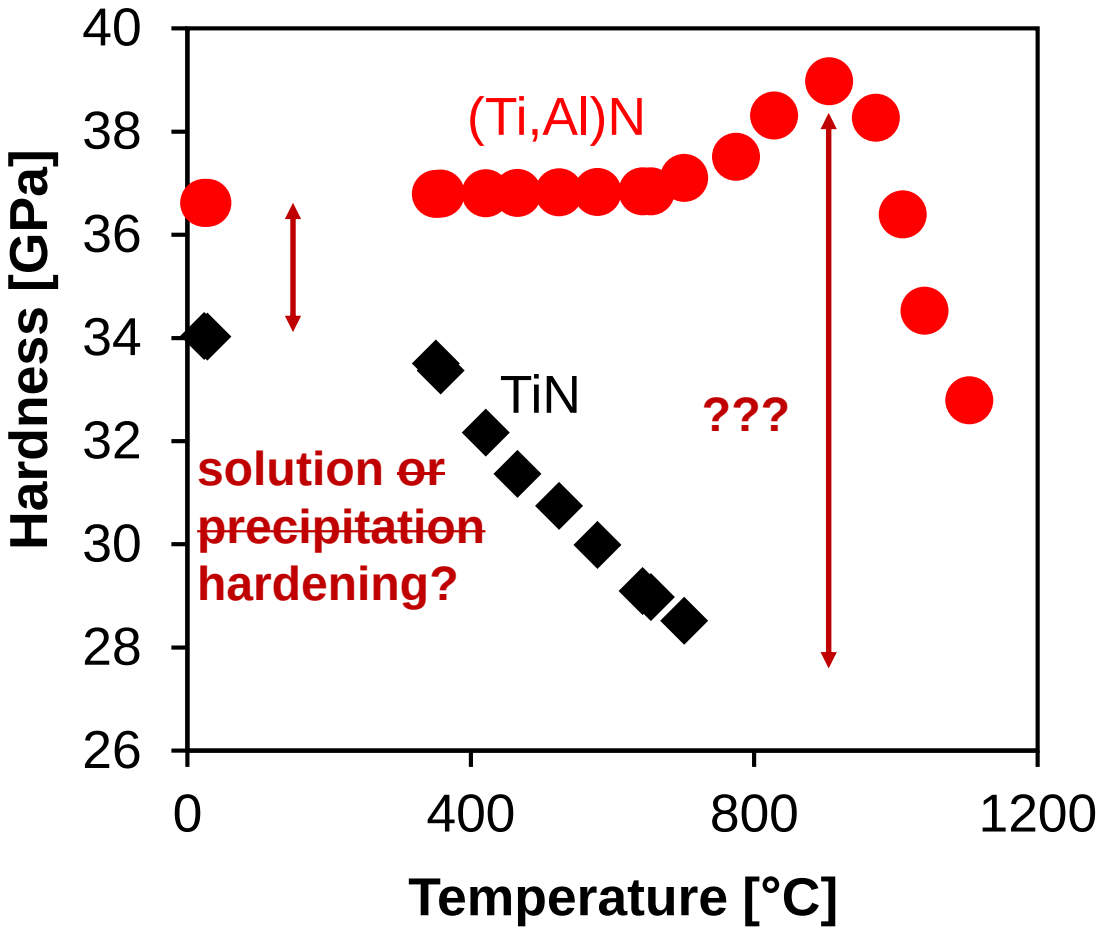
In real solutions, atoms form short-range order to minimize G:

clustering in case of $\Omega > 0$ or

ordering in case of $\Omega < 0$.

This ordering can be observed!

Application: (Ti,Al)N coatings for cutting tools



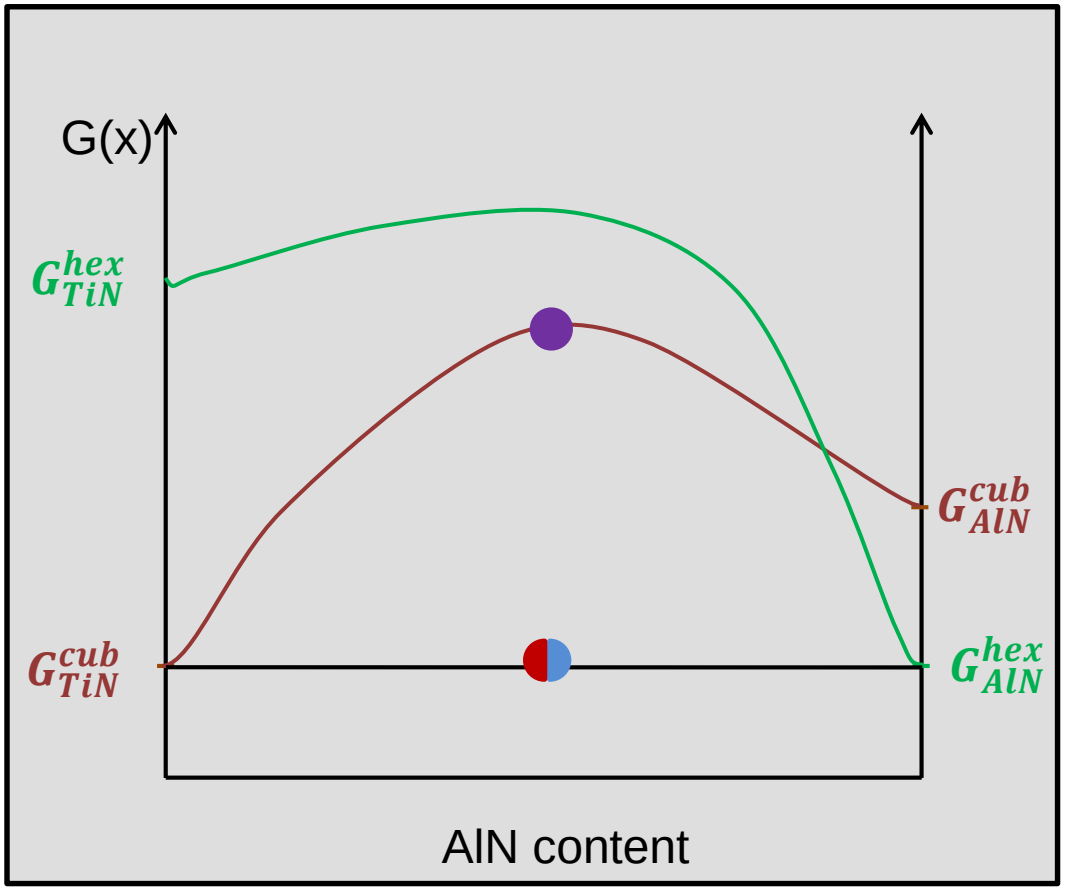
H increases by Al addition!

But WHY?

Let‘s look at G(x) curves!

Mayrhofer, Rachbauer, Rovere, Schneider, *Protective Transition Metal Nitride Coatings* (2012).

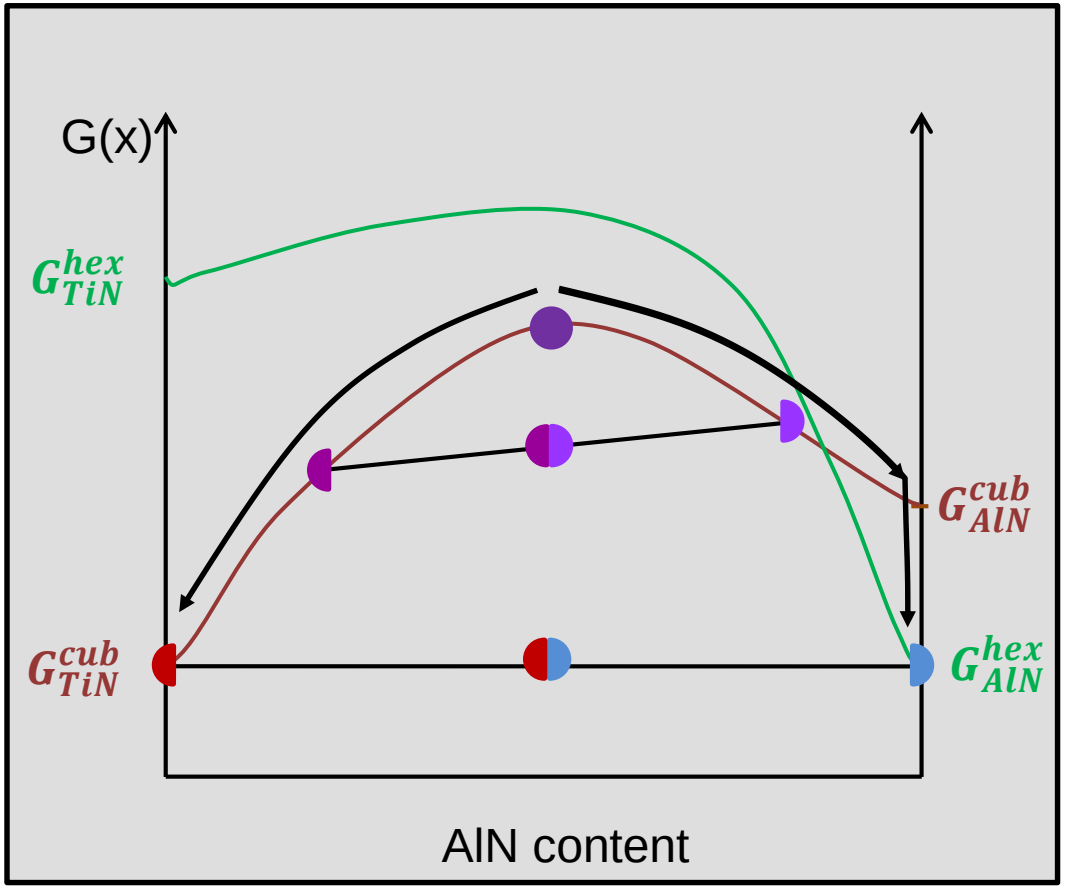
Annealing of a metastable phase: How can the Gibbs energy be lowered?

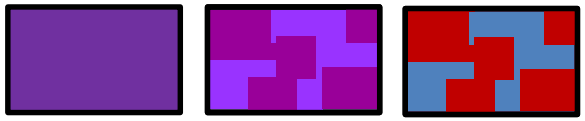


1. What is the stable state for $Ti_{0.5}Al_{0.5}N$?

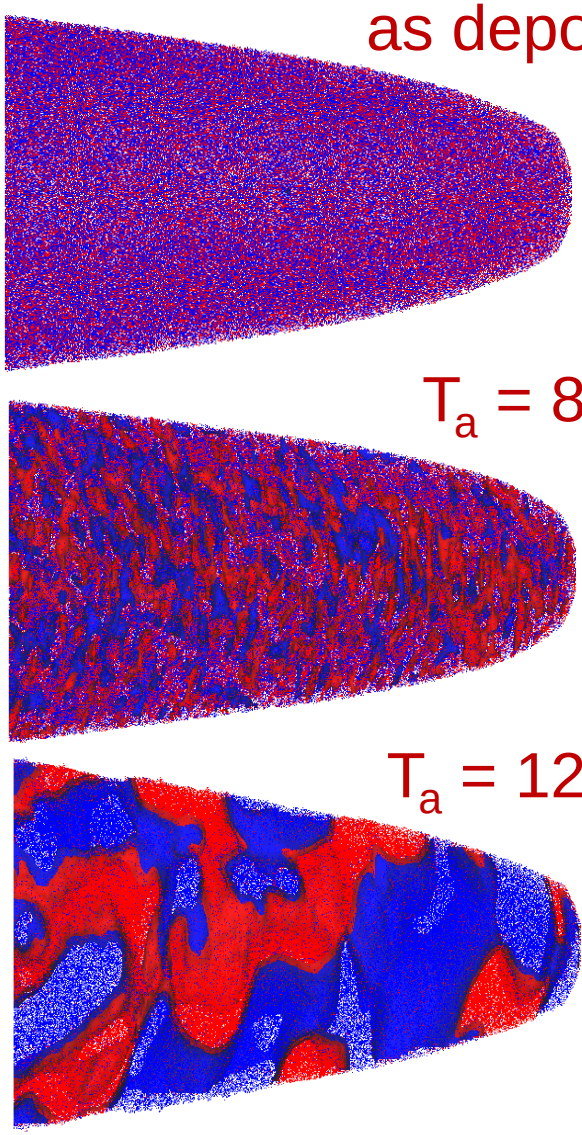
→ cub-TiN + hex-AlN

Annealing of a metastable phase: How can the Gibbs energy be lowered?



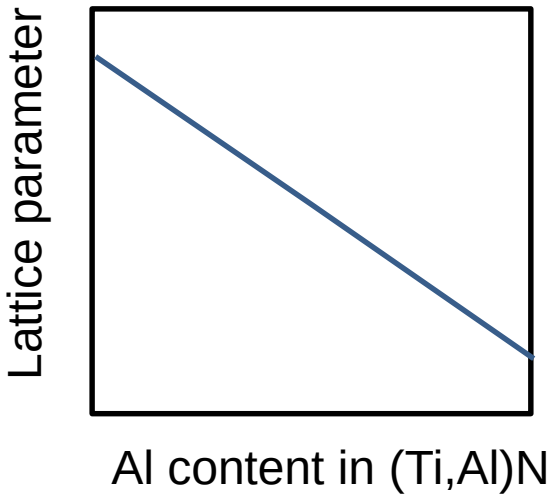


E_A(de-mixing) = E_A(diffusion)



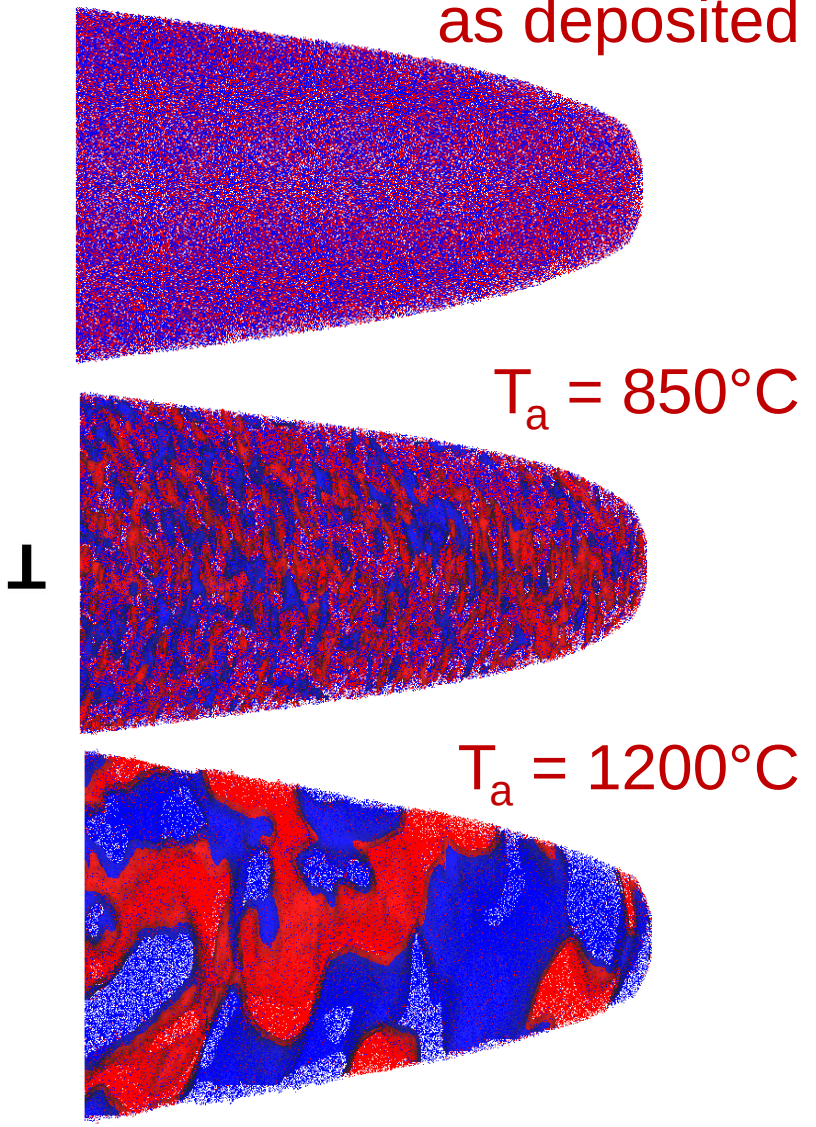
to Baben et al., Materials Research Letters (2016).

Annealing of a metastable phase: Implications on mechanical properties



→ Composition variation leads to variation of lattice parameter.

→ Strain field!



Mayrhofer et al., J. Appl. Phys. 100 (2006) 094906.

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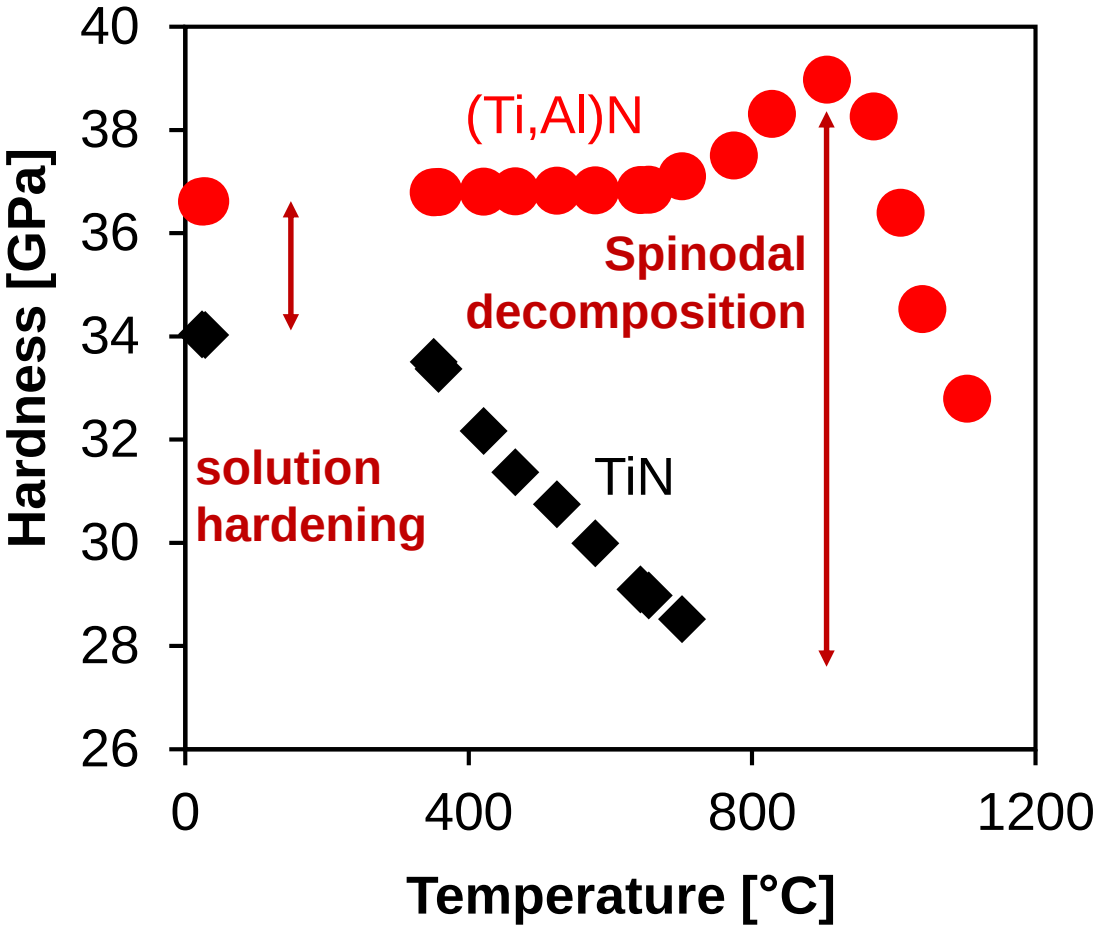

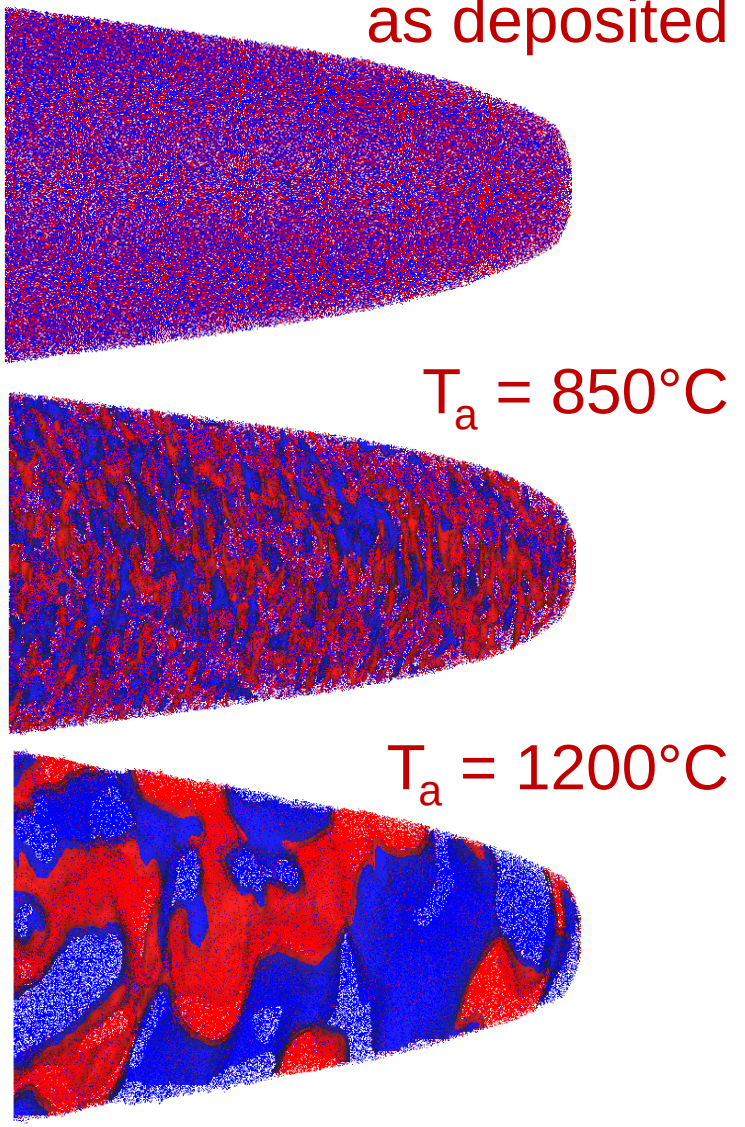

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Outline

1. Understanding processes&materials based on G(x,T,p)

QUALITATIVE APPLICATION OF MC II

2. Modelling G(x,T,p) based on theory&experiment

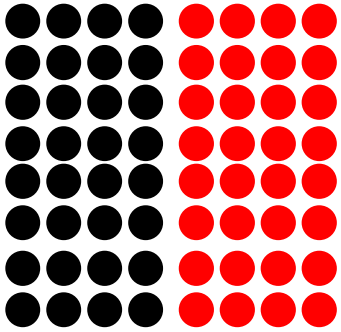
QUALITATIVE → QUANTITATIVE

3. Modelling processes&materials based on G(x,T,p)

QUANTITATIVE APPLICATION OF MC II

Strategy:

$$G_{total} = X_A G_A + X_B G_B$$
$$= X_A(H_A - TS_A) + X_B(H_B - TS_B)$$
$$- T\Delta S_{mix}$$
$$+ \Delta H_{mix}$$
$$+ \Delta G_{excess}$$



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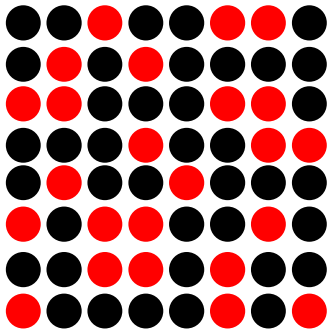

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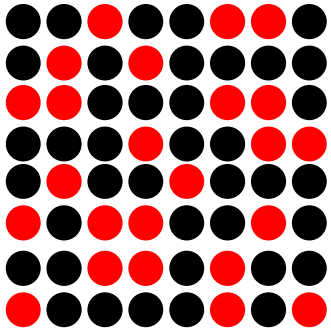

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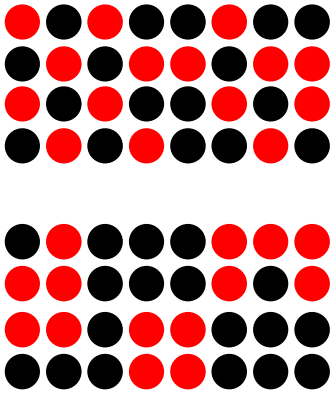

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What thermodynamic property describes the temperature dependence of the enthalpy?

A) entropy

B) thermal expansion coefficient

C) heat capacity

D) volume

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A) entropy

B) thermal expansion coefficient

C) heat capacity

D) volume

$C_P = dH/dT$

$$H(T) = H^{298K} + \int_{298K}^{T} C_P dT$$

What expression describes the temperature dependence of the entropy?

A) $dS/dT = C_P$

B) $dS/dT = T*C_P$

C) $dS/dT = C_P/T$

D) $dS/dT = T*\ln(C_P)$

What expression describes the temperature dependence of the entropy?

A) $dS/dT = C_P$

B) $dS/dT = T*C_P$

C) $dS/dT = C_P/T$

$$S(T) = S^{298K} + \int_{298K}^{T} \frac{C_P}{T} dT$$

D) $dS/dT = T*\ln(C_P)$

CalPhaD: Modelling G(T)

$$G(T) = H(T) - TS(T)$$

$$= H^{298K} + \int_{298K}^{T} C_P dT - T\left[S^{298K} + \int_{298K}^{T} \frac{C_P}{T} dT\right]$$

What thermodynamic data is needed to model G(T)?

→ H^{298K}, S^{298K}, $C_P(T)$

CalPhaD: Modelling G(T)

In 1991, the SGTE (Scientific Group Thermodata Europe, a large consortium of groups working on thermodynamic databases), agreed on a set of

$$H^{298K},\ S^{298K},\ C_P(T)$$

for the elements in different crystal structures

→ Dinsdale, CALPHAD 15 (1991) 317.

What thermodynamic property describes the pressure dependence of the Gibbs energy?

A) entropy

B) thermal expansion coefficient

C) heat capacity

D) volume

What thermodynamic property describes the pressure dependence of the Gibbs energy?

A) entropy

B) thermal expansion coefficient

C) heat capacity

D) volume

$V = dG/dp$

CalPhaD: Modelling G(p)

$dG/dp = V$

What thermodynamic data is needed to model G(p)?

→ molar volume and compressibility or bulk modulus

→ i.e. V(p)

Strategy:

$G_{total} = X_A G_A + X_B G_B$

$= X_A(H_A - TS_A) + X_B(H_B - TS_B)$ ✓

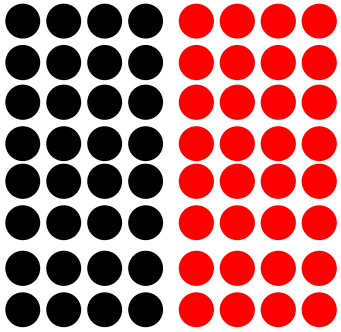
$- T\Delta S_{mix}$ ✓

$+RT\sum X_i \ln X_i$

$+ \Delta H_{mix}$ ✓

$+\Omega X_A X_B$

$+ \Delta G_{excess}$?



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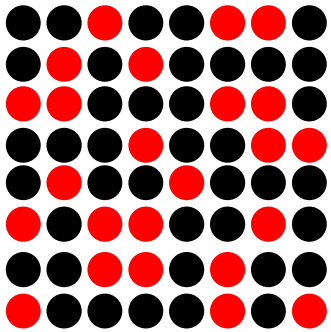

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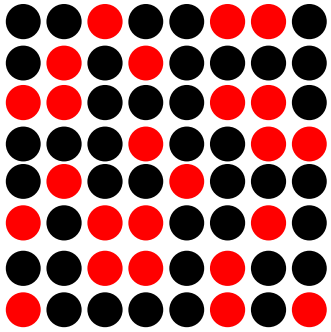

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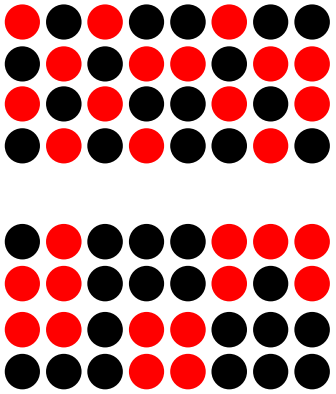
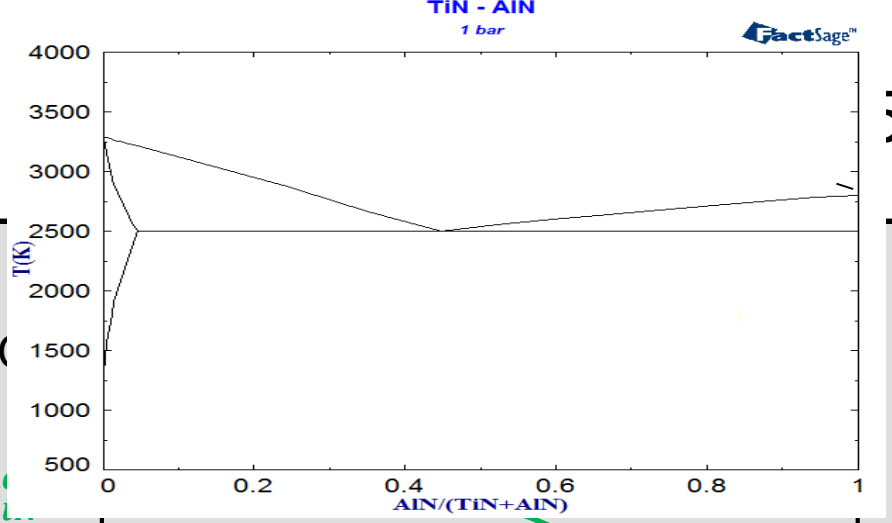
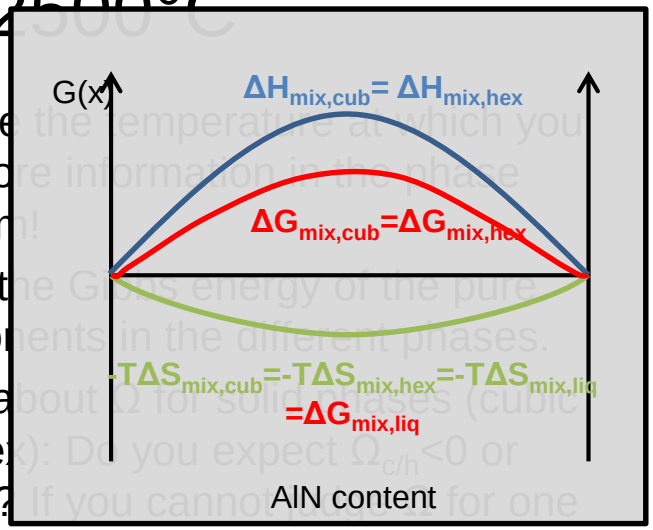


real solution ordering/clustering A-A+B-B << 2A-B A-A+B-B >> 2A-B

50°C and 2500°C



1. Choose the temperature at which you find more information in the phase diagram!
2. Order the Gibbs energy of the pure components in the different phases.
3. Think about Ω for solid phases (cubic and hex): Do you expect $\Omega_{c/h}<0$ or $\Omega_{c/h}>0$? If you cannot decide for one phase, assume $\Omega_c=\Omega_h$.
4. Do you expect $|\Delta H_{mix}| < |T\Delta S_{mix}|$ or $|\Delta H_{mix}| > |T\Delta S_{mix}|$?
5. Draw ΔH_{mix}, $-T\Delta S_{mix}$ and ΔG_{mix} for all phases. Assume ΔH_{mix}(liquid) ≈ 0.
6. Draw G(x) for the solid phases.
7. Draw G(x) for the liquid phase, taking into account position of the eutectic. Eventually adjust G(x) for the solid phases to match solubility limits.
8. Repeat the steps for the other temperature.



Low/virtually no solubility → $|\Delta H_{mix}| > |T\Delta S_{mix}|$

TiN: $G_{cubic} << G_{liquid} < G_{hex}$

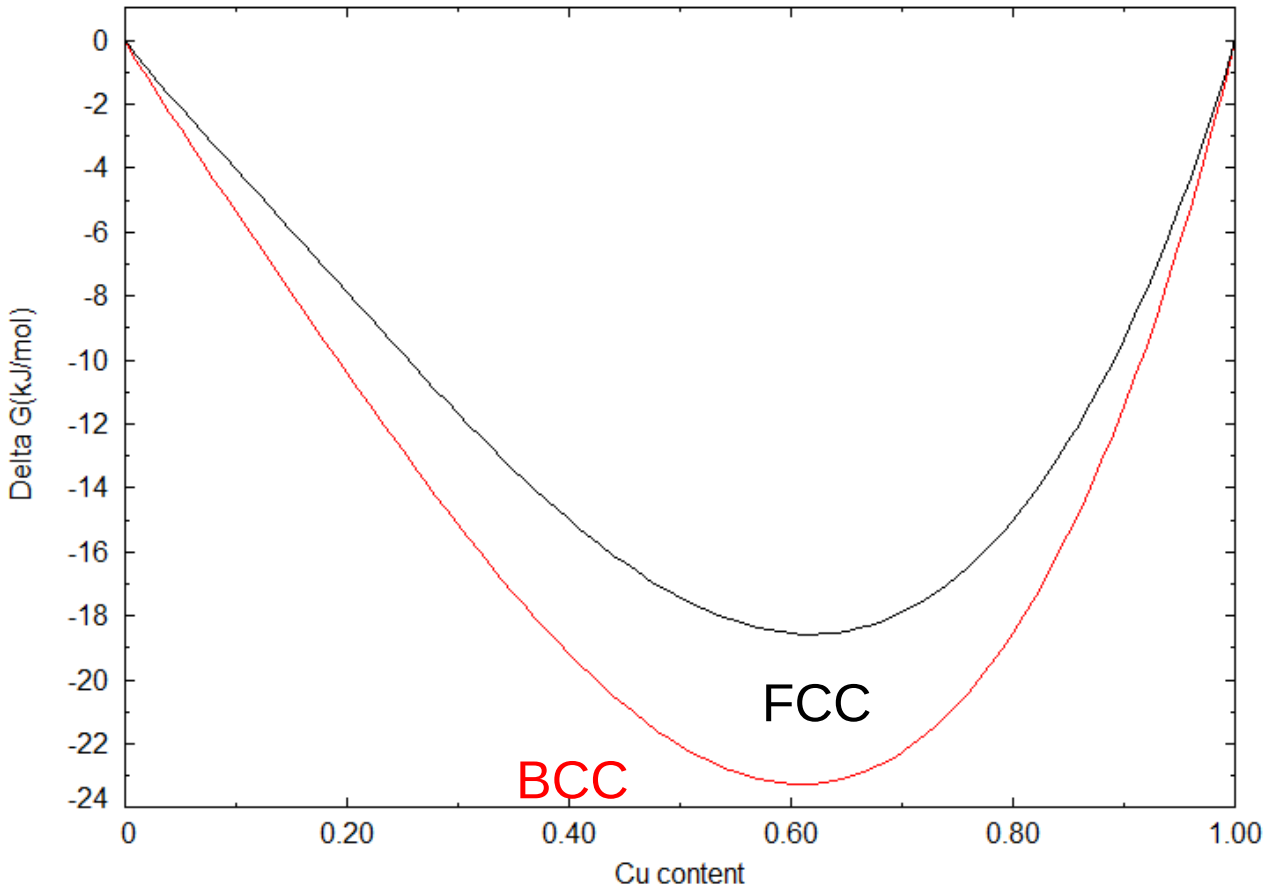
$\Omega_{cubic} = \Omega_{hex} > 0$ $\Delta G_{TiN} > \Delta G_{AlN}$

AlN: $G_{hex} < G_{liquid} < G_{cubic}$

What information can be extracted from the Al-Cu phase diagram?

A) $\Omega_{fcc} < \Omega_{bcc}$

B) $\Omega_{fcc} > \Omega_{bcc}$



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$G_{total} = X_A G_A + X_B G_B$

$= X_A(H_A - TS_A) + X_B(H_B - TS_B)$ ✓

$- T\Delta S_{mix}$ ✓

$+RT\sum X_i \ln X_i$

$+ \Delta H_{mix}$ ✓

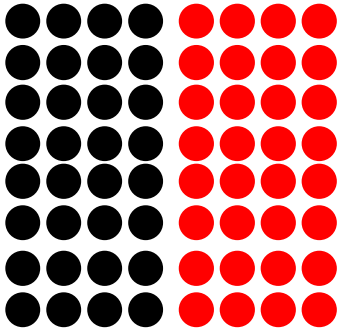
$+X_A X_B {}^*\Omega$

✓

e.g. Redlich-Kister

$+ X_A X_B {}^*\Omega_v {}^*(X_A - X_B)^v$

$+ \Delta G_{excess}$



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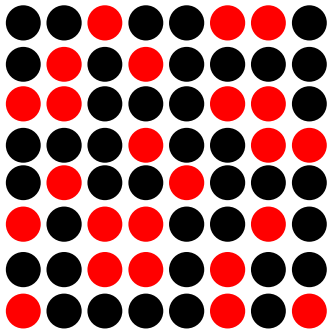

ideal solution
randomly mixed
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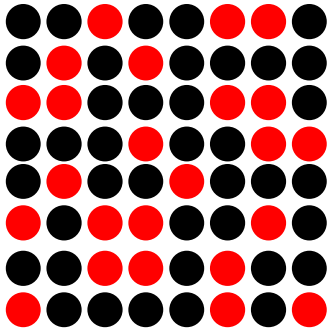

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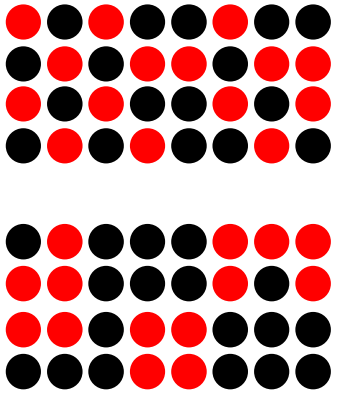
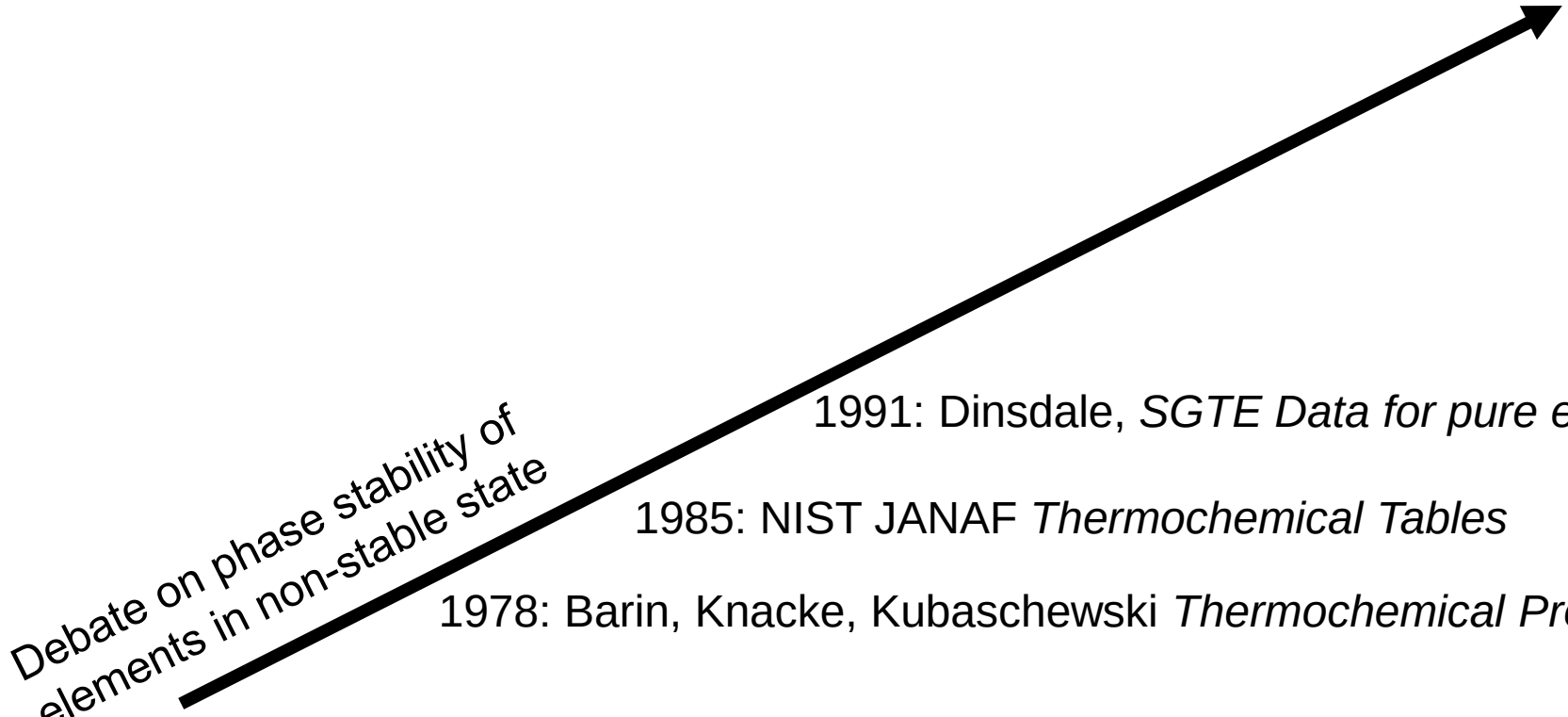


real solution
ordering/clustering
A-A+B-B << 2A-B
A-A+B-B >> 2A-B

History of computational thermodynamics and thermodynamic databases



1957 First ternary phase diagram calculation (Ni-Cr-Cu)

Strategy:

$G_{total} = X_A G_A + X_B G_B$

$= X_A(H_A - TS_A) + X_B(H_B - TS_B)$ ✓

$- T\Delta S_{mix}$ ✓

$+RT\sum X_i \ln X_i$

$+ \Delta H_{mix}$ ✓

$+X_A X_B {}^*\Omega$

e.g. Redlich-Kister ✓

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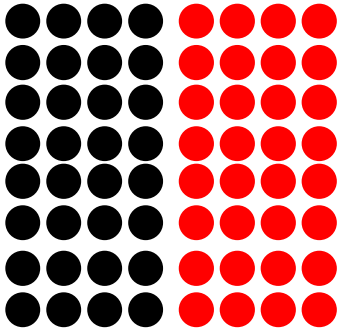

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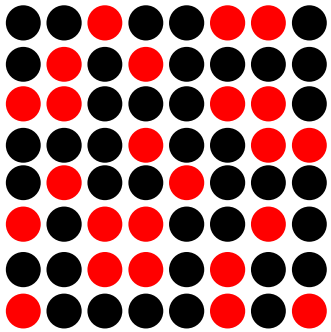

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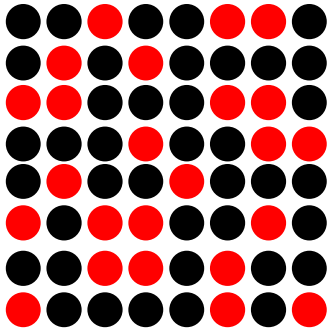

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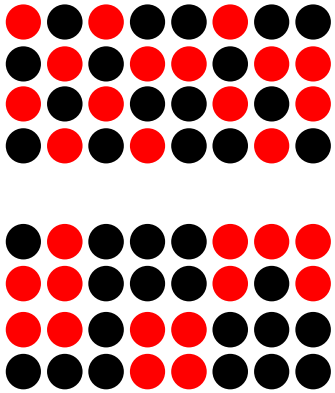

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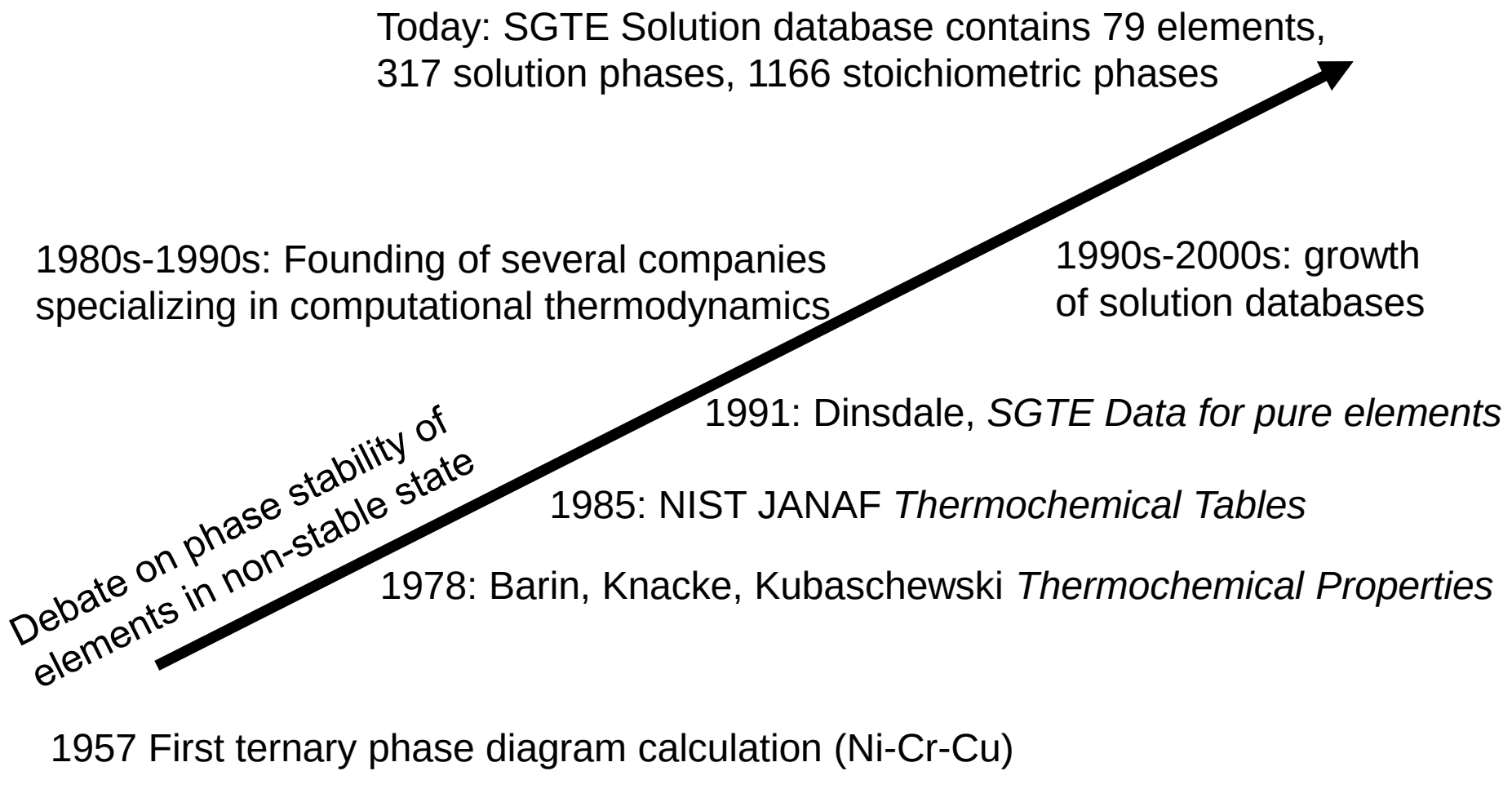
History of computational thermodynamics and thermodynamic databases



History of computational thermodynamics and thermodynamic databases

Today: SGTE Solution database contains 79 elements, 317 solution phases, 1166 stoichiometric phases
Allows description of
577 binary systems,
141 ternary systems,
15 higher order systems

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sc	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds								

~70 non-radioctive, non-noble gas elements
→ *70*69/2 = 2415 binary systems*
→ *70*69*68/6 = 54740 ternary systems*

Materials Genome Initiative (MGI) launched in 2011

Executive Summary

Vision: *Advanced materials are essential to economic security and human well-being and have applications in multiple industries, including those aimed at addressing challenges in clean energy, national security, and human welfare. To meet these challenges, the Materials Genome Initiative will enable discovery, development, manufacturing, and deployment of advanced materials at least twice as fast as possible today, at a fraction of the cost.*

https://www.mgi.gov/sites/default/files/documents/mgi_strategic_plan_-_dec_2014.pdf

Materials Genome Initiative (MGI) launched in 2011

Achieving this vision requires successfully addressing four key challenges:

(1) Leading a culture shift in materials research to encourage and facilitate an integrated team approach that links computation, data, and experiment and crosses boundaries between academia, National and Federal laboratories, and industry;

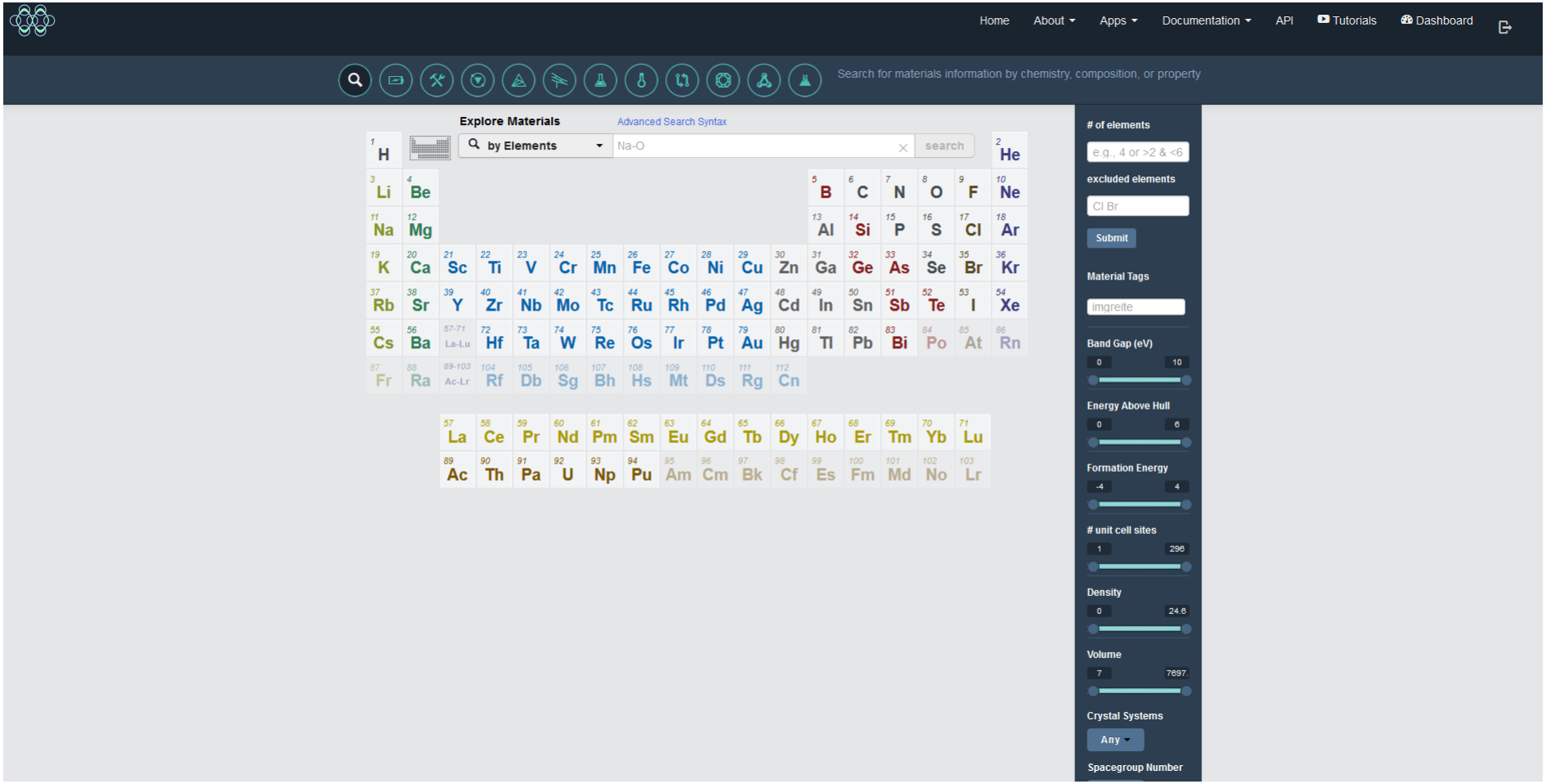
(2) Integrating experiment, computation, and theory and equipping the materials community with the advanced tools and techniques to work across materials classes and along the materials development continuum from research to industrial application; = MC II

(3) Making digital data accessible in = www.materialsproject.org, www.oqmd.org, to a searchable materials data infrast www.aflowlib.org, www.nomad-coe.eu… able to others;

= you!

(4) Creating a world-class materials workforce that is trained for careers in academia or industry, including high-tech manufacturing jobs.

https://www.mgi.gov/sites/default/files/documents/mgi_strategic_plan_-_dec_2014.pdf



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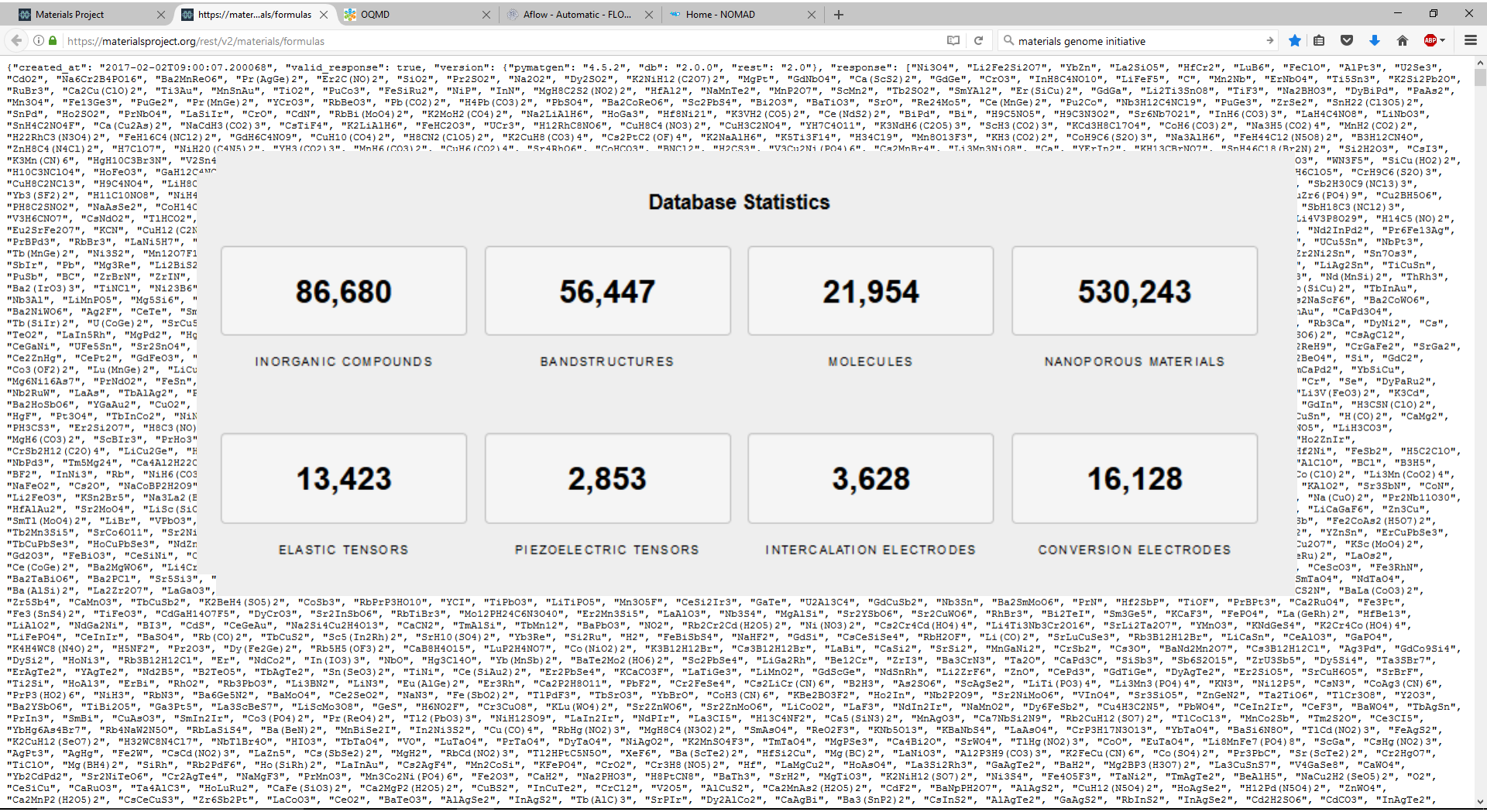


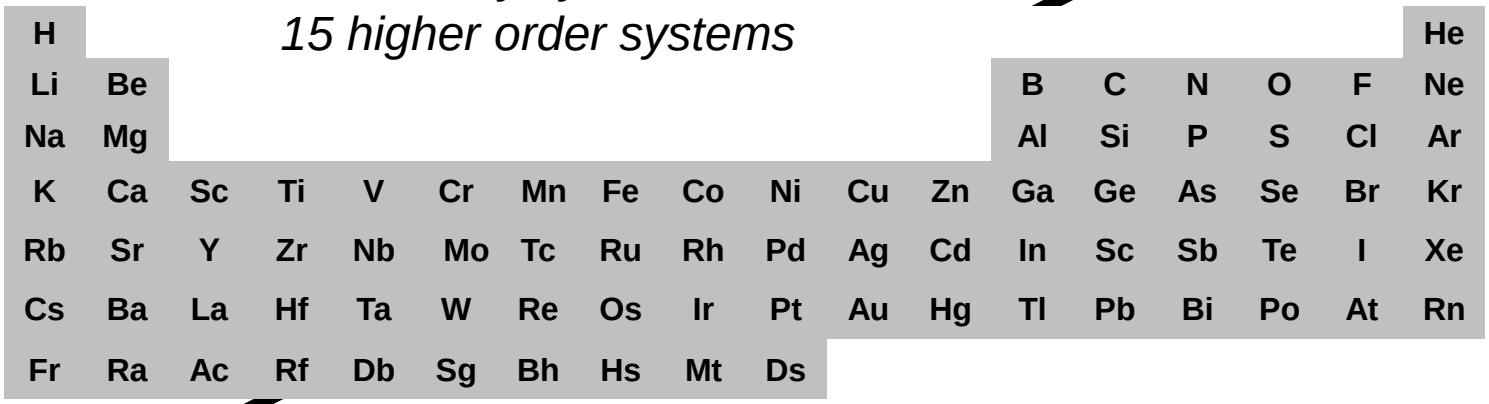
https://materialsproject.org/rest/v2/materials/formulas

History of computational thermodynamics and thermodynamic databases

$G(T,X_i)$

Today: SGTE Solution database contains 79 elements, 317 solution phases, 1166 stoichiometric phases

Allows description of
577 binary systems,
141 ternary systems,
15 higher order systems



~70 non-radioctive, non-noble gas elements

→ *70*69 = 4830 binary systems*

→ *70*69*68 = 328440 ternary systems*

Materials Project | https://mater...als/formulas | OQMD | Aflow - Automatic - FLO... | Home - NOMAD

https://materialsproject.org/rest/v2/materials/formulas

materials genome initiative

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"Mn3O4", "Fe13Ge3", "PuGe2", "Pr(MnGe)2", "YCrO3", "RbBeO3", "Pb(CO2)2", "H4Pb(CO3)2", "PbSO4", "Ba2CoReO6", "Sc2PbS4", "Bi2O3", "BaTiO3", "SrO", "Re24Mo5", "Ce(MnGe)2", "Pu2Co", "Nb3H12C4NC19", "PuGe3", "ZrSe2", "SnH22(ClSO5)2",
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"SnH4C2NO4F", "Ca(Cu2As)2", "NaCdH3(CO2)3", "CsTiF4", "K2LiAlH6", "FeHC2O3", "UCr3", "H12RhC8NO6", "CuH8C4(NO3)2", "CuH3C2NO4", "YH7C4O11", "K3NdH6(C2O5)3", "ScH3(CO2)3", "KCd3H8C17O4", "CoH6(CO3)2", "Na3H5(CO2)4", "MnH2(CO2)2",
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"CuH8C2NCl3", "H9C4NO4", "LiH8C", "Sb2H30C9(NCl3)3",
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G(0 K)

Database Statistics

86,680	56,447	21,954	530,243
INORGANIC COMPOUNDS	BANDSTRUCTURES	MOLECULES	NANOPOROUS MATERIALS

13,423	2,853	3,628	16,128
ELASTIC TENSORS	PIEZOELECTRIC TENSORS	INTERCALATION ELECTRODES	CONVERSION ELECTRODES

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Programme | Desktop | DEU | 18:00 | 02.02.2017

https://materialsproject.org/rest/v2/materials/formulas

OQMD:

The Open Quantum Materials Database

Home Materials Analysis Documentation Download

Newsflash: OQMD v1.1 is out! (Download it here.)

Welcome to the Open Quantum Materials Database

The OQMD is a database of DFT-calculated thermodynamic and structural properties. This online interface is for convenient, small-scale access; for a more powerful utilization of the data, we recommend downloading the entire database and the API for interfacing with it, from the link below.

Current status

OQMD v1.1 has been released! Download it here.
The database now contains 563247 entries. In addition, calculations of new structures are constantly ongoing!
Recently added compounds include: EuPaBe PrPaFe PaReHg AcLaPa KPaMo

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You can...

Search for materials by composition,
Create phase diagrams using the thermochemical data in OQMD,
Determine ground state compounds at any composition,
Visualize crystal structures, or
Download the entire database (and the API) for your own use!

Tweet @TheOQMD to ask what is stable at a composition, or to get a simple phase diagram!

The OQMD was created in Chris Wolverton's group at Northwestern University.

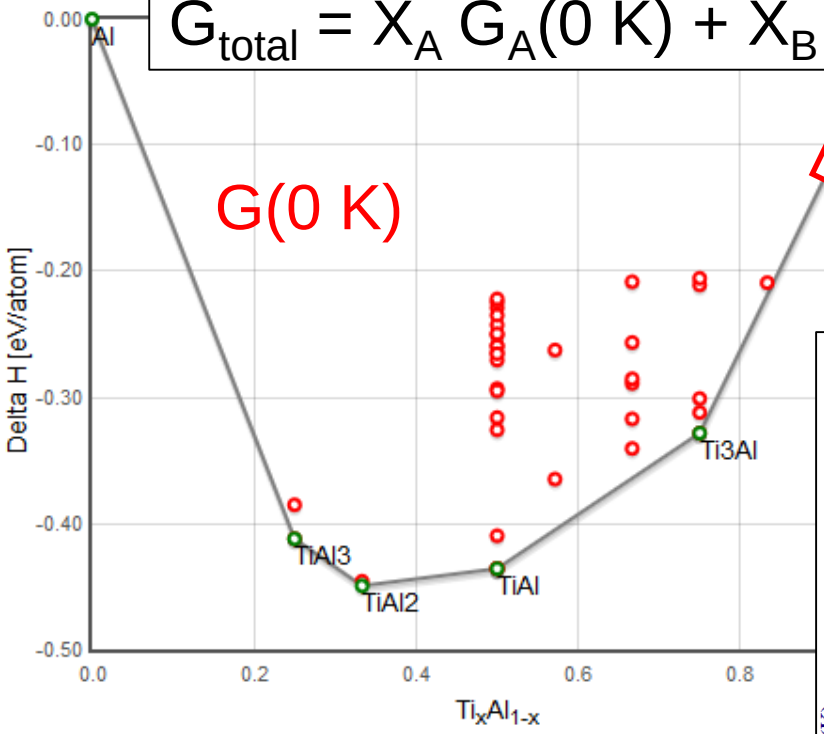
Contact us by e-mail

If you are using any results from this website, please reference this work as shown here

http://oqmd.org/

Phase diagram creation

$$G_{total} = X_A G_A(0\ K) + X_B G_B(0\ K)$$



$C_p(T)$, $G(T,X_i)$

$- T\Delta S_{mix}$ $+ \Delta H_{mix}$ $+ \Delta G_{excess}$

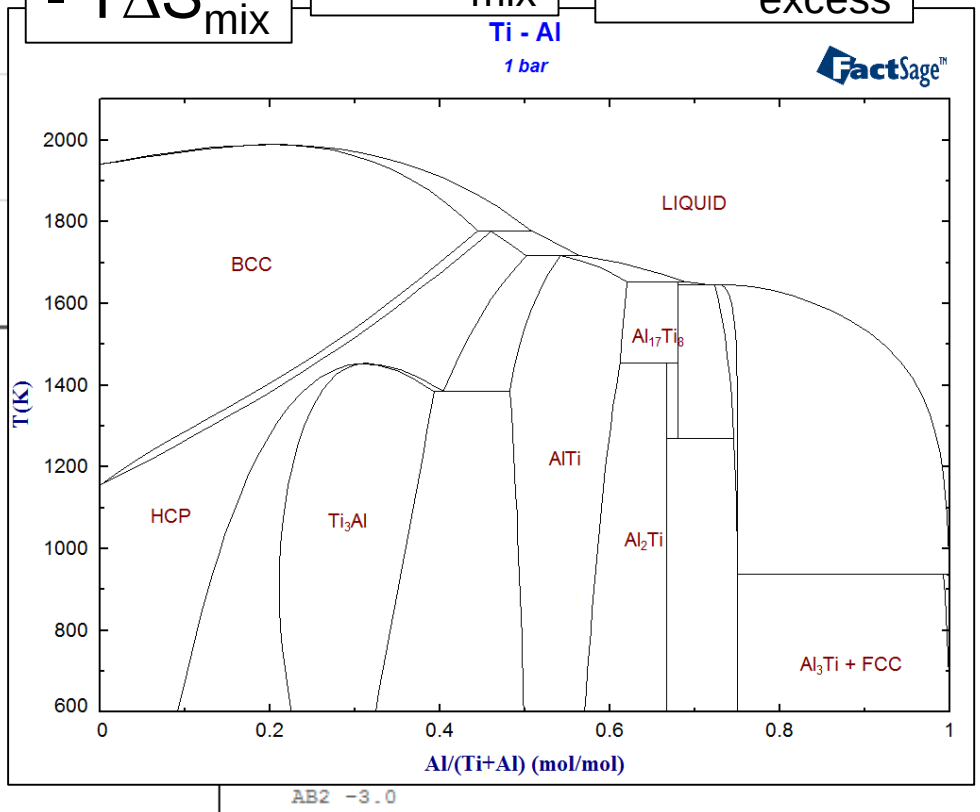
Specify a region of phase space:

mples:

Fe-O

Li-H-O

Li2O-Fe2O3



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Enter a Compound Name, ICSD Number, Aflowlib Unique IDentifier or advanced search string (ie. Mg & Sn & Cu).

ICSD#, AUID#, element combos...

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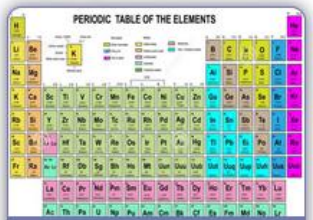
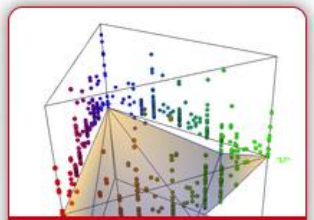
Advanced search

Apps and Docs



MendeLIB search



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Dysprosium-doped cadmium oxide as a gateway material for mid-infrared plasmonics

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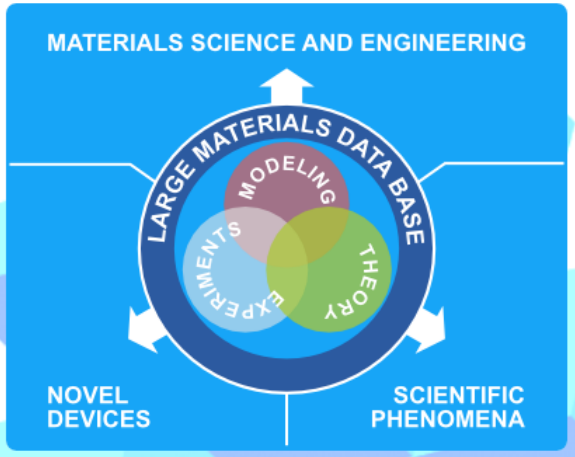
The Novel Materials Discovery (NOMAD) Laboratory develops a *Materials Encyclopedia* and *Big-Data Analytics* and *Advanced Graphics Tools* for materials science and engineering.

Eight complementary computational materials science groups and four high-performance computing centers form the synergetic core of this Centre of Excellence.



Latest News

Feb 2, 2017
NOMAD Summer School

Jan 27, 2017
New Tools Developed at NOMAD Hackathon

Jan 26, 2017
Presentation on NOMAD Visualizations at Technical University of Luleå

Jan 12, 2017
NOMAD presented at Tianjin University

Jan 3, 2017
NOMAD Hackathon, 18 - 20 Jan 2017

MATERIALS ENCYCLOPEDIA | BIG-DATA ANALYTICS | ADVANCED GRAPHICS | HPC INFRASTRUCTURE | OUTREACH

H2020 NOMAD
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https://www.nomad-coe.eu/

Application: (Ti,Al)N coatings for cutting tools

You are interested to learn something about thermodynamics of your material system during BSc/MSc/PhD thesis / at work: What do you do?

CHECK PHASE DIAGRAMS/MATERIALS DATA E.G. AT

www.springermaterials.com **www.factsage.com**
www.materialsproject.org **www.oqmd.org**
www.aflowlib.org **www.nomad-coe.eu**

...

History of computational thermodynamics and thermodynamic databases

Debate on phase stability of compounds based on experimental and *ab initio* methods

10/2017: first purely ab initio based thermodynamic database

Today: SGTE Solution database contains 79 elements,
317 solution phases, 1166 stoichiometric phases

1980s-1990s: Founding of several companies
specializing in computational thermodynamics

Debate on phase stability of
elements in non-stable state

EXCITING YEARS TO COME!!!
WILL WE SEE THE THERMODYNAMIC MATERIALS GENOME?

…3: growth
…ion databases

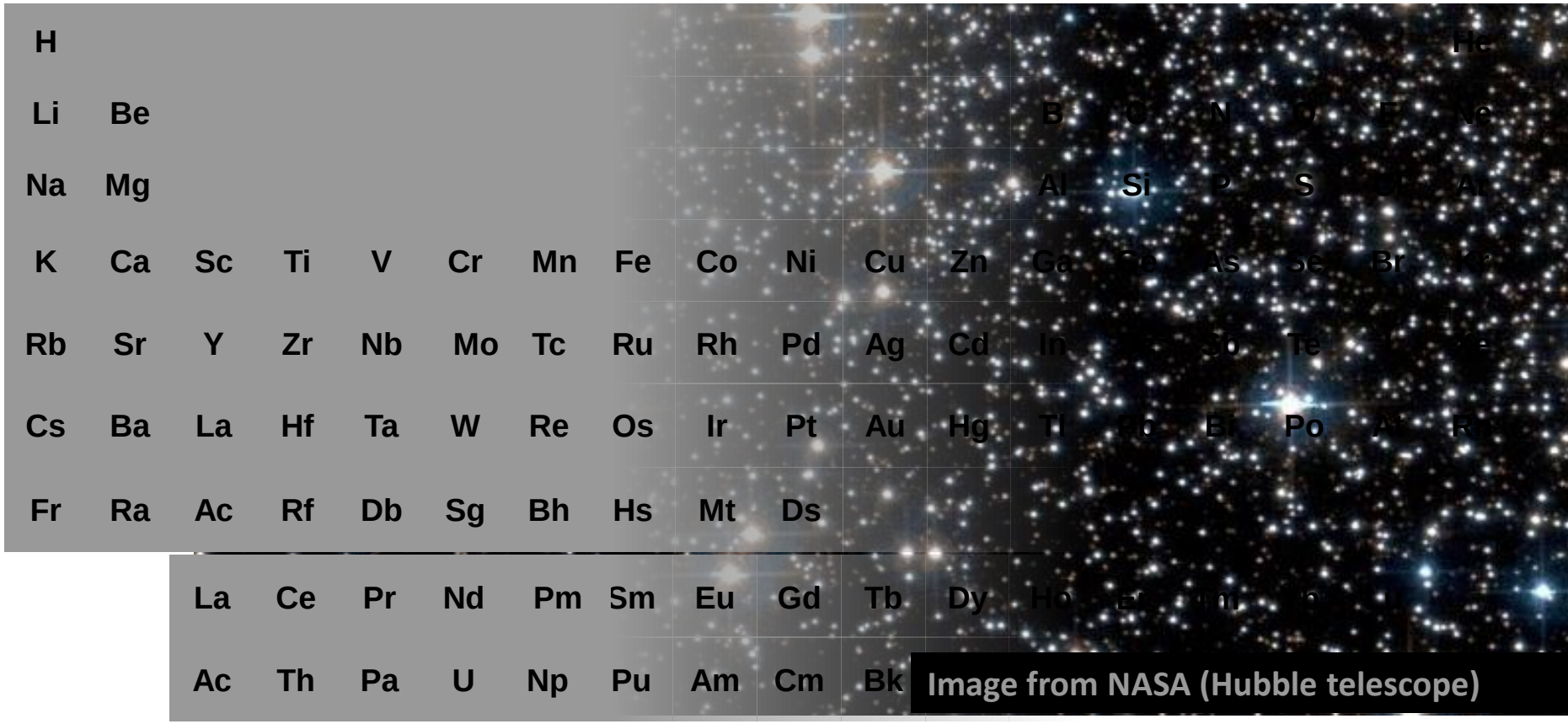
…e, *SGTE Data for pure elements*

JANAF *Thermochemical Tables*

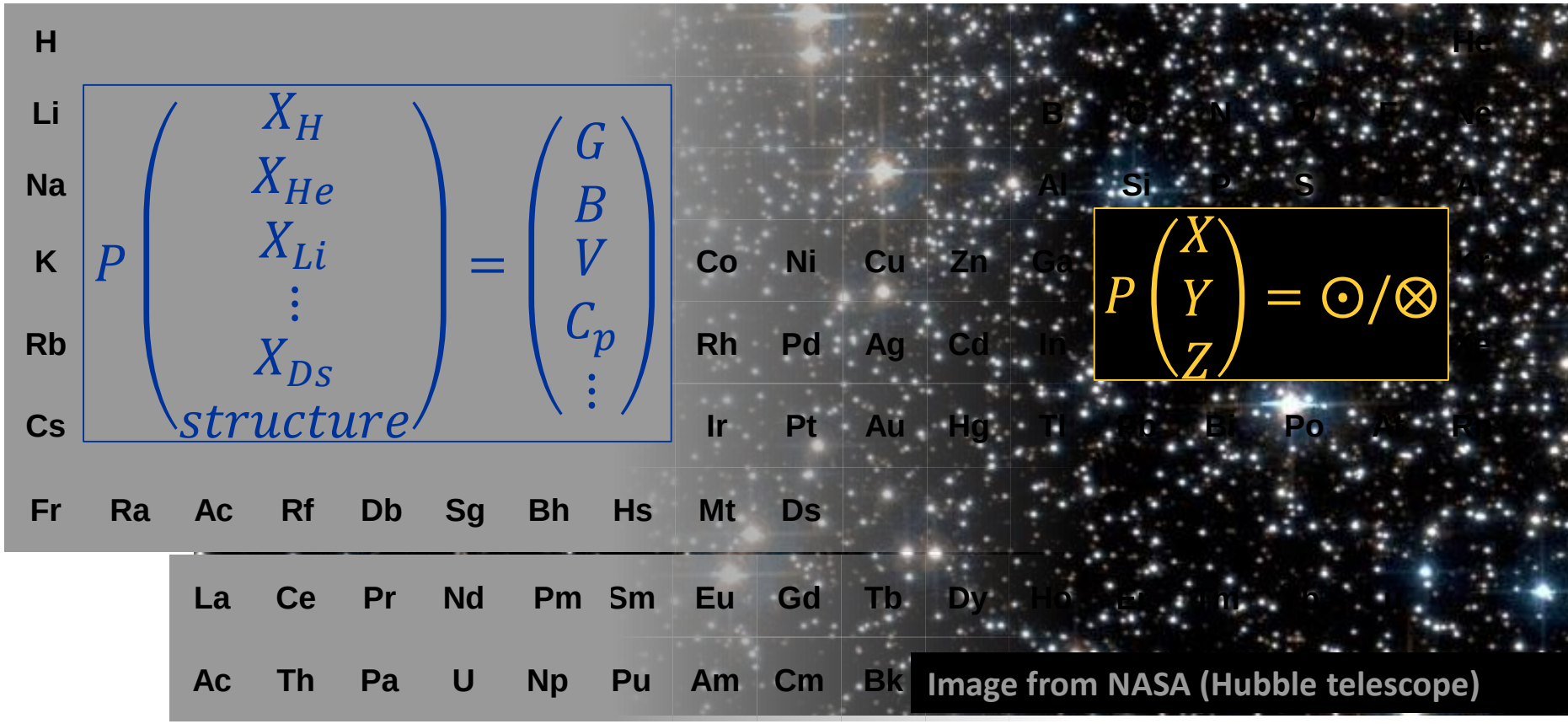
…, Knacke, Kubaschewski *Thermochemical Properties*

1957 First ternary phase diagram calculation (Ni-Cr-Cu)

Vision: Map of Chemical Space

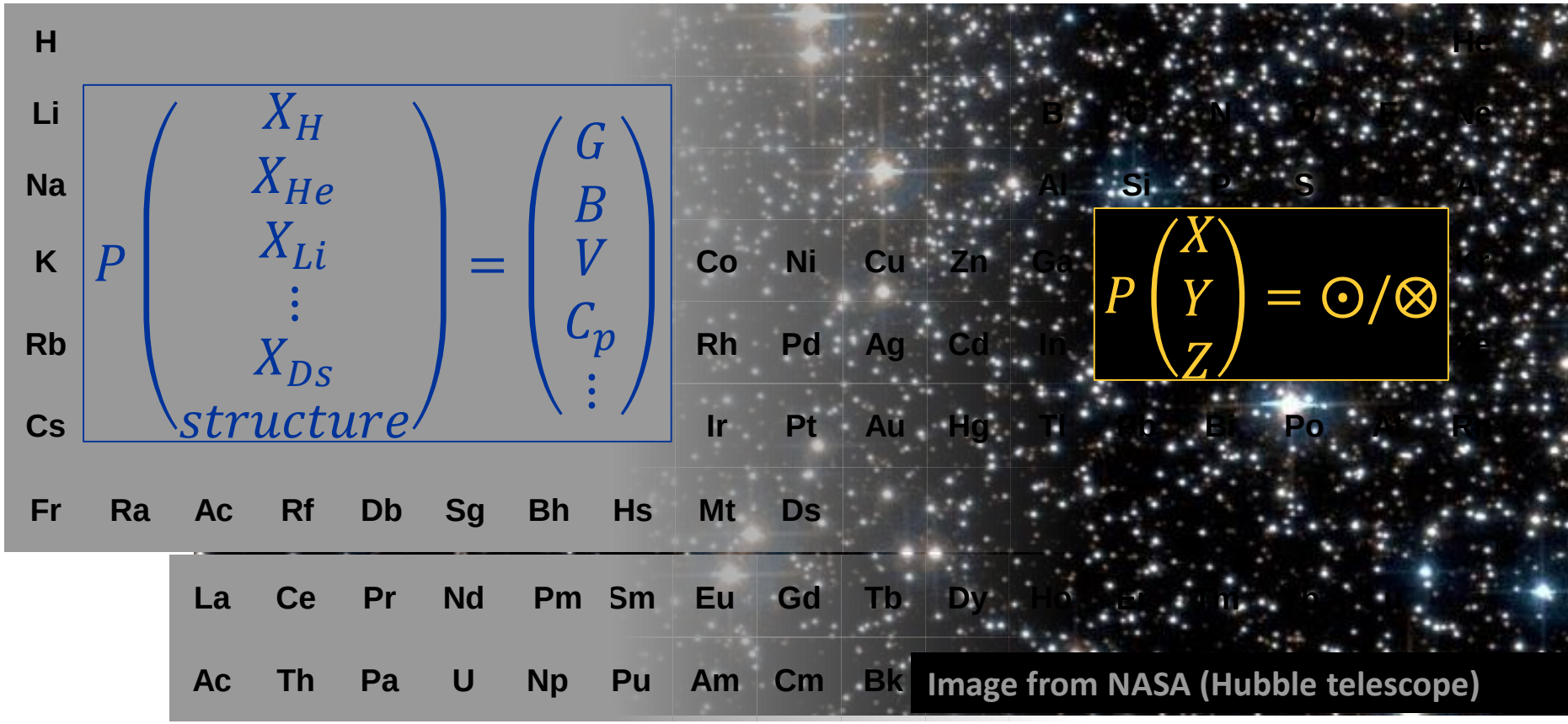


Vision: Map of Chemical Space



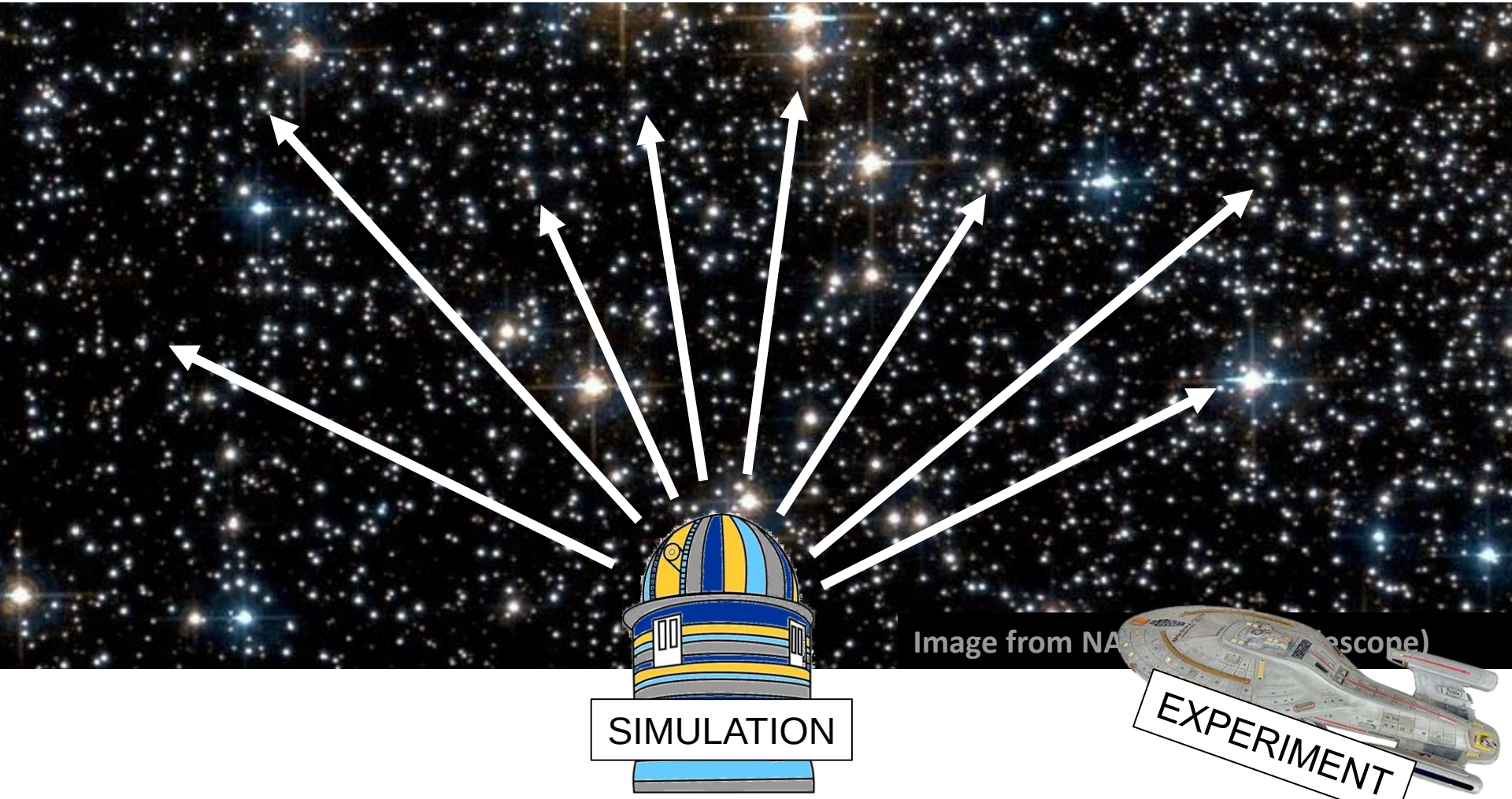
Vision: Map of Chemical Space

How do you navigate?



Vision: Map of Chemical Space

→ MATERIALS INFORMATICS



Thank you for your attention!