

3-D Representation of Phase Diagrams and other Property Diagrams for Multi-component Systems

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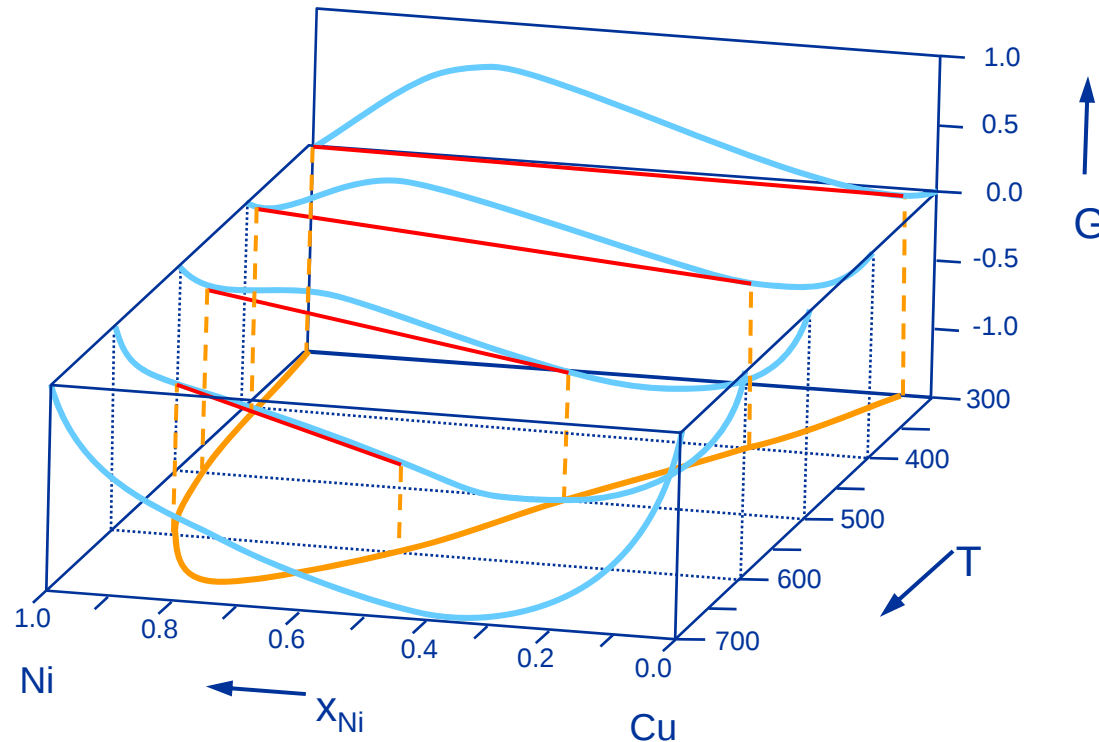


Where will 3-D representation help?

- From Gibbs energy to phase diagram
- Thermodynamic properties in ternaries, e.g. isothermal activities
- Liquidus projections
- Quaternary phase diagrams

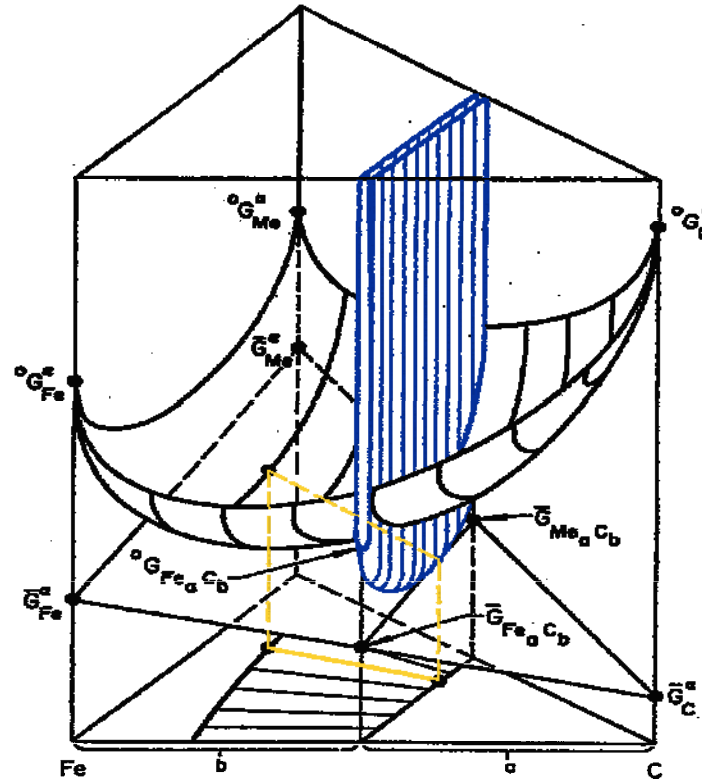


Phase diagrams as projections from Gibbs Energy plots



Binary system: projection in G-T-x diagram, $p = \text{const.}$

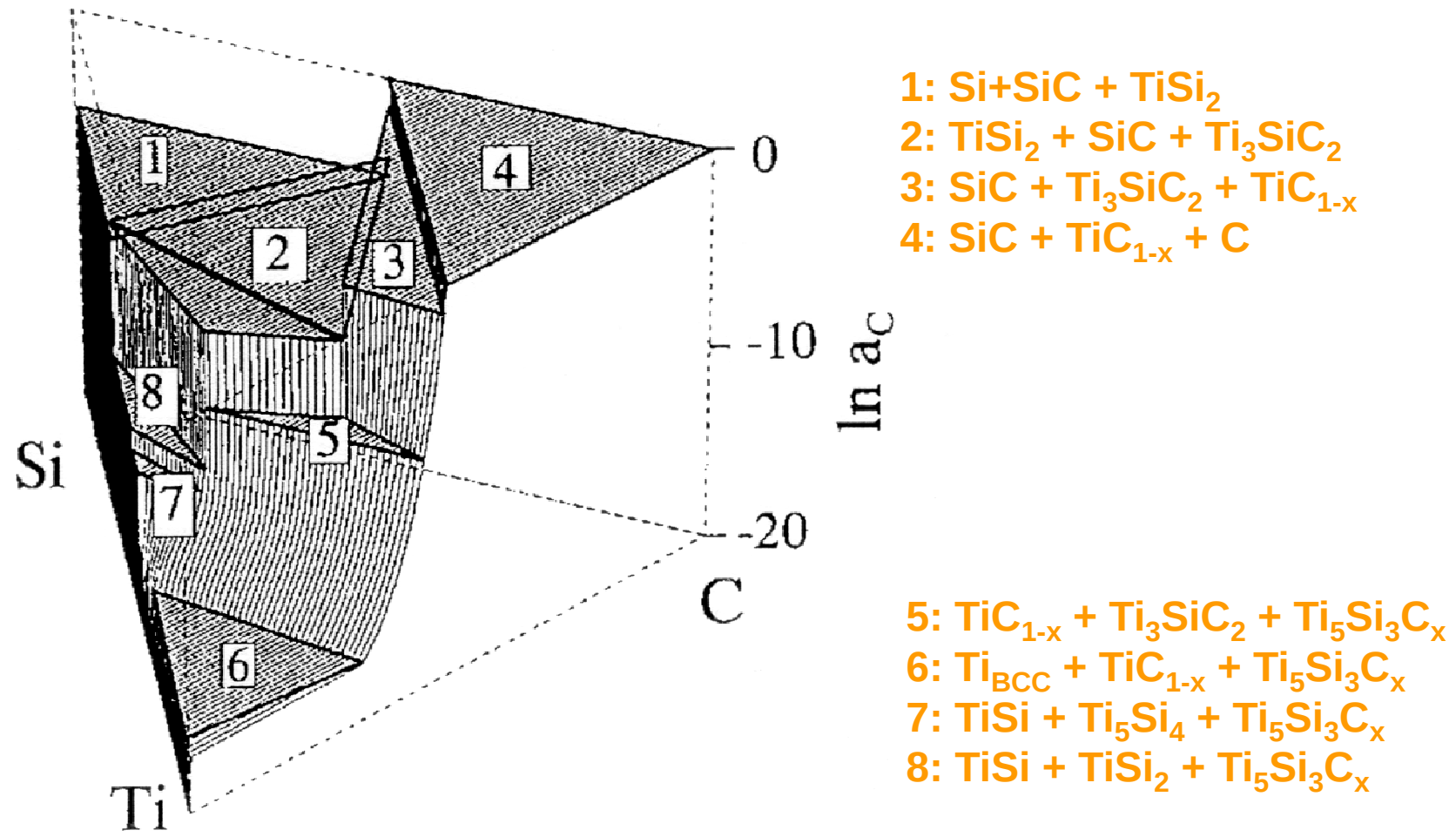
Phase diagrams as projections from Gibbs energy plots



Ternary system: projection in G - x_1 - x_2 diagram,
 $T = \text{const}$ and $p = \text{const}$

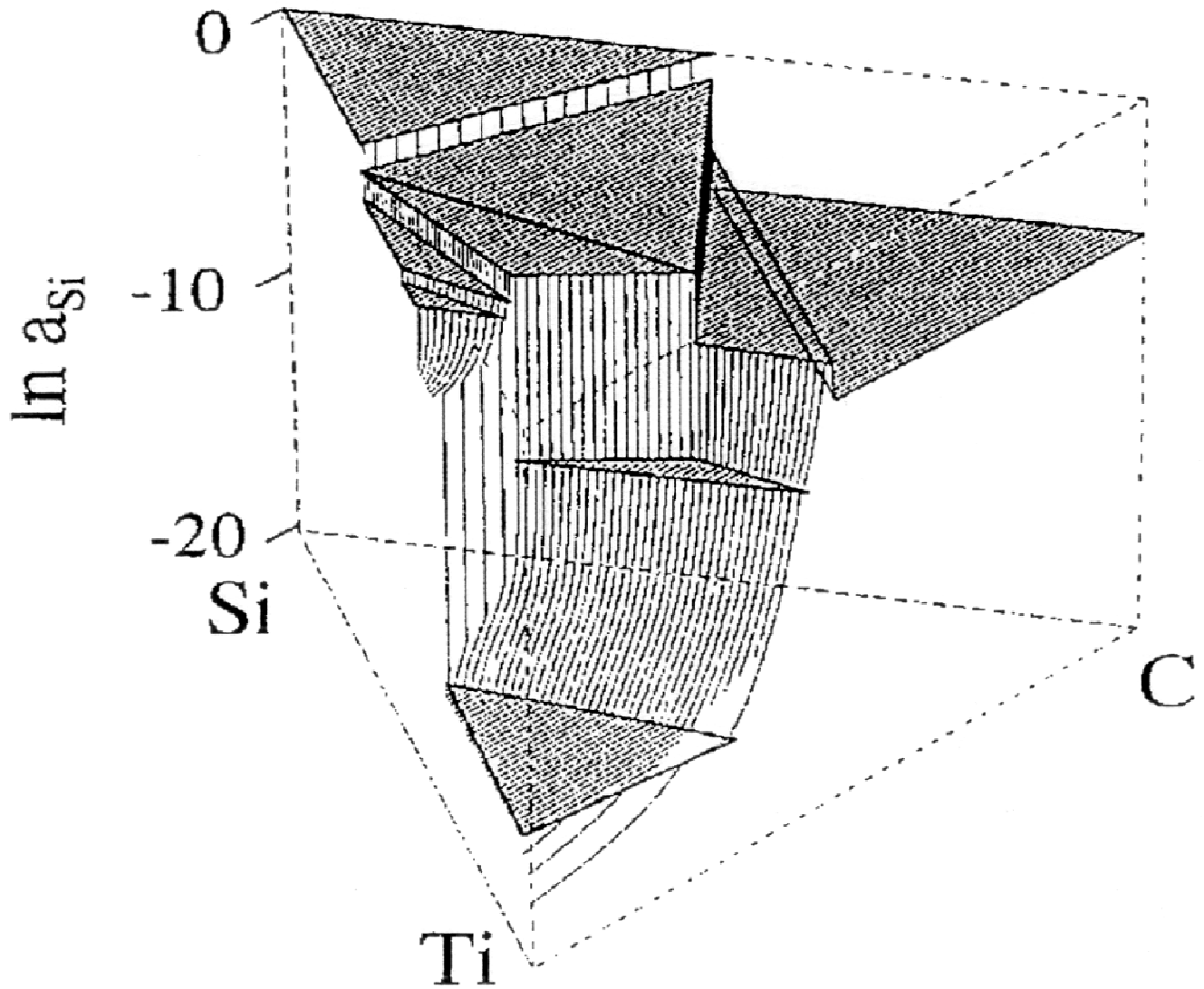
Perspective Representation of Isothermal Activity Plots for the System Ti-Si-C





Carbon activity in system Ti-Si-C
for $T = 1200^\circ \text{C}$





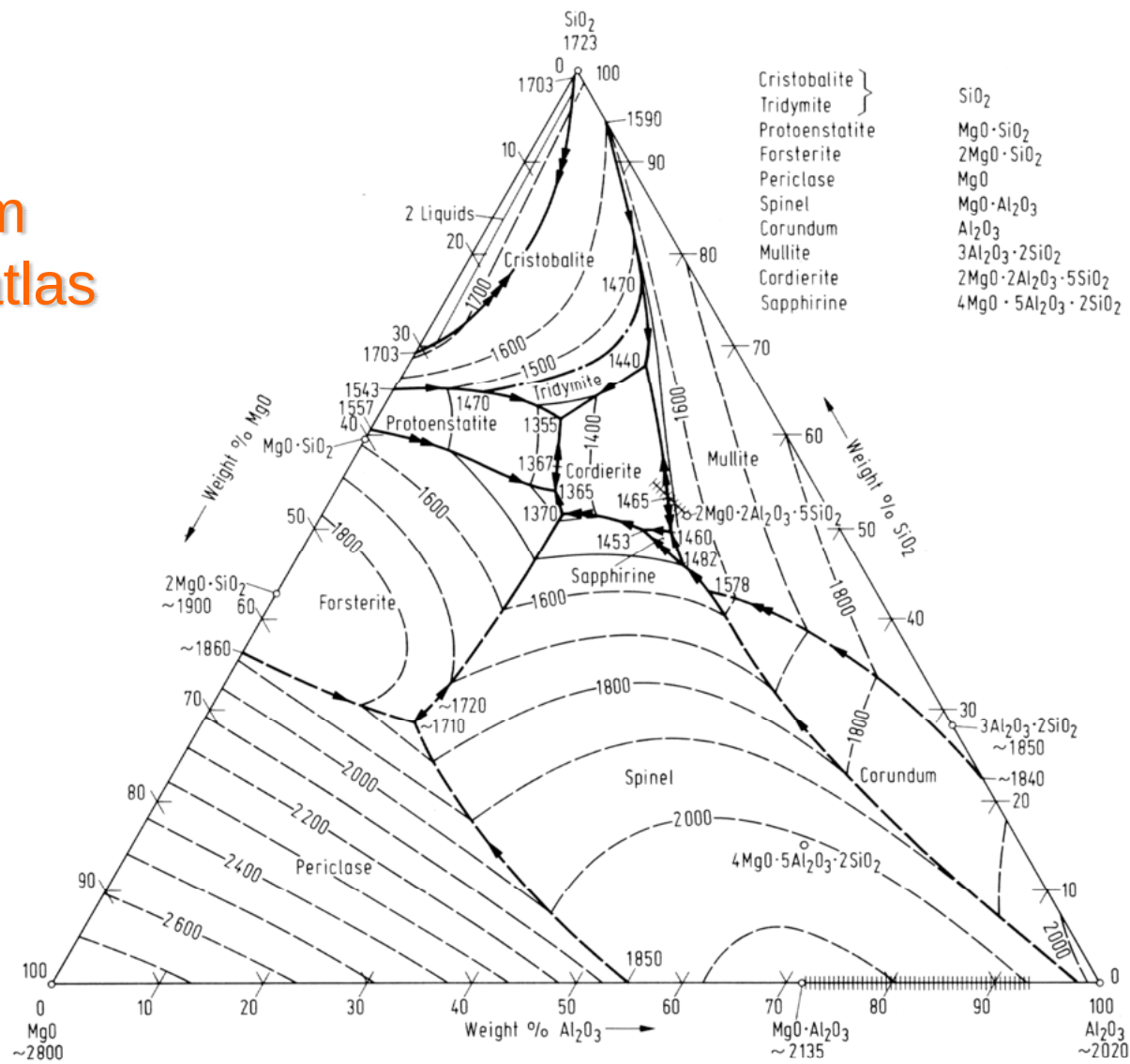
Silicon activity in system Ti-Si-C for $T = 1200^\circ\text{C}$



Liquidus Projection for the System $\text{MgO-Al}_2\text{O}_3\text{-SiO}_2$



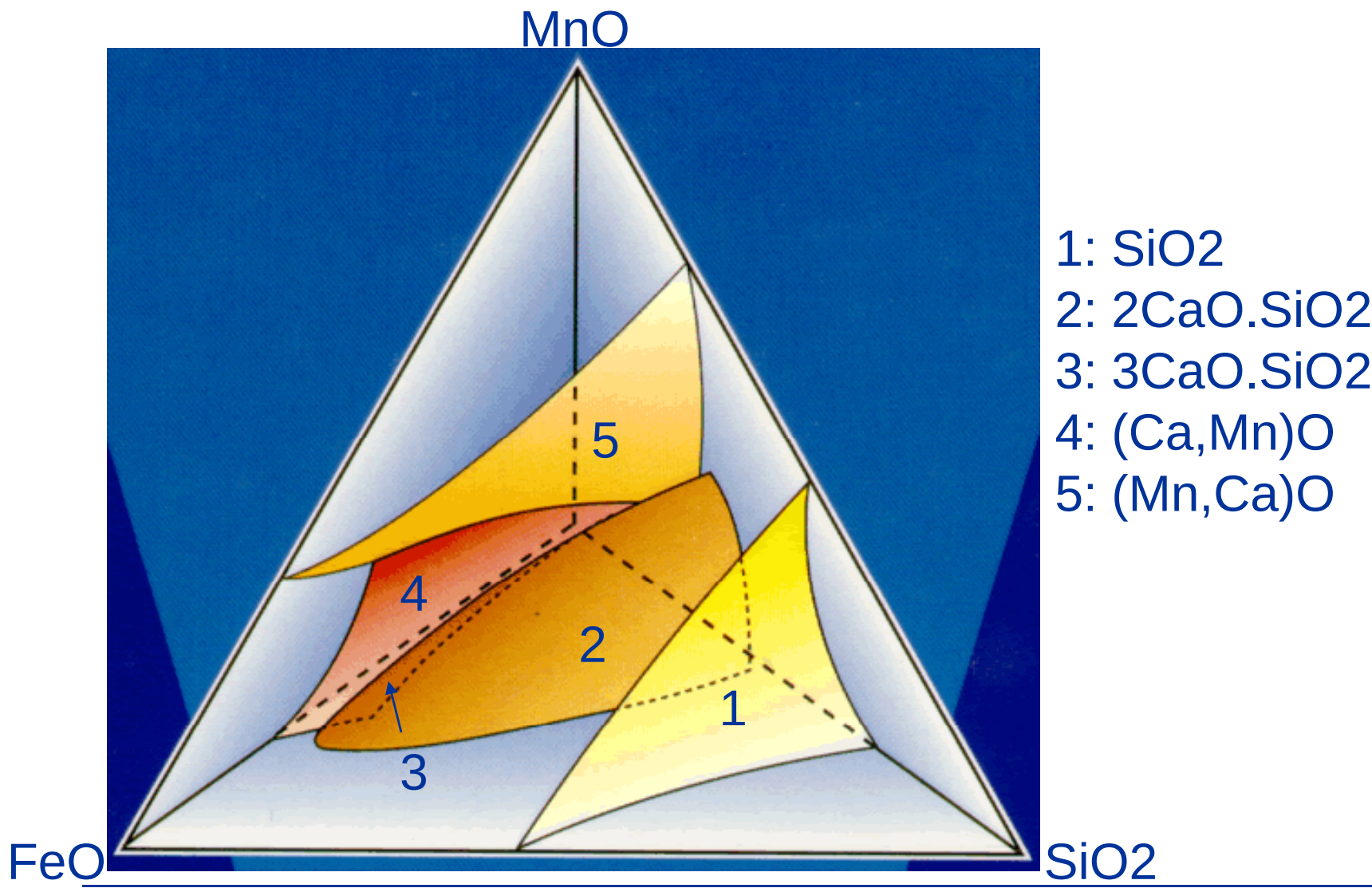
From
Slag atlas



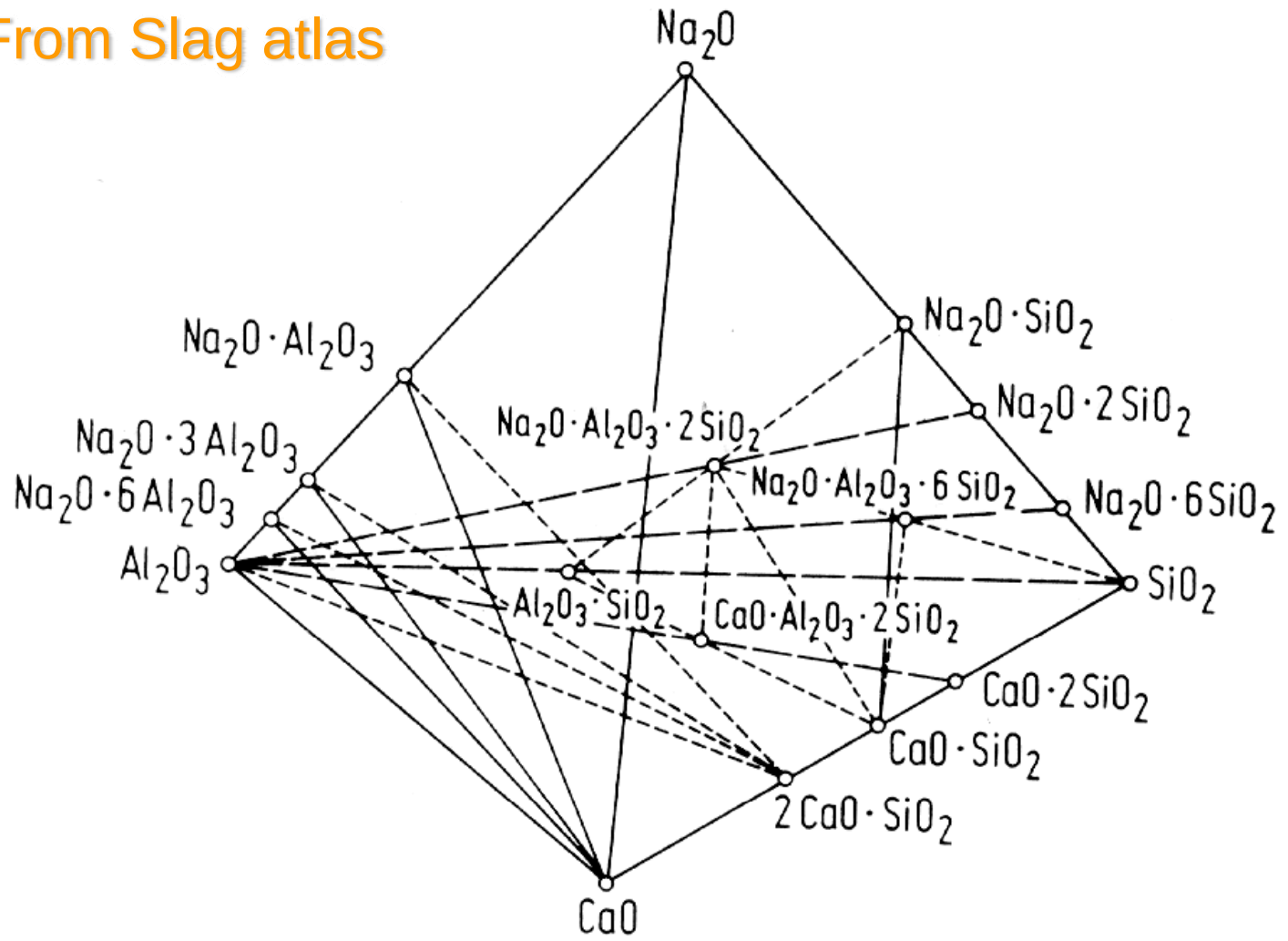
Quaternary Phase Diagrams



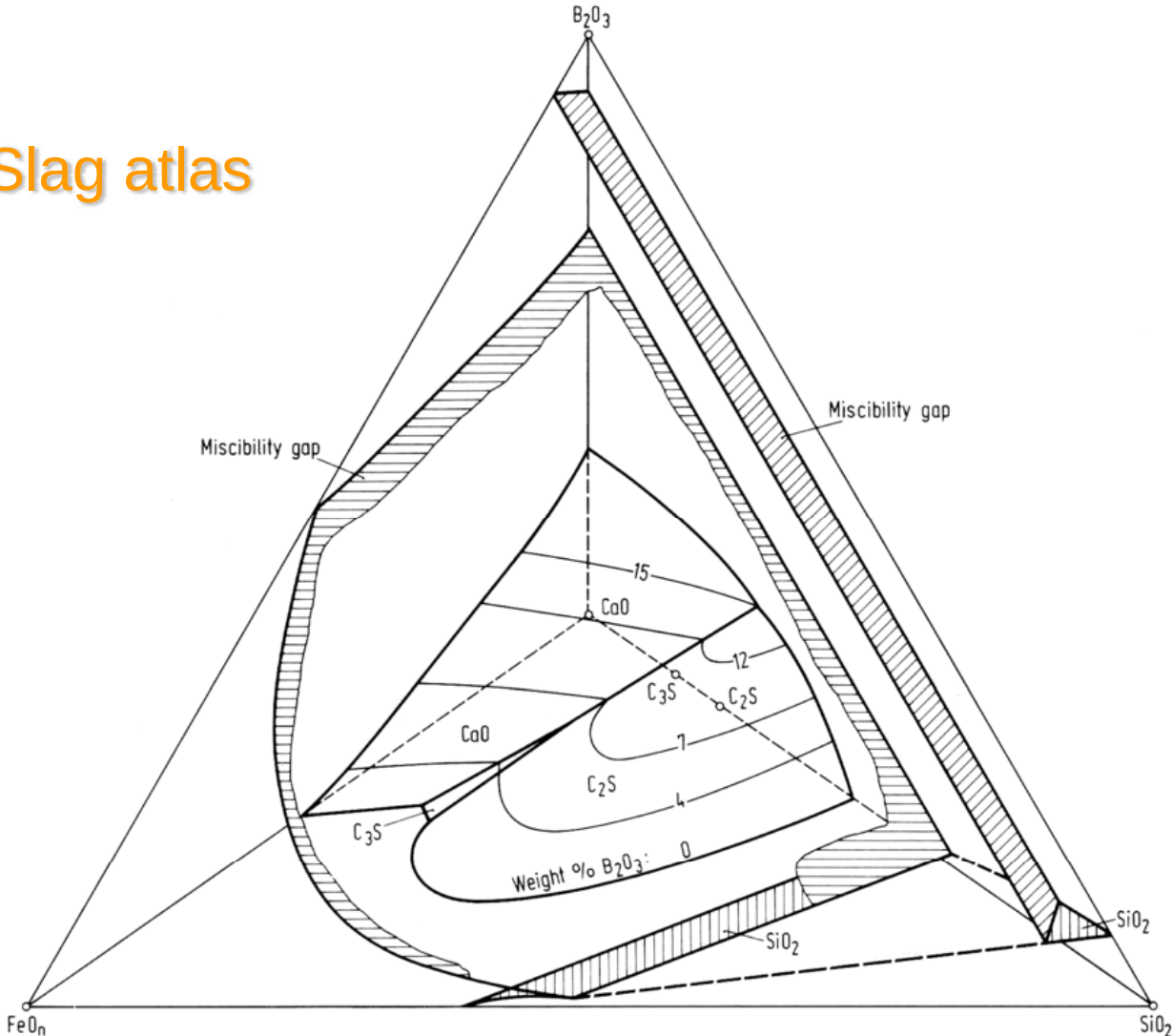
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From Slag atlas



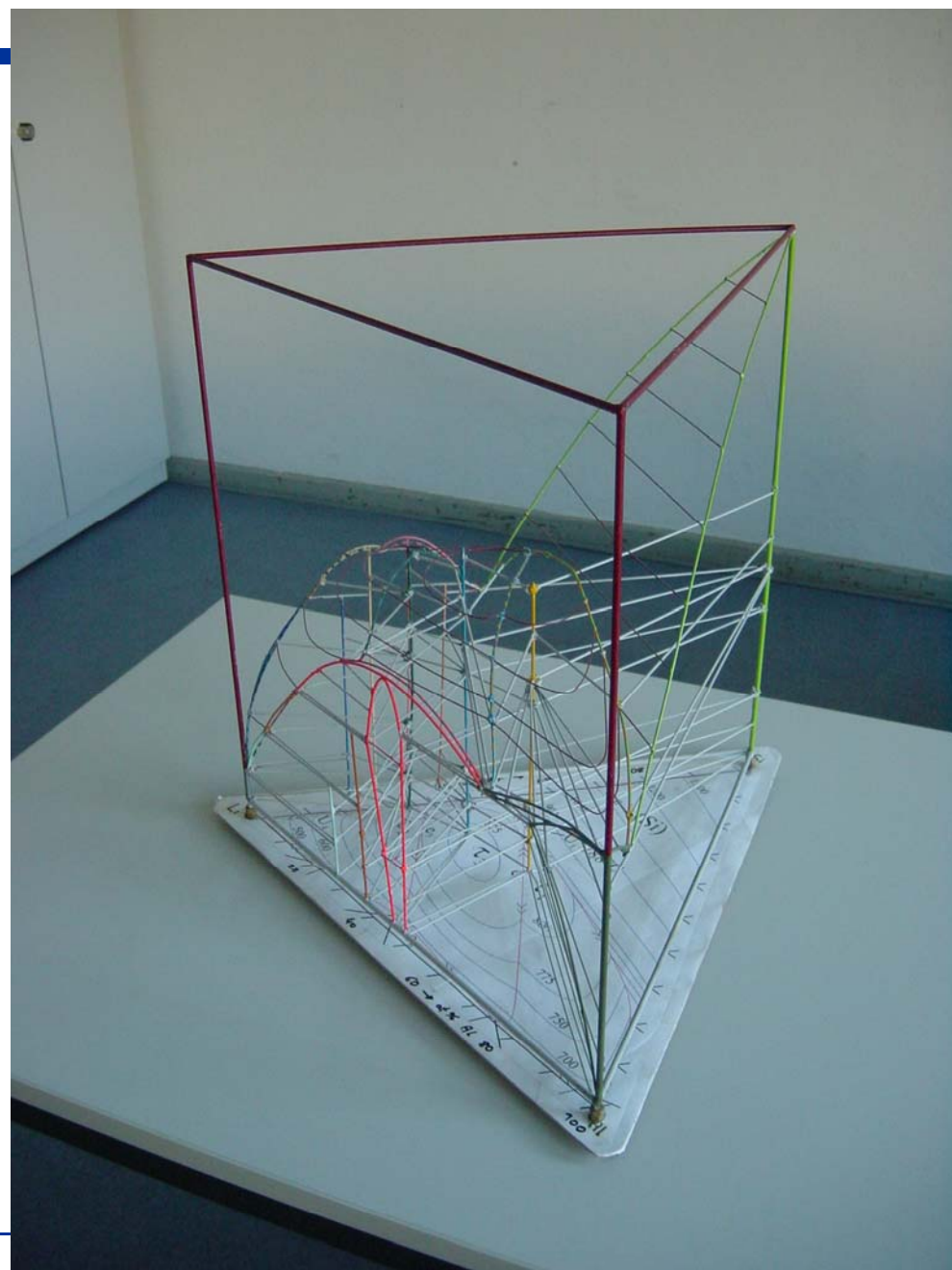
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Wire Models



Wire model for the system Al-Li-Si



(R.Schmid-Fetzer, TU-Clausthal)



Wire model for the system Co-Fe-Mo-Ni, T=1373K

Intermediate Summary

The routine 3D-visualisation of phase diagrams and also property diagrams would contribute considerably to the understanding of multi-dimensional relationships in material systems.



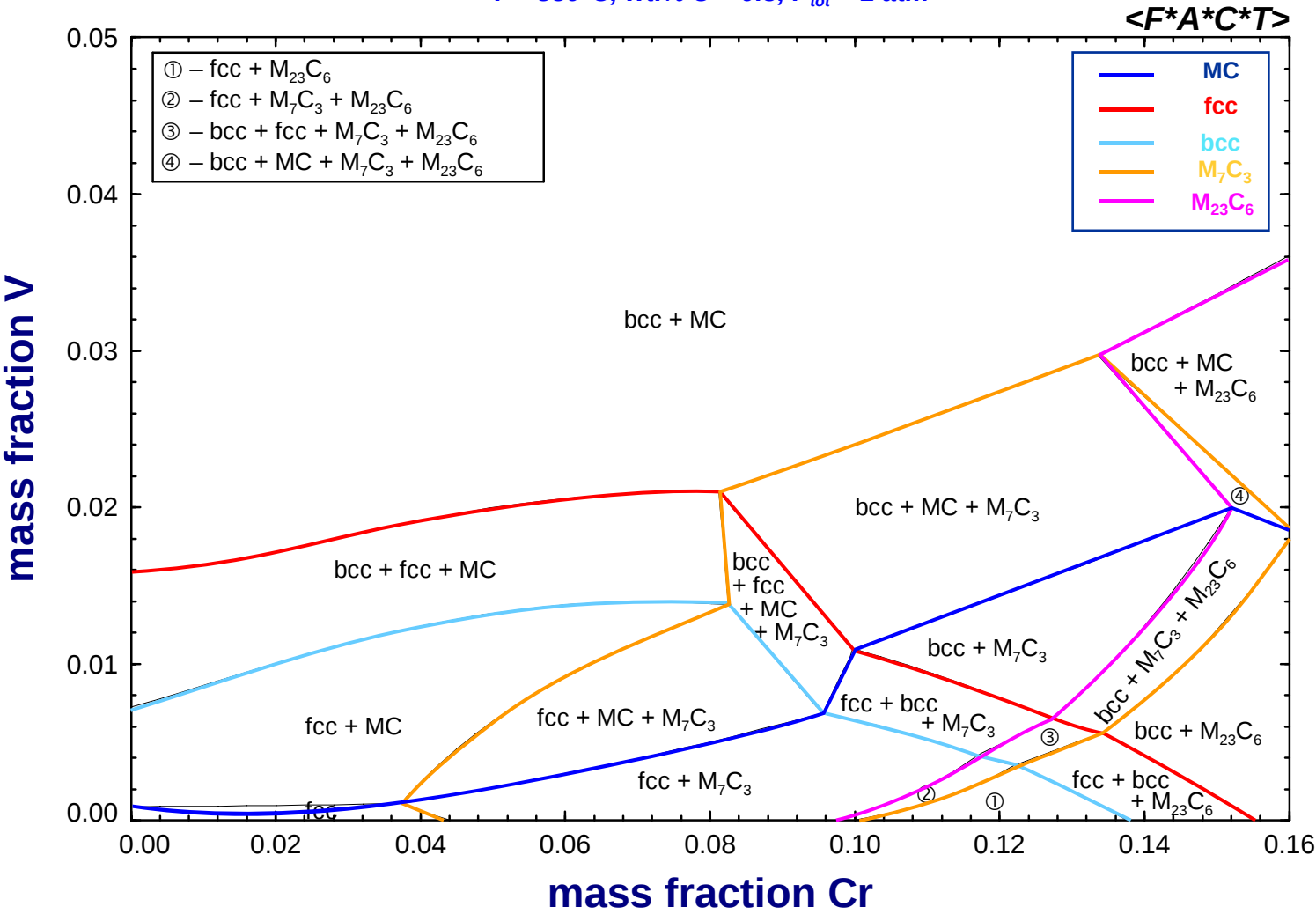
Results of thermochemical calculations Part 1

Isothermal isobaric isopleth sections



Fe - Cr - V - C System

$T = 850^{\circ}\text{C}$, $\text{wt.\% C} = 0.3$, $P_{\text{tot}} = 1 \text{ atm}$

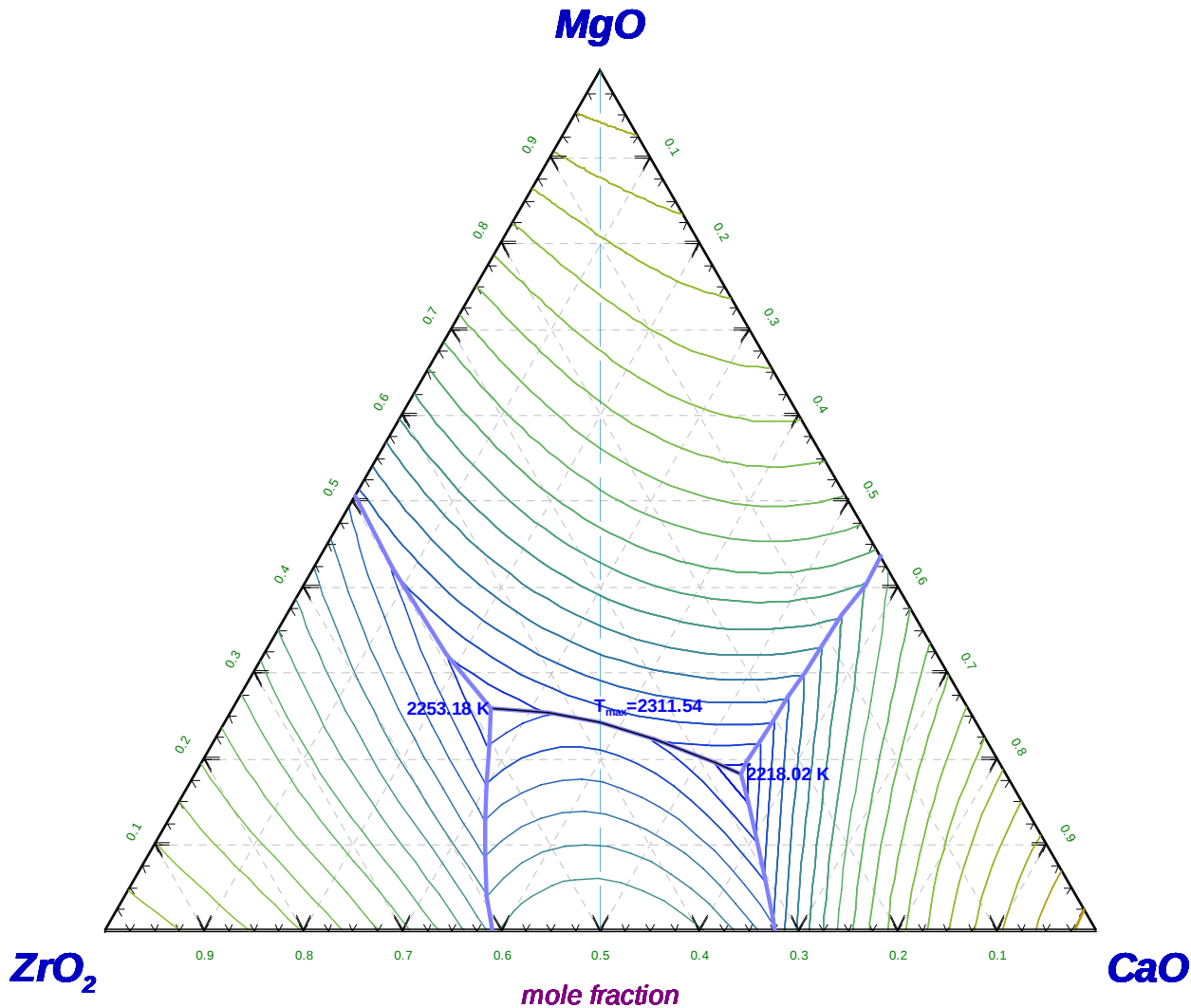


Results of thermochemical calculations Part 2

Liquidus projections



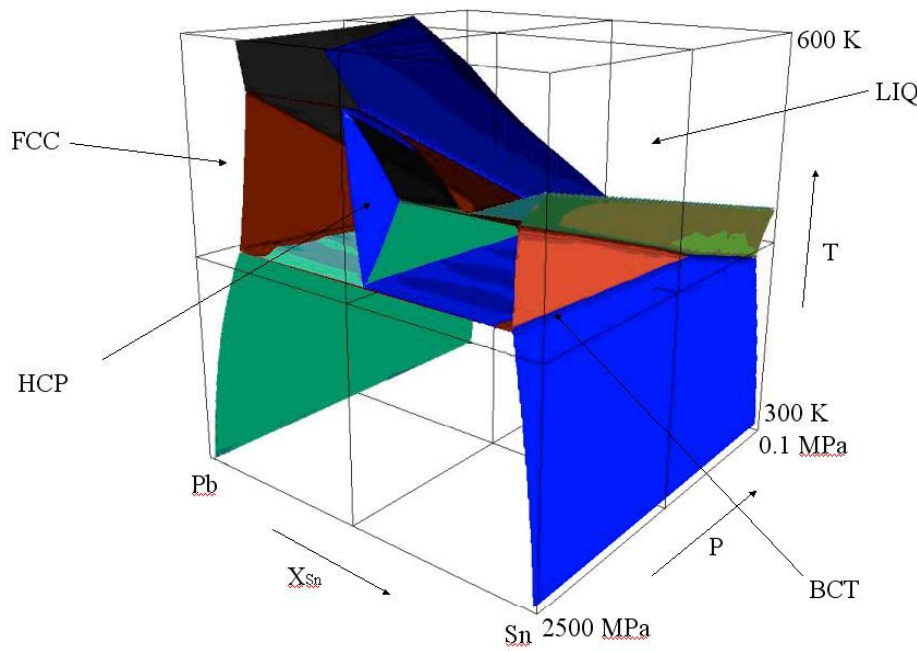
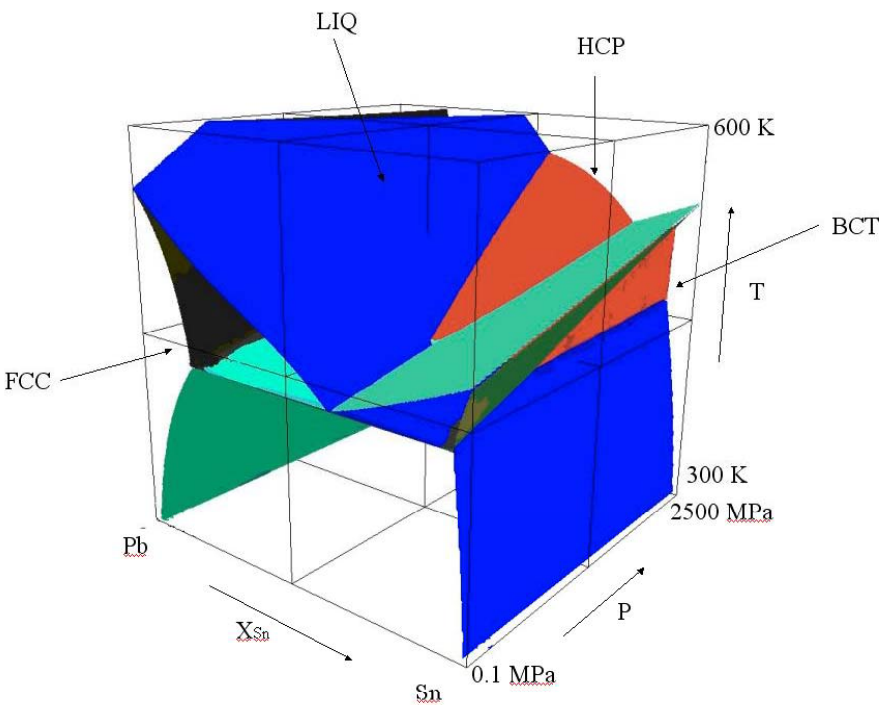
MgO - CaO - ZrO₂
Polythermal projection 2200 - 3500



Results thermochemical calculations Part 3

Binary composition-temperature-pressure
cube





The Pb-Sn T-P-x Phase Diagram
left: from low to high pressure
right: from high to low pressure



Results of thermochemical calculations

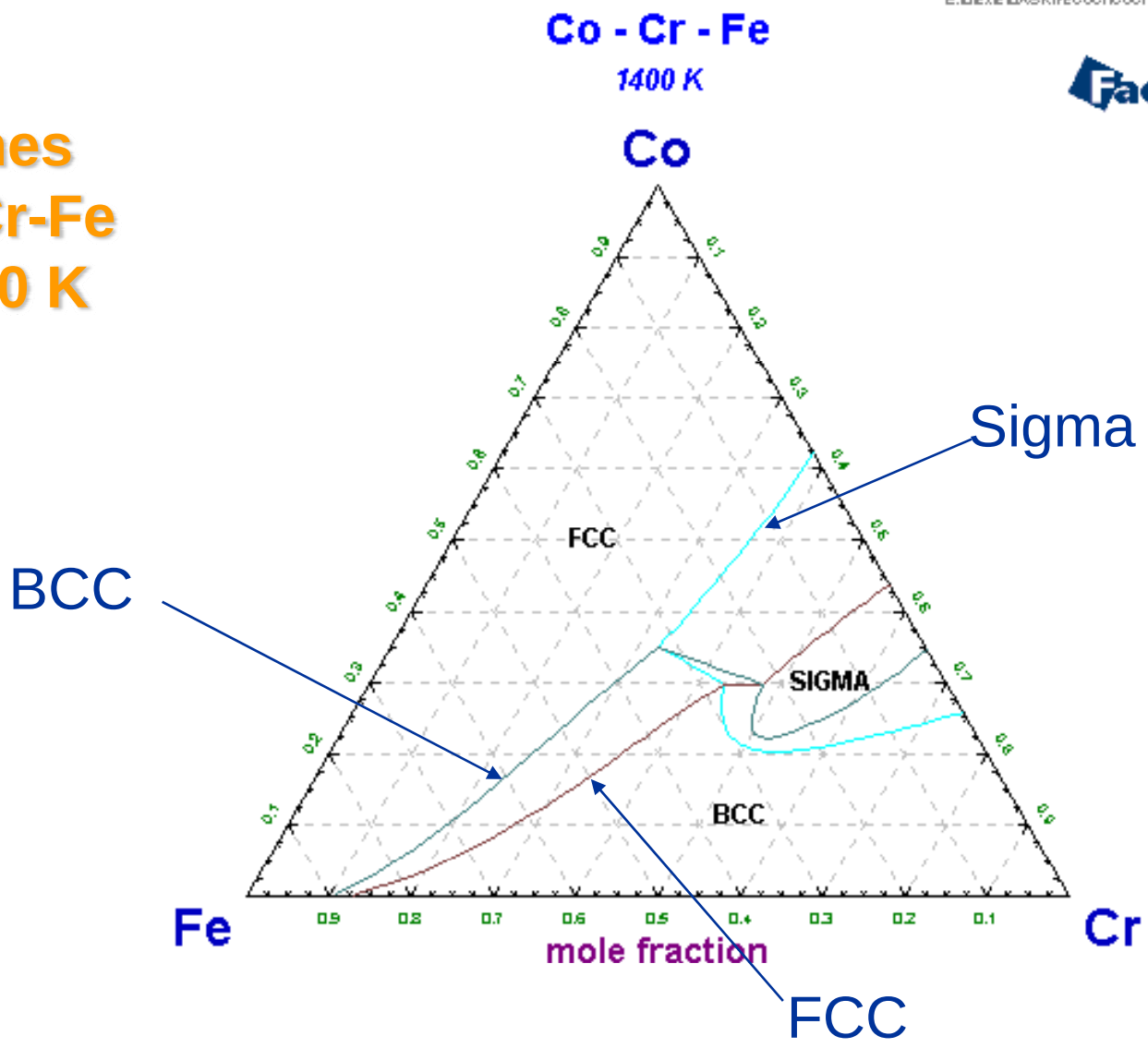
Part 4

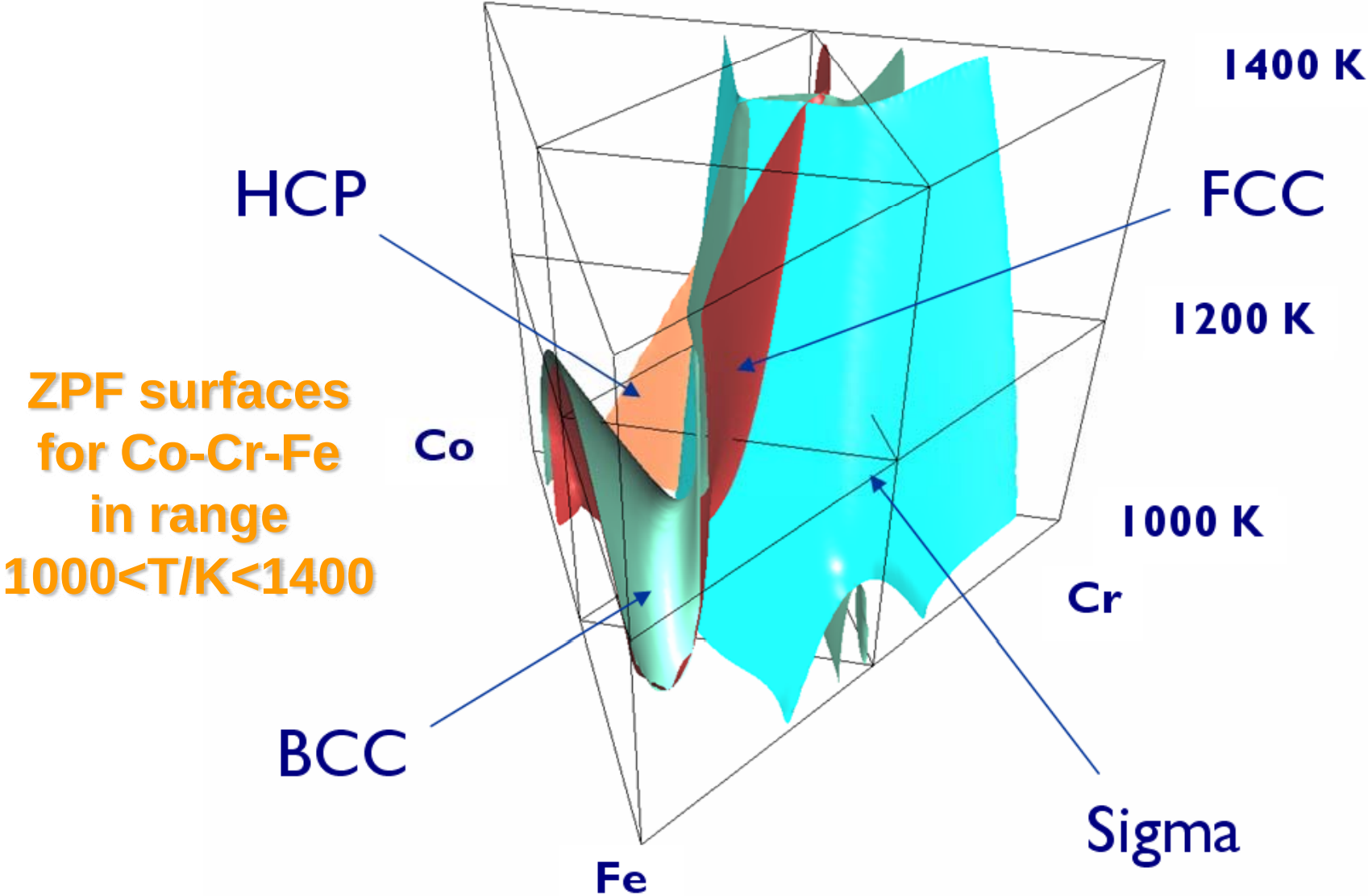
Ternary composition-temperature prism





ZPF lines
for Co-Cr-Fe
T = 1400 K





Results of thermochemical calculations

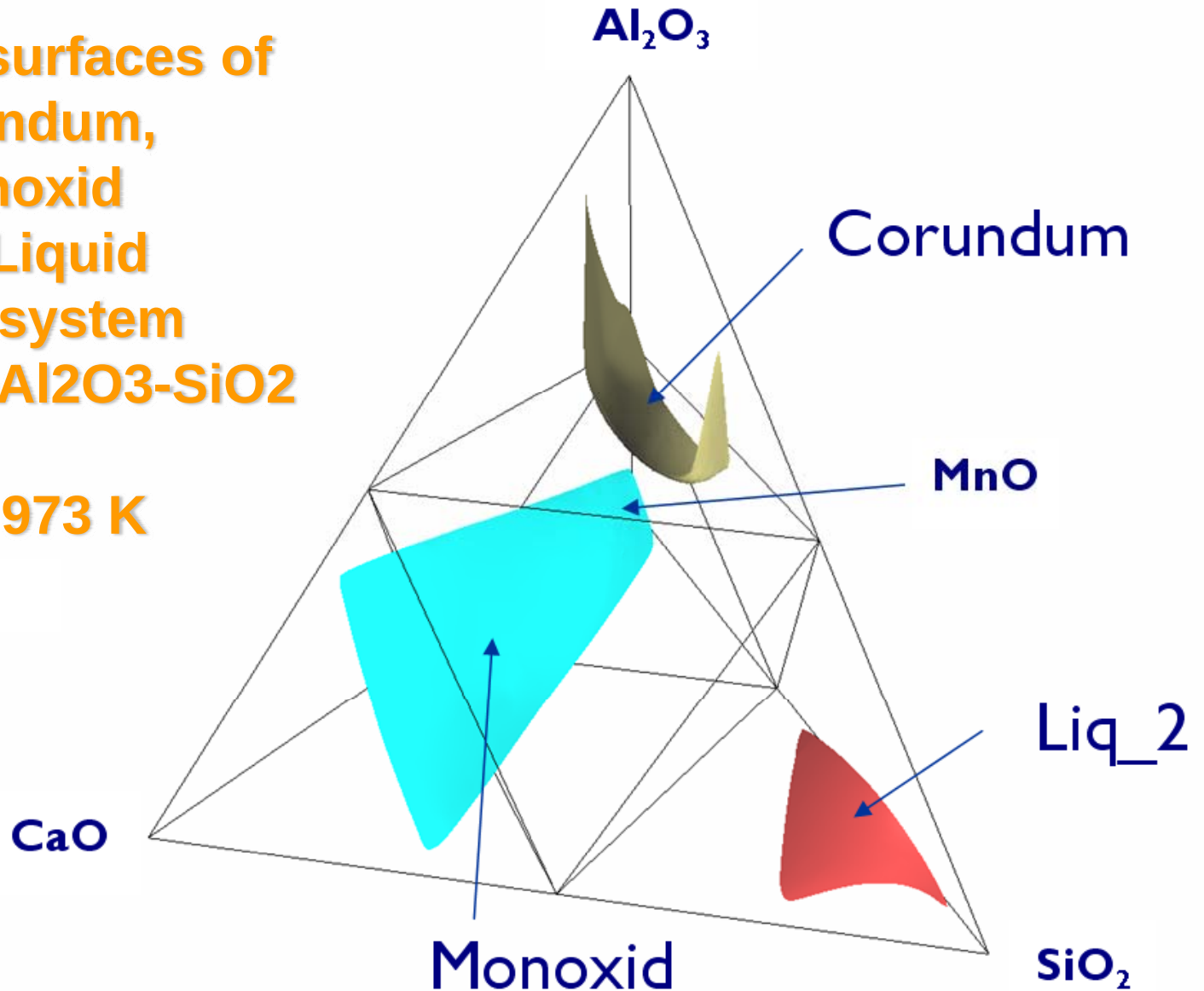
Part 5

Quaternary composition tetrahedron

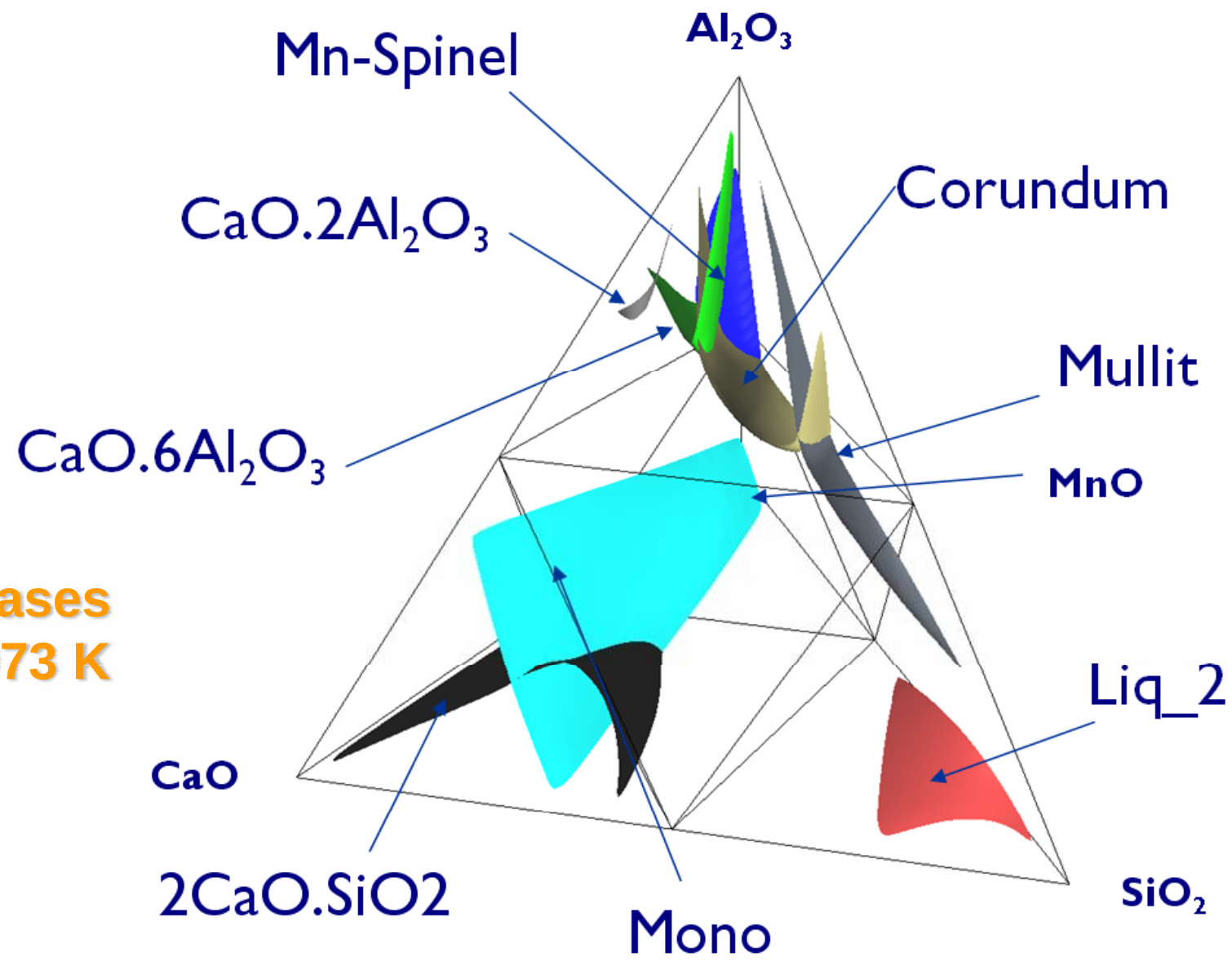


The ZPF surfaces of
Corundum,
Monoxid
and Liquid
in the system
 $\text{CaO-MnO-Al}_2\text{O}_3\text{-SiO}_2$

$T = 1973 \text{ K}$



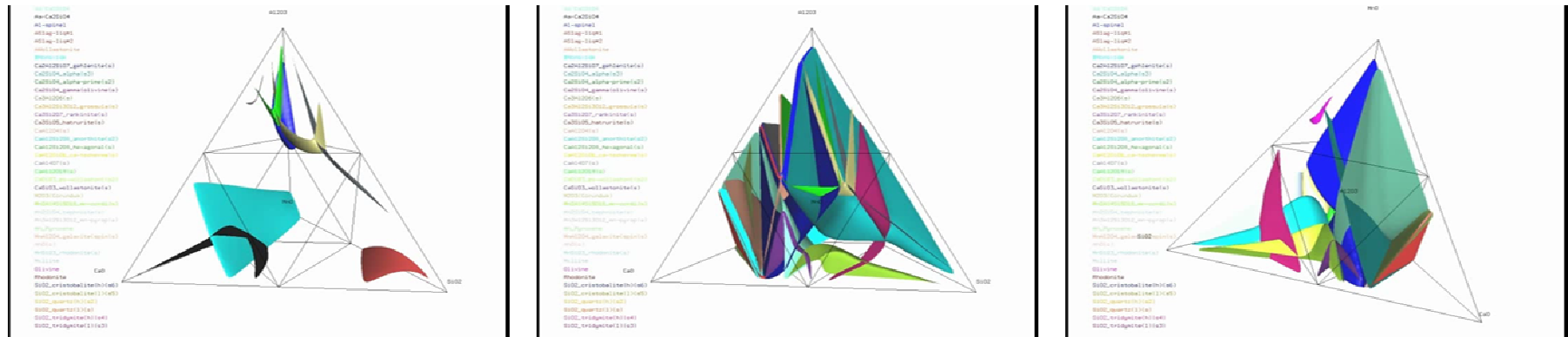
All phases
T = 1973 K



Results of thermochemical calculations

Part 6

4D: Quaternary composition tetrahedron with variable temperature



Summary

- Gibbs Energy thermodynamics (Software and Databases) permit quantitative calculation of systems with „arbitrarily“ high number of components.
- Regarding time (animation) as an additional parameter it is even possible to generate *four dimensional* representations.
- Up-to-date graphics soft- and hardware provides tools for real 3D-representation.



Thank you for your attention !

**We would be happy to welcome
You in the 3D cave of
RWTH computer center, Aachen !!!**

Polarisation glasses will be made available.

