CALCULATION AND INTERPRETATION OF PROJECTIONS OF THE TEMPERATURE OF FIRST MELTING

Gunnar Eriksson[1], Christopher W. Bale[2] and Arthur D. Pelton[2]

1. GTT-Technologies, Kaiserstraße 100, D-52134 Herzogenrath, Germany

2. CRCT – Centre de Recherche en Calcul Thermochimique, Département de Génie Chimique, École Polytechnique, C.P. 6079, Succ. 'Centre Ville', Montréal, Québec, H3C 3A7 Canada

Outline

- Solidus projection (6.3)
- First-melting-temperature projection (6.4)

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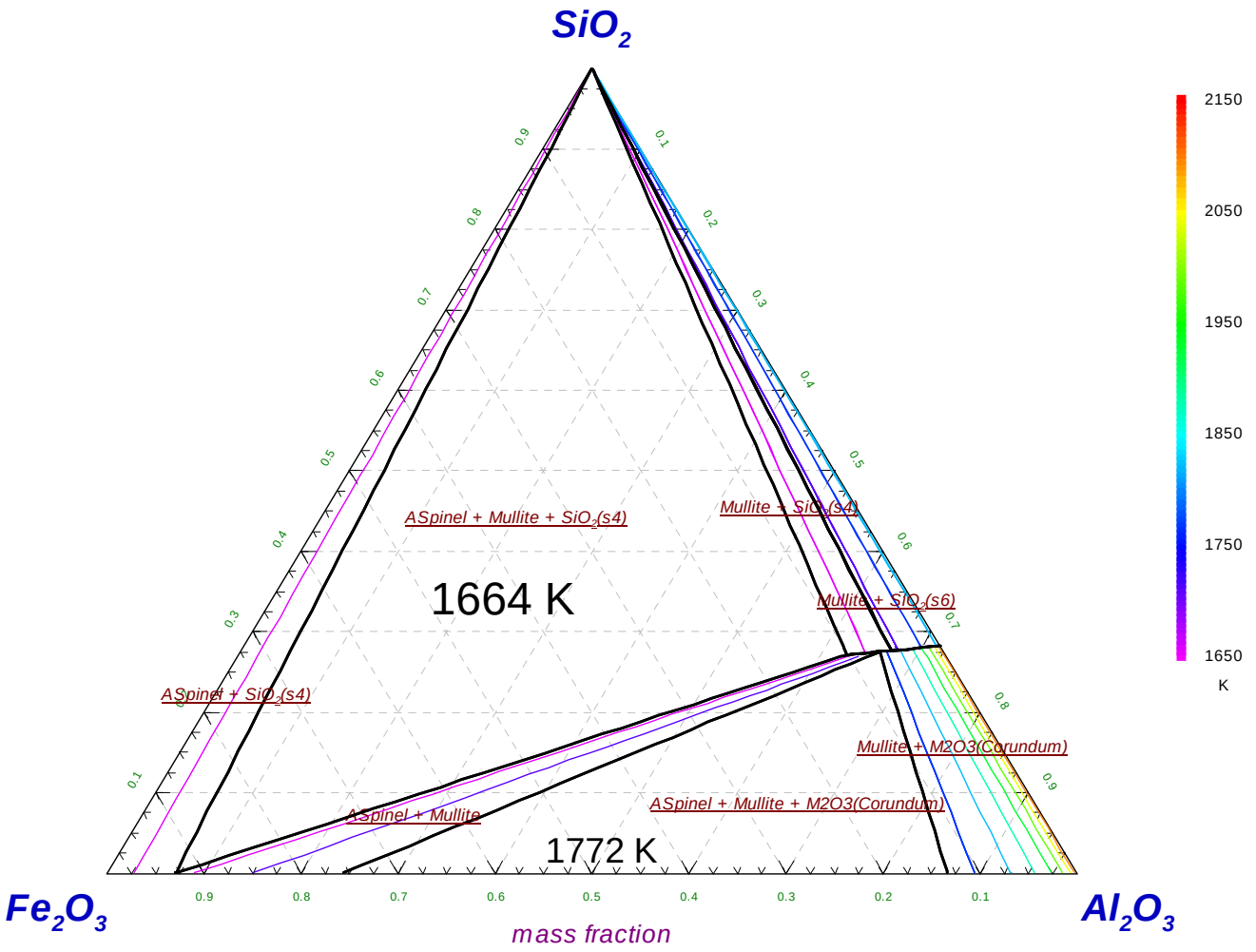
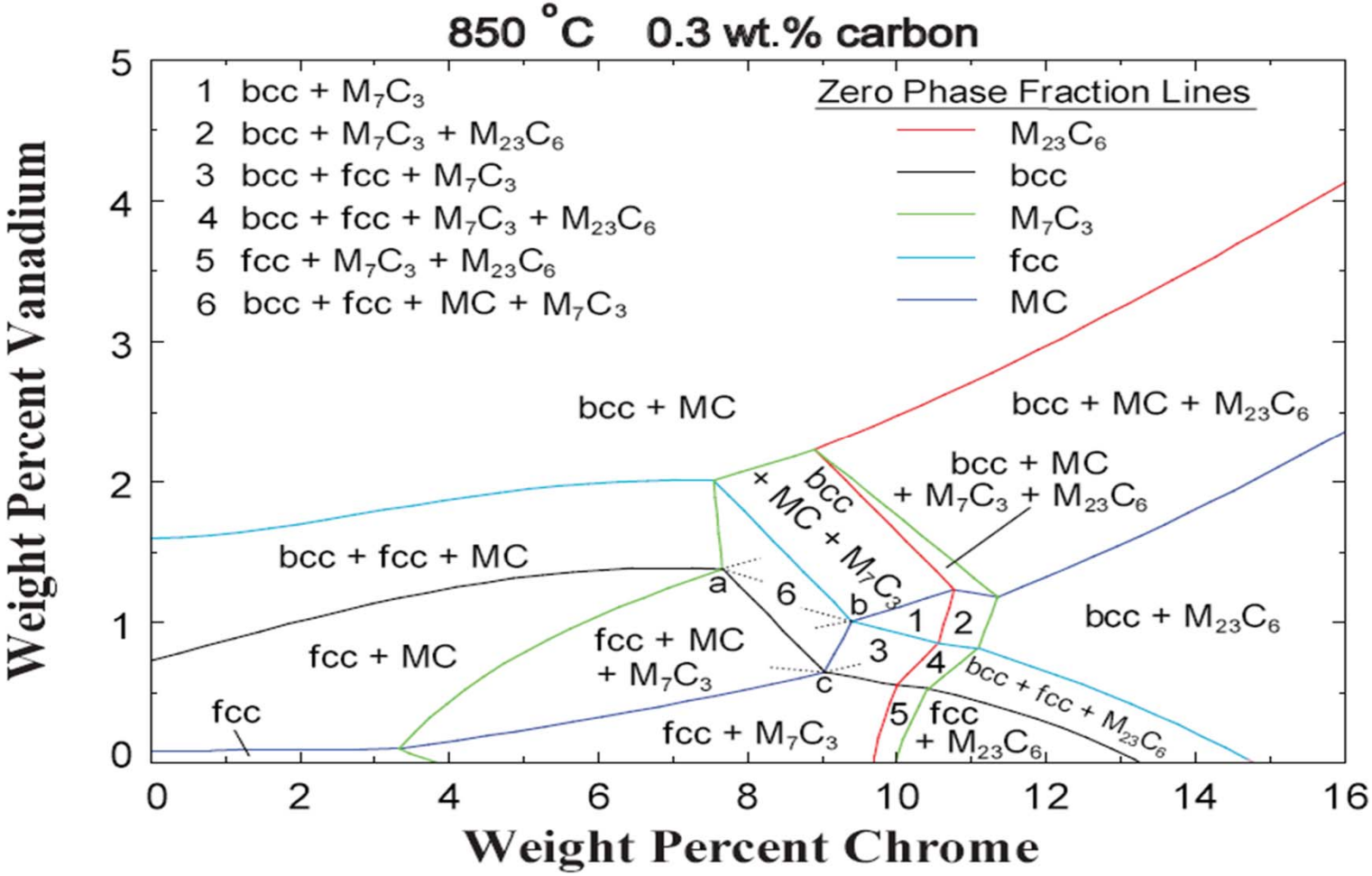
Fe_2O_3 - Al_2O_3 - SiO_2 - O_2

Projection - formation (ASlag-liq), p(O_2) = 0.21 bar, 1 bar



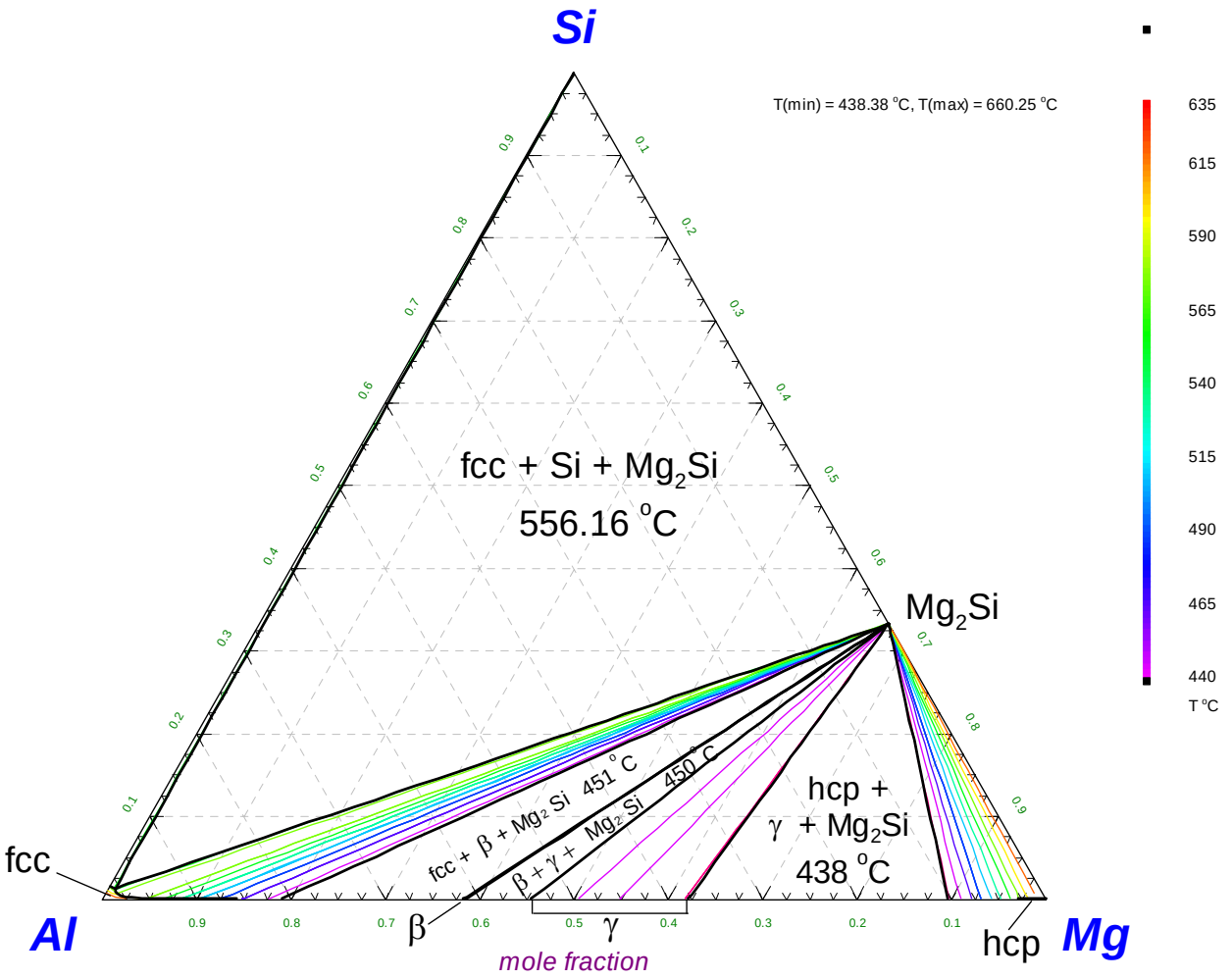
Fe-Cr-V-C isothermal section illustrating Zero-Phase-Fraction (ZPF) lines



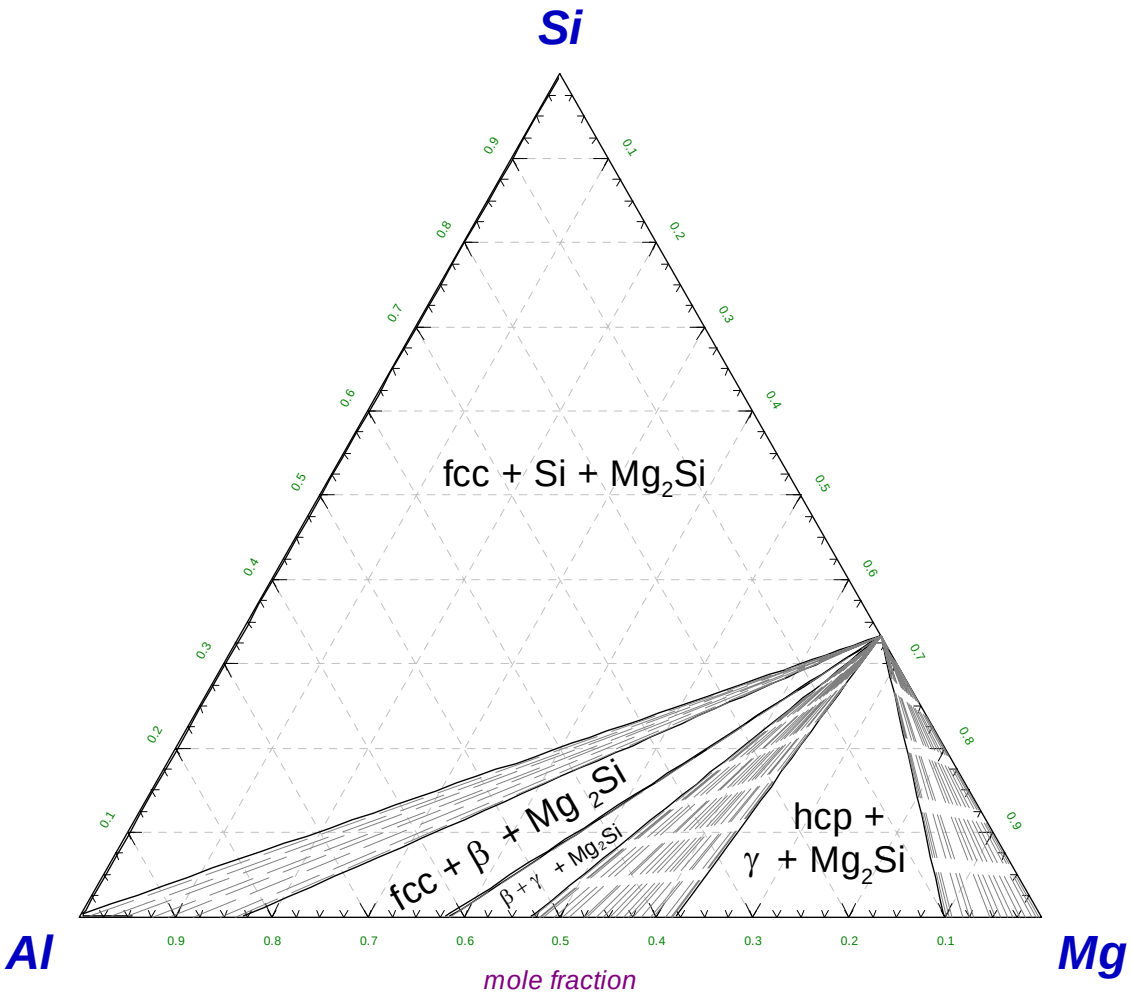
FactSage will calculate phase diagrams with solid projection by the same strategy of following Zero-Phase-Fraction (ZPF) lines as for all other types of phase diagrams.

Input parameters for a phase diagram calculation can be chosen such that phase fields might be overlapping. Such phase diagram types are not permitted in FactSage, the reason being that the ZPF-line method will then not work properly.

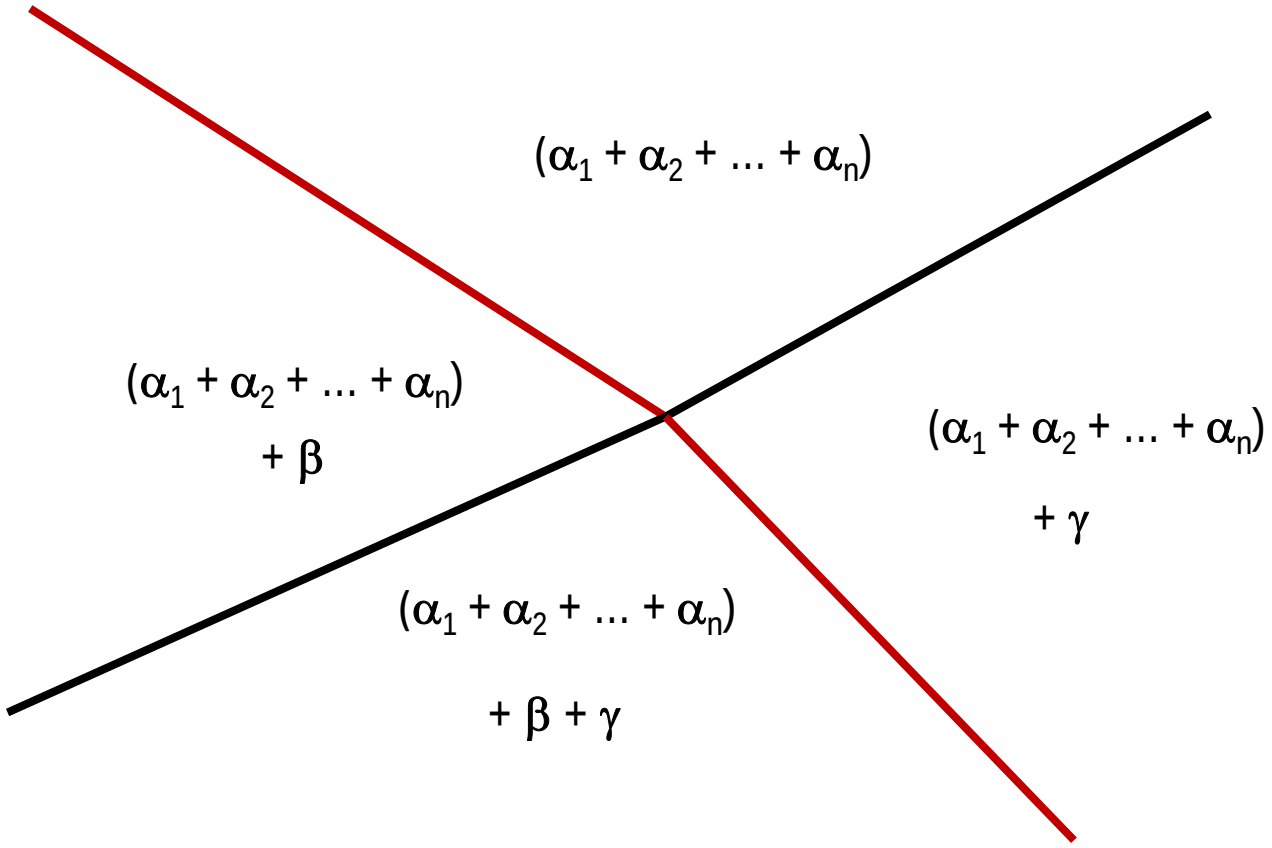
SOLIDUS PROJECTION



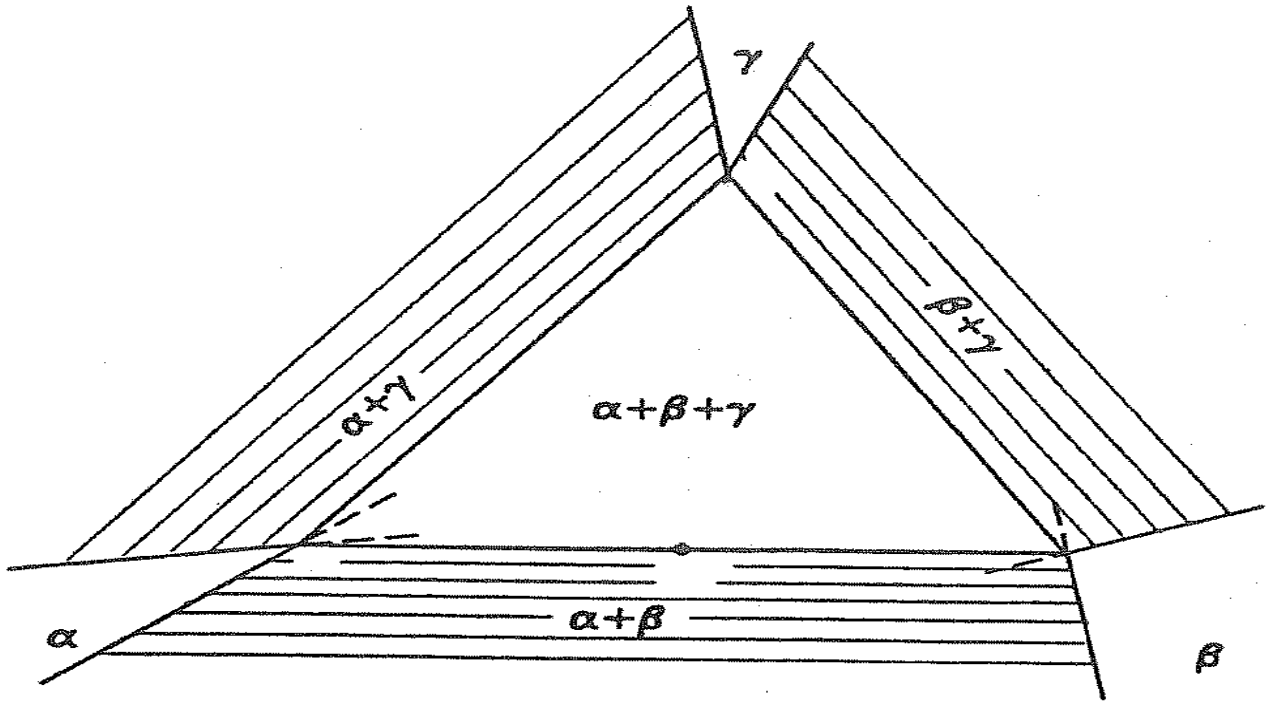
ISOTHERMAL SECTION 430°C



A node in a general phase diagram section or a solidus projection

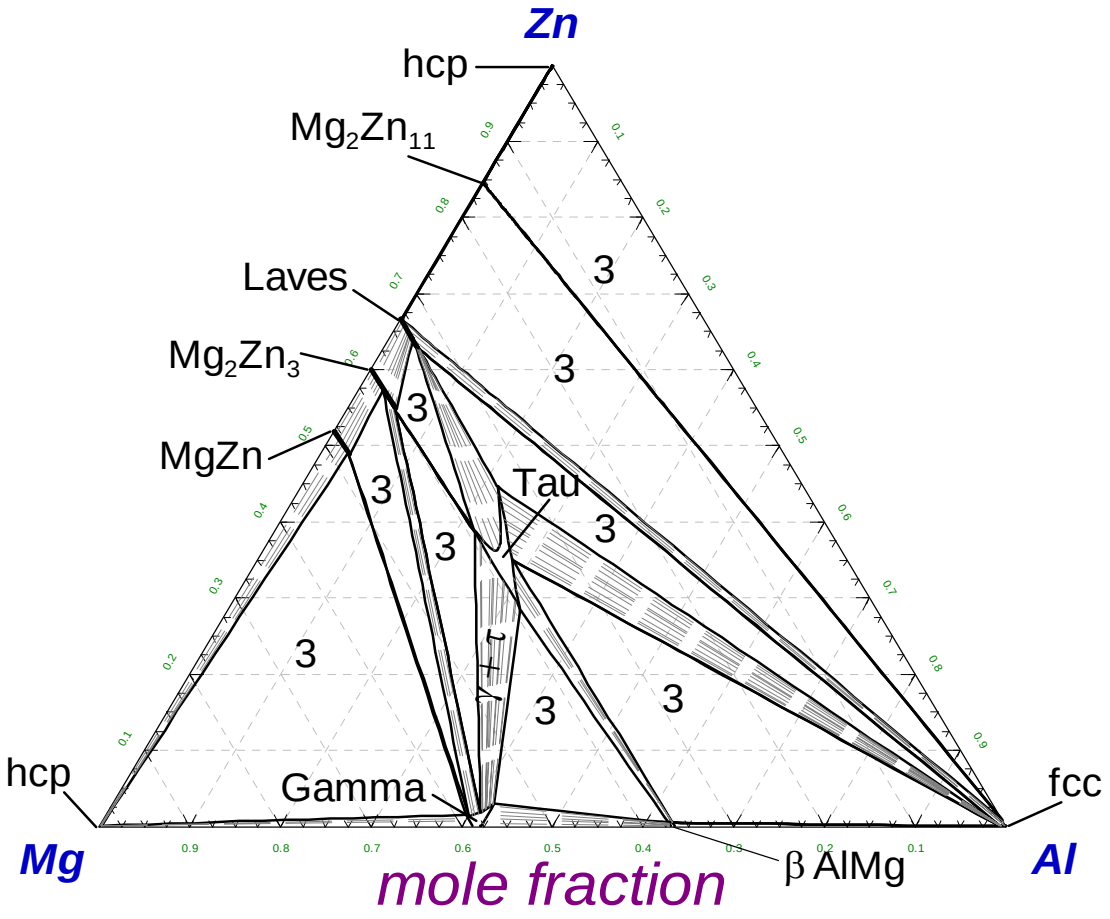


Tie triangle in a ternary isothermal section or in a ternary solidus projection

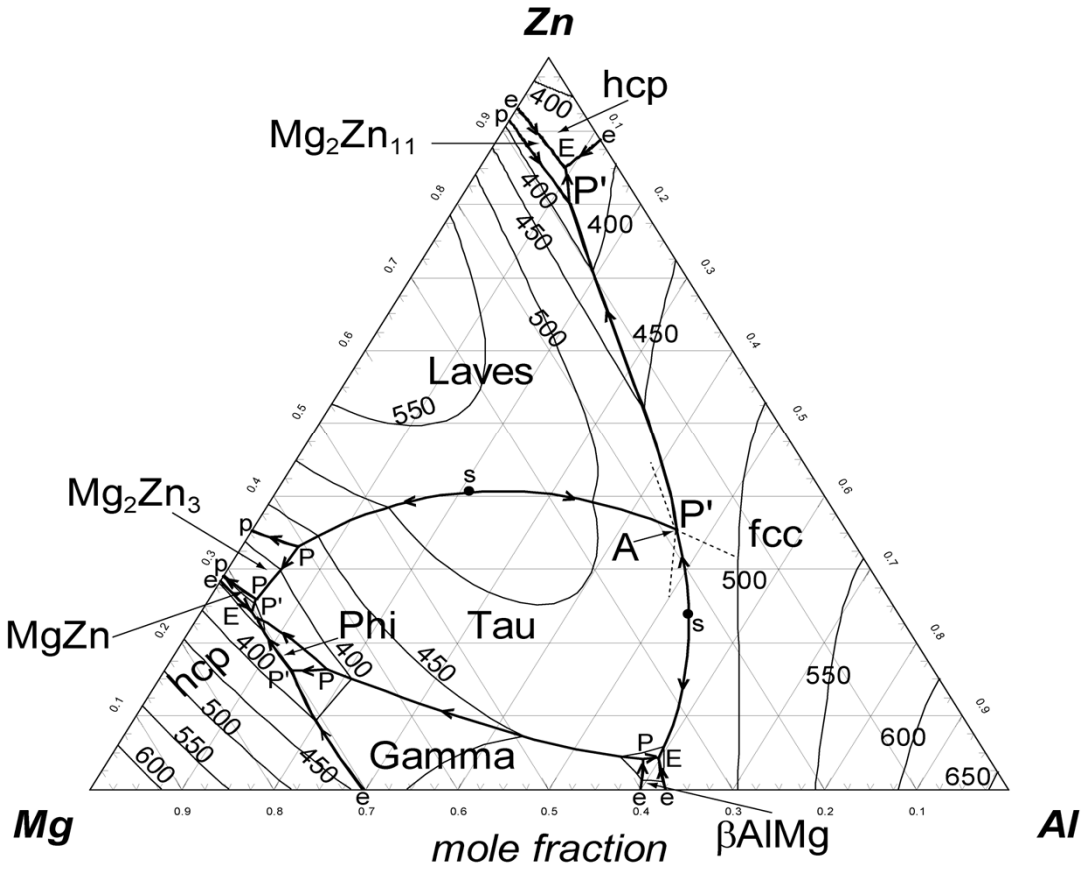


Schreinemakers‘ Rule

Zn - Mg - Al
Isothermal section at 25 °C

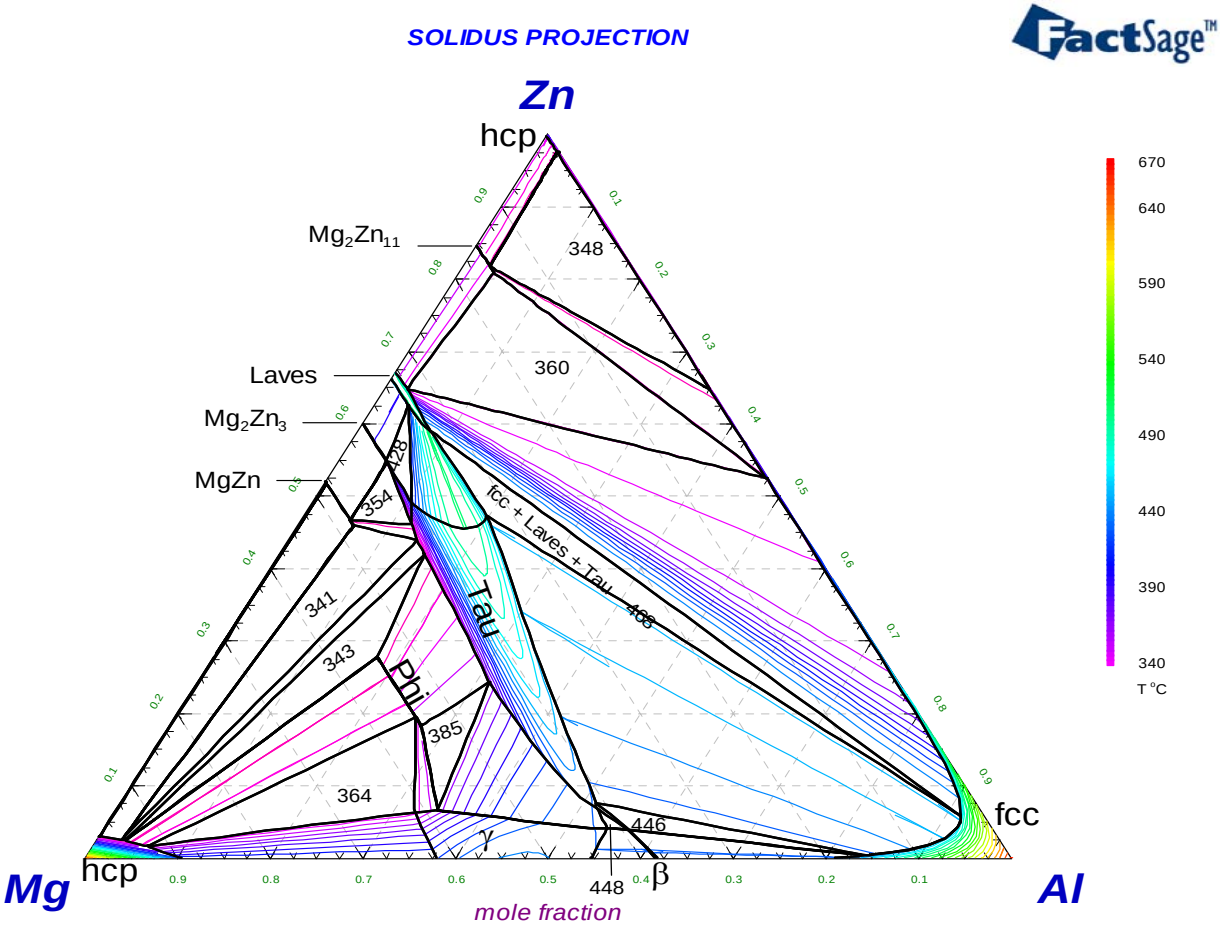


Zn-Mg-Al liquidus projection



Each ternary invariant (P=peritectic, E=eutectic) point on the liquidus projection corresponds to a tie-triangle on the solidus projection

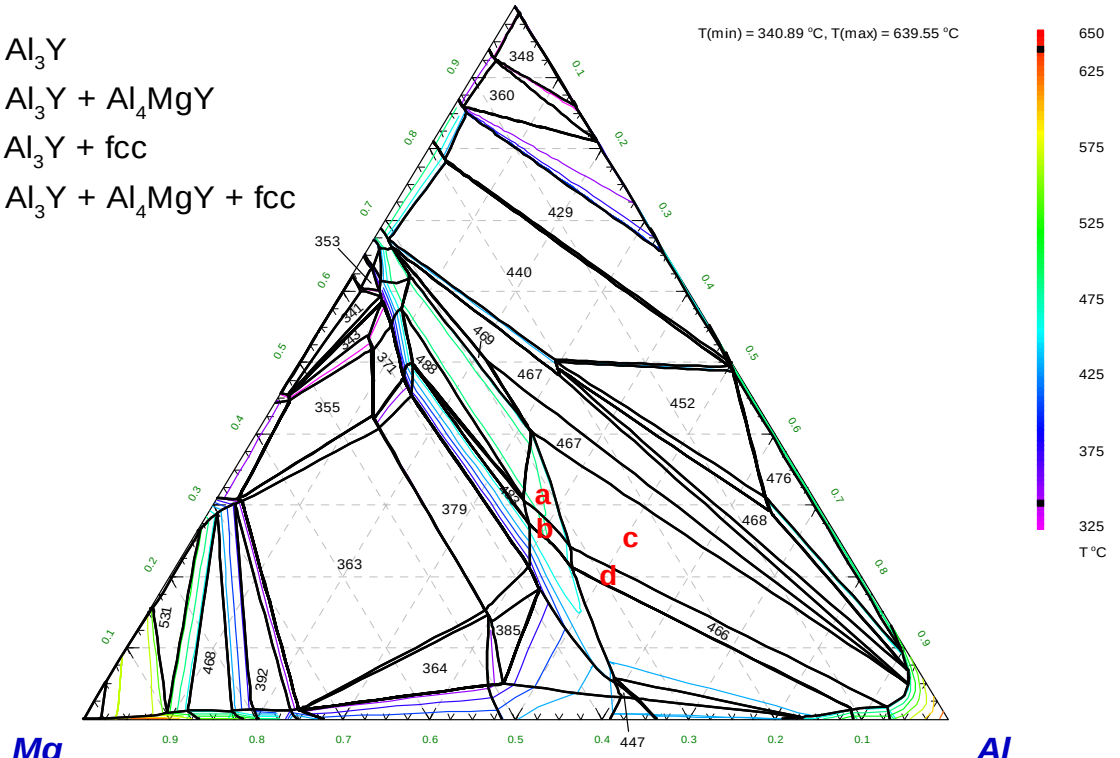
Zn-Mg-Al solidus projection



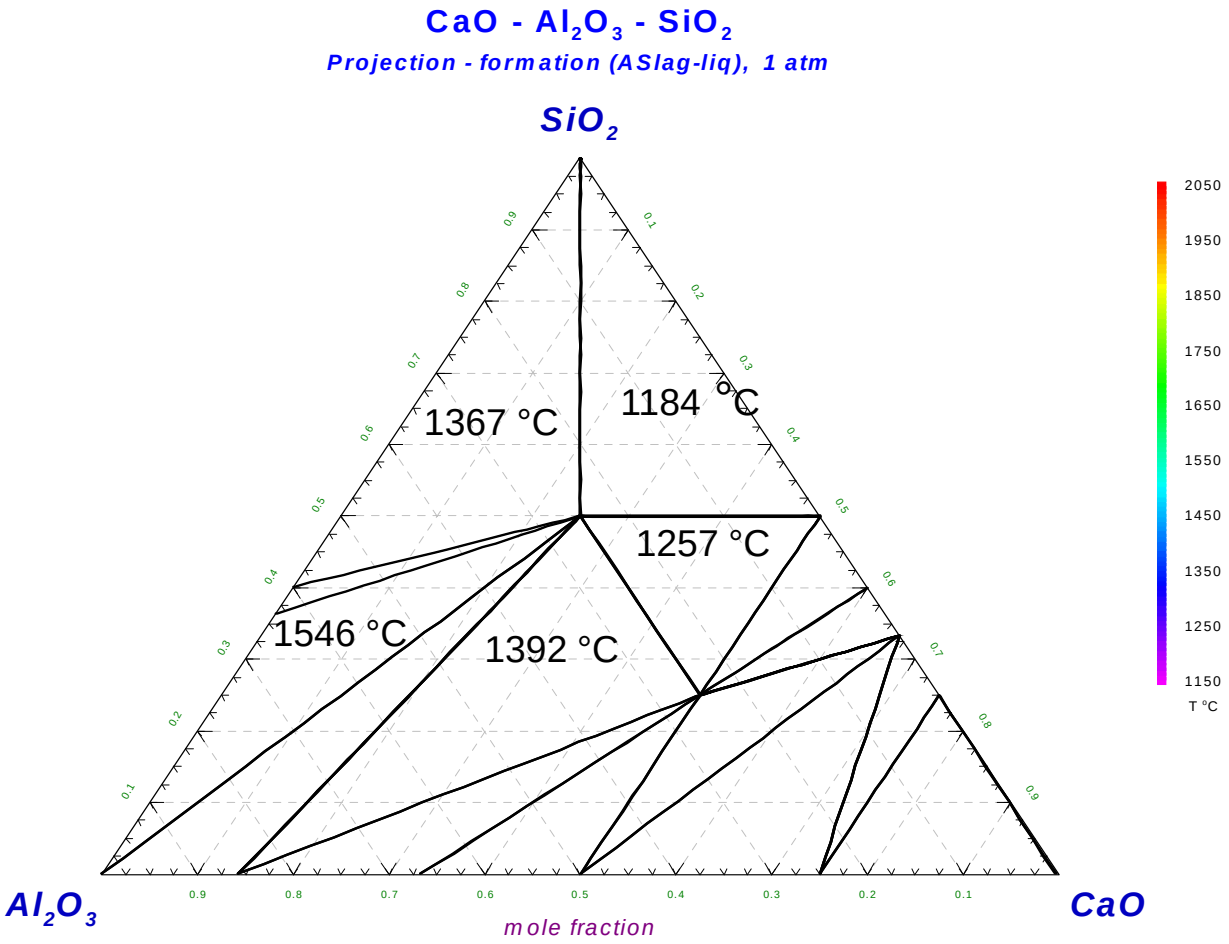
Zn-Mg-Al-Y

SOLIDUS PROJECTION, mole fraction Yttrium = 0.05

a = Tau + Al_3Y
b = Tau + Al_3Y + Al_4MgY
c = Tau + Al_3Y + fcc
d = Tau + Al_3Y + Al_4MgY + fcc



Solidus projection when stable ternary compounds



Outline

- Solidus projection (6.3)
- First-melting-temperature projection (6.4)

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Exceptions and challenges

- In systems with catatectics or retrograde solubilities, a liquid phase can resolidify upon heating.

- In such systems, phase fields on a solidus projection can overlap.

- However, phase fields on a 'first-melting-temperature' projection never overlap. These are calculated automatically by the ZPF strategy.

- If a system contains no catatectics or retrograde solubilities (as is the case in the great majority of systems), the first-melting-temperature and solidus projections are identical.

- Note: For systems exhibiting catactectics or retrograde solubility, the usual phase diagram rules are not necessarily obeyed in those composition ranges where liquid resolidifies upon heating.

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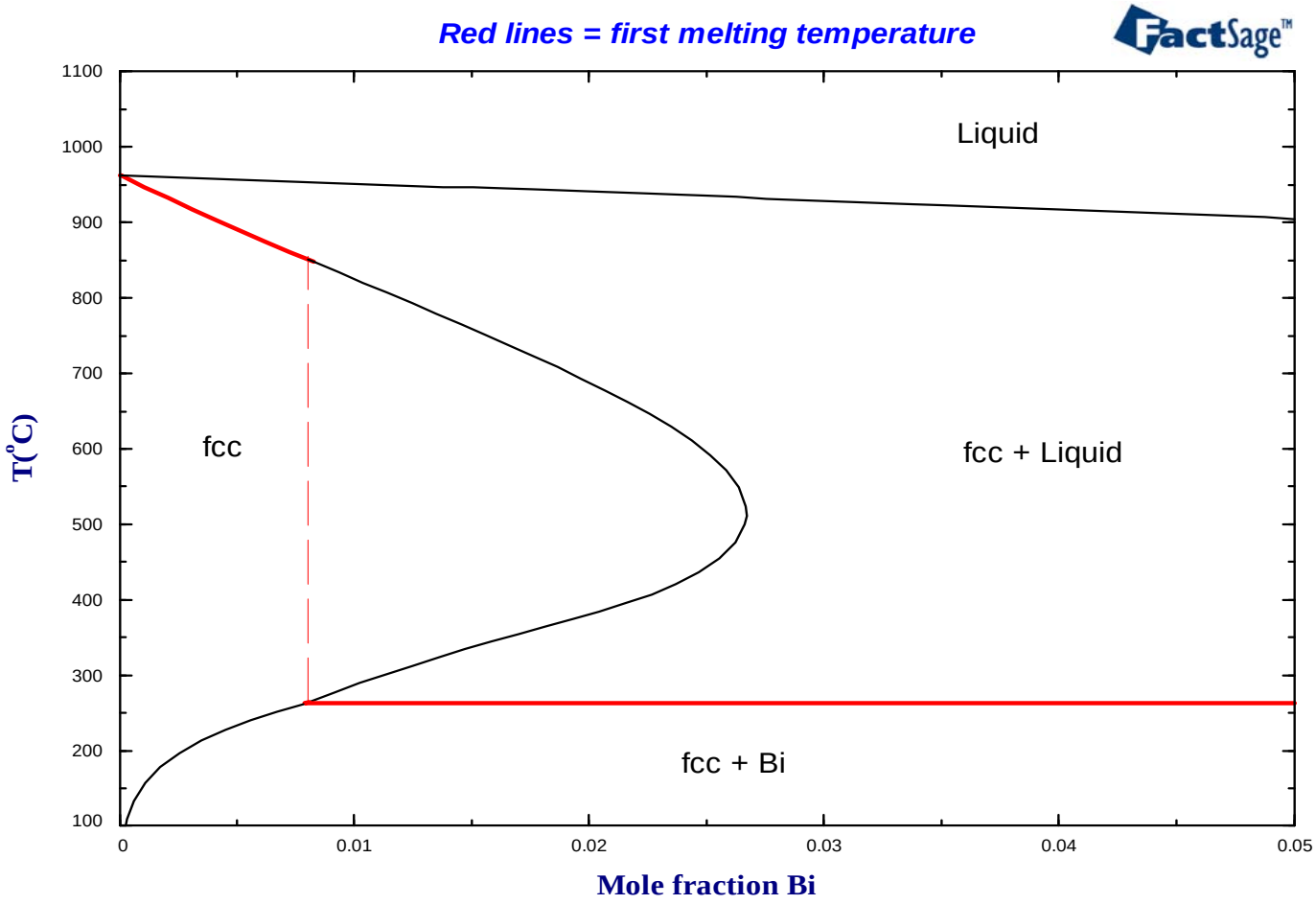
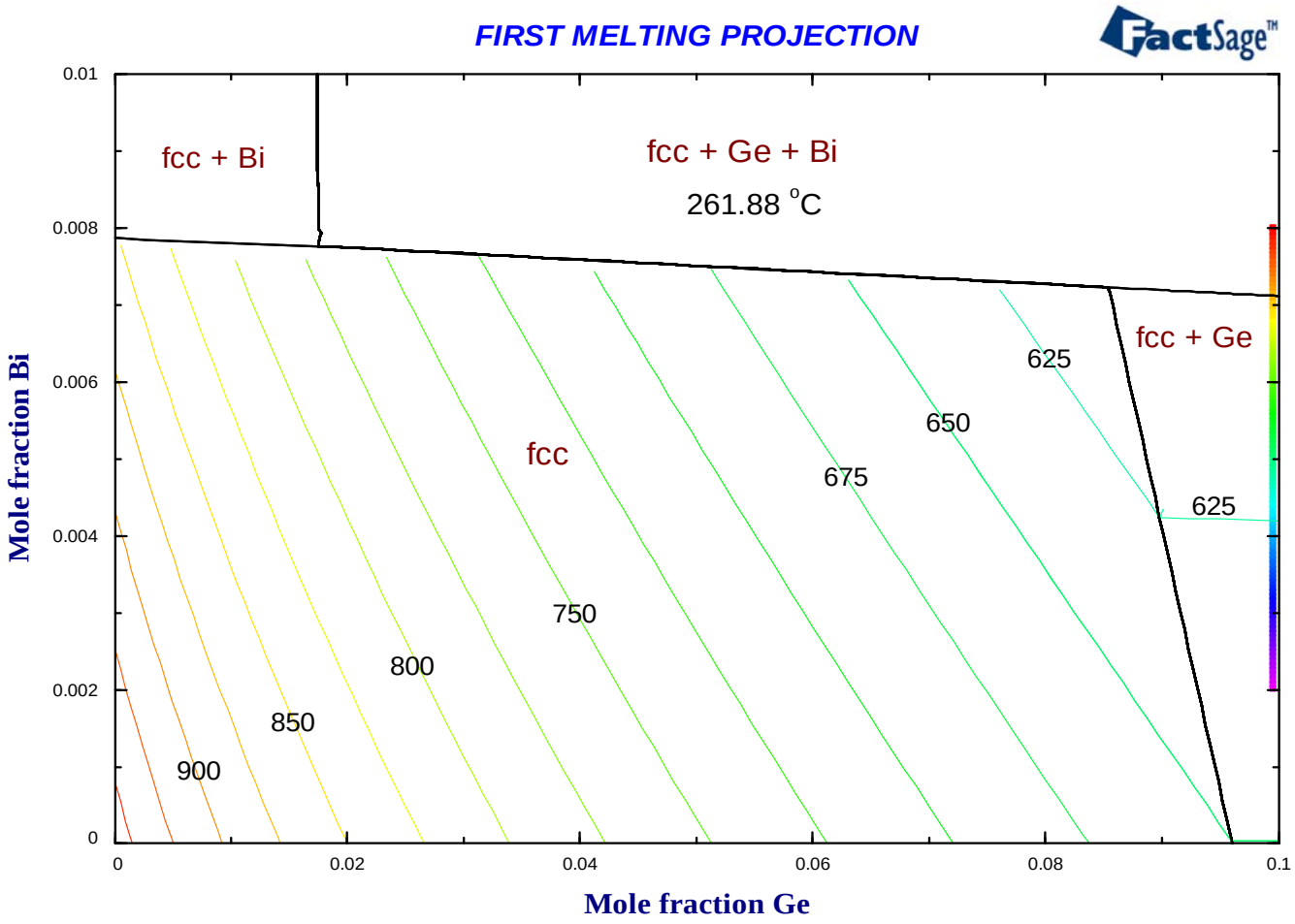
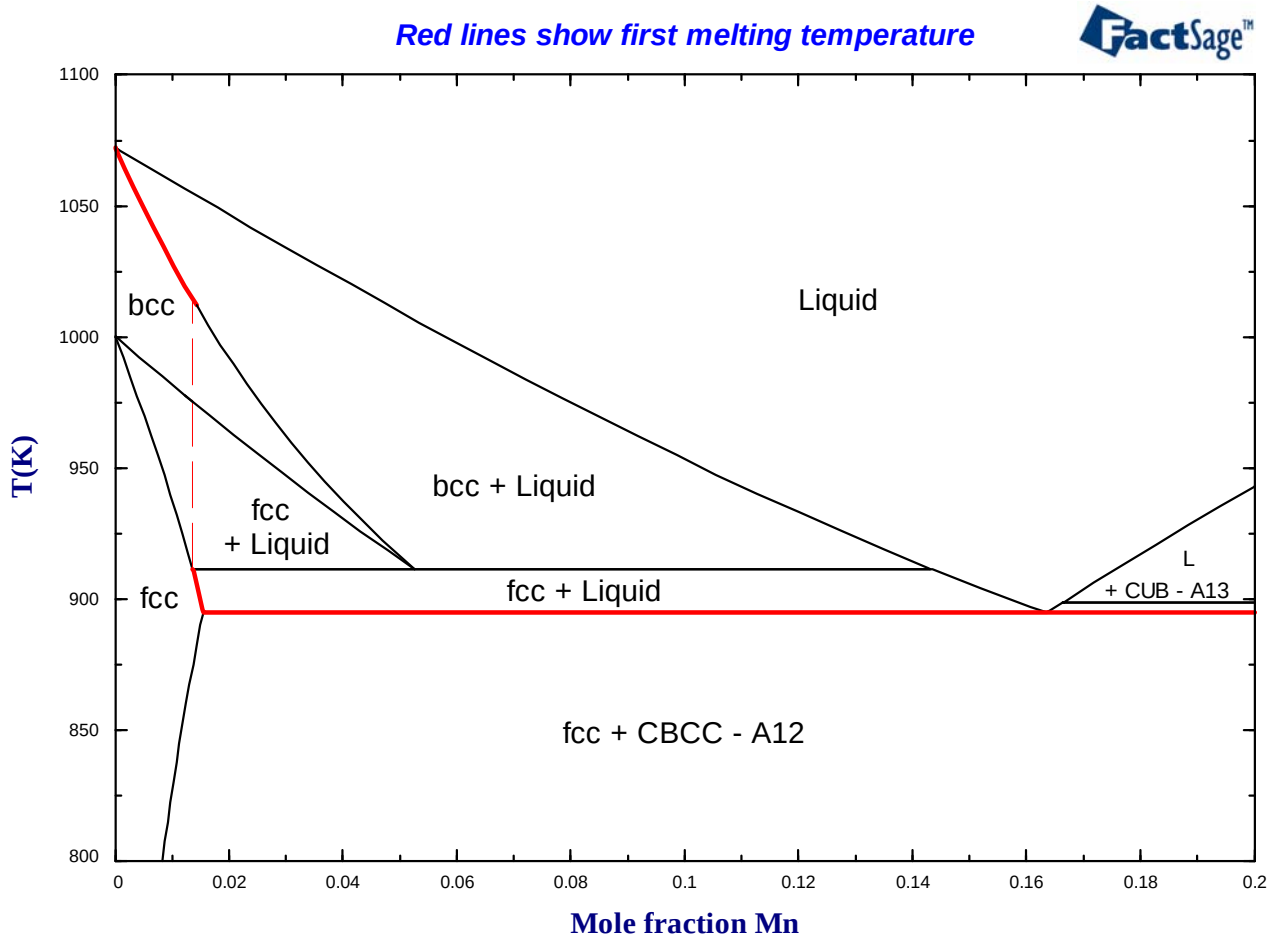
Ag-Bi with a retrograde solubility



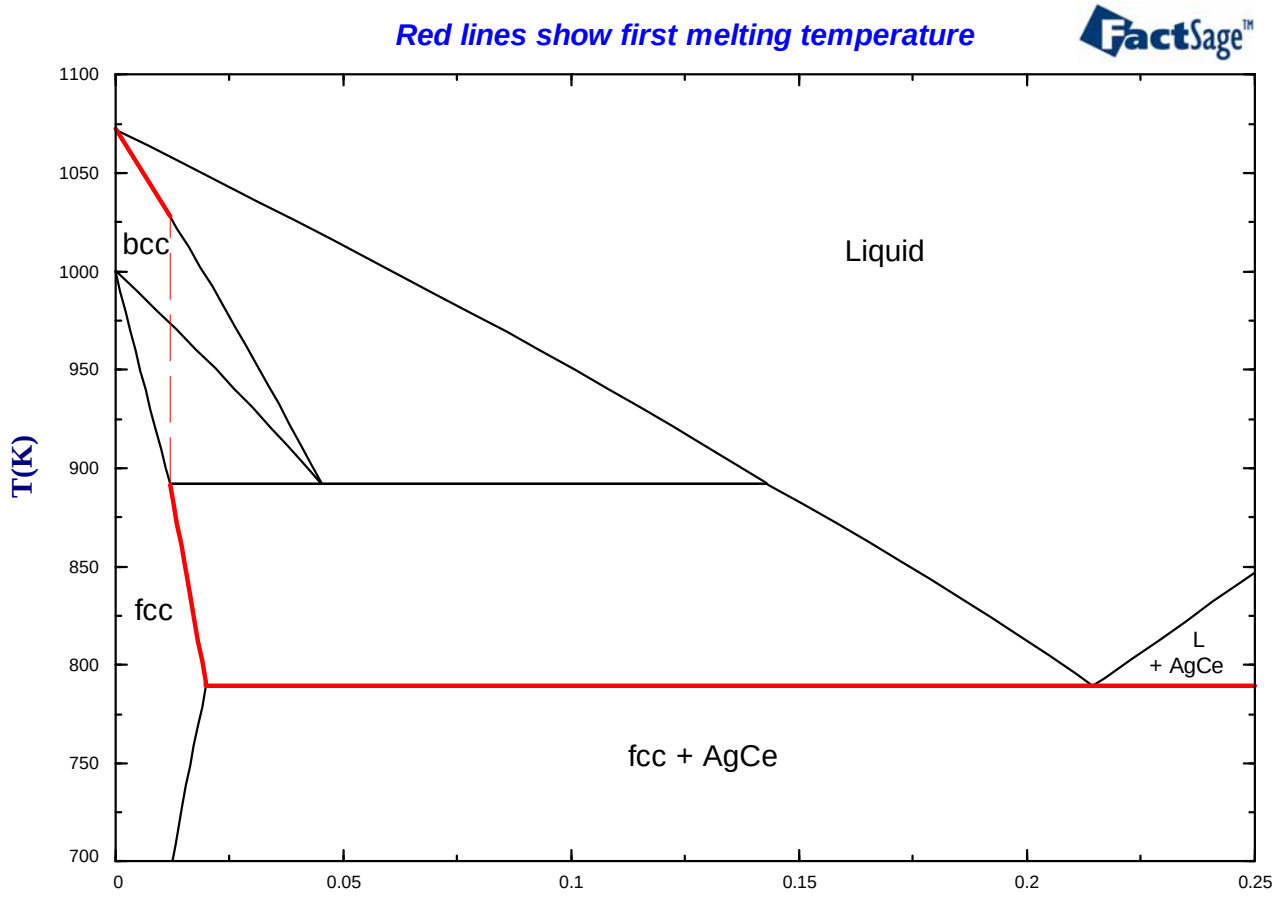
Ag-Bi-Ge

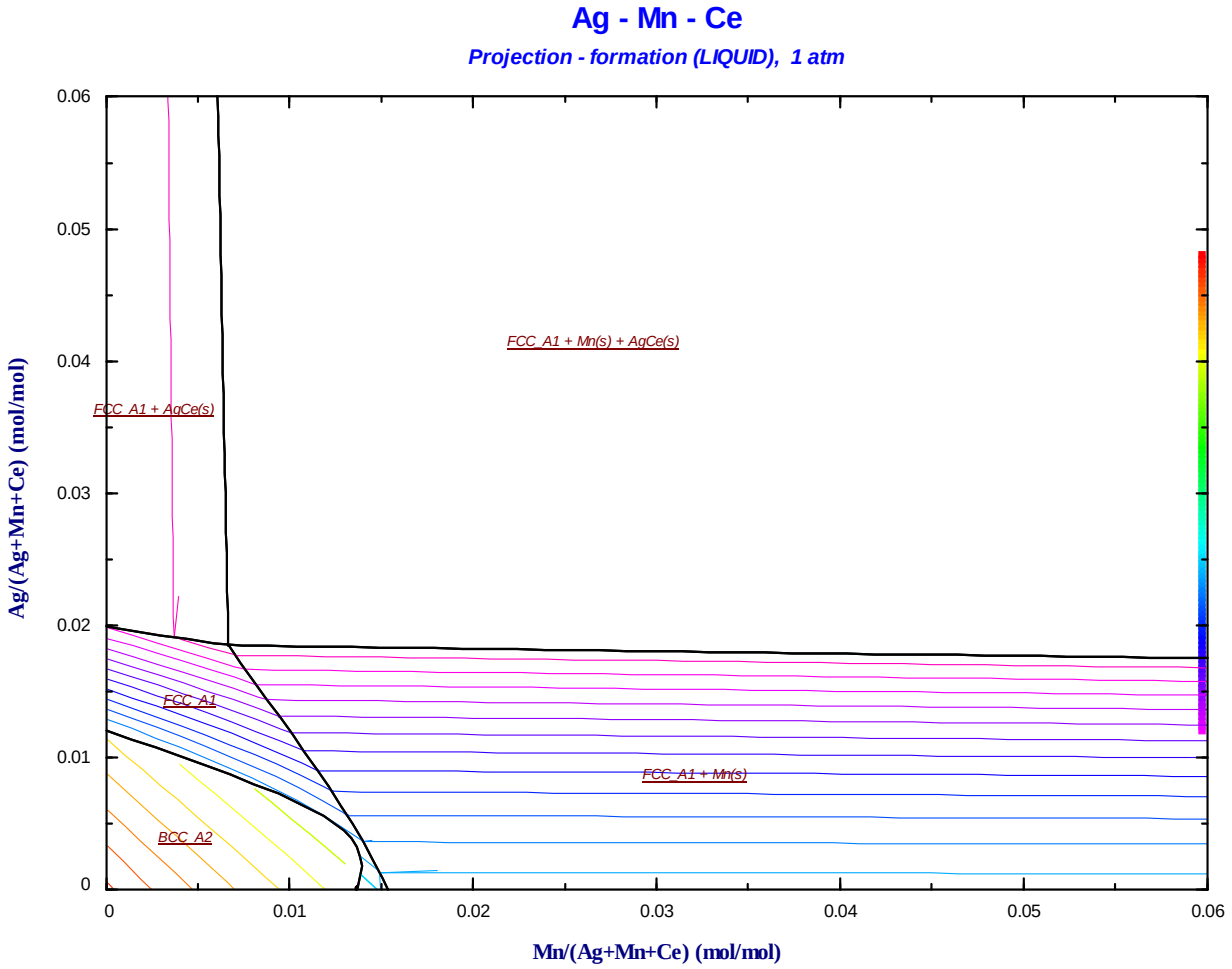

FIRST MELTING PROJECTION
FactSage™
fcc + Bi
fcc + Ge + Bi
261.88 °C
fcc + Ge
fcc
625
650
675
625
750
800
850
900
Mole fraction Bi
Mole fraction Ge
0.01
0.008
0.006
0.004
0.002
0
0
0.02
0.04
0.06
0.08
0.1

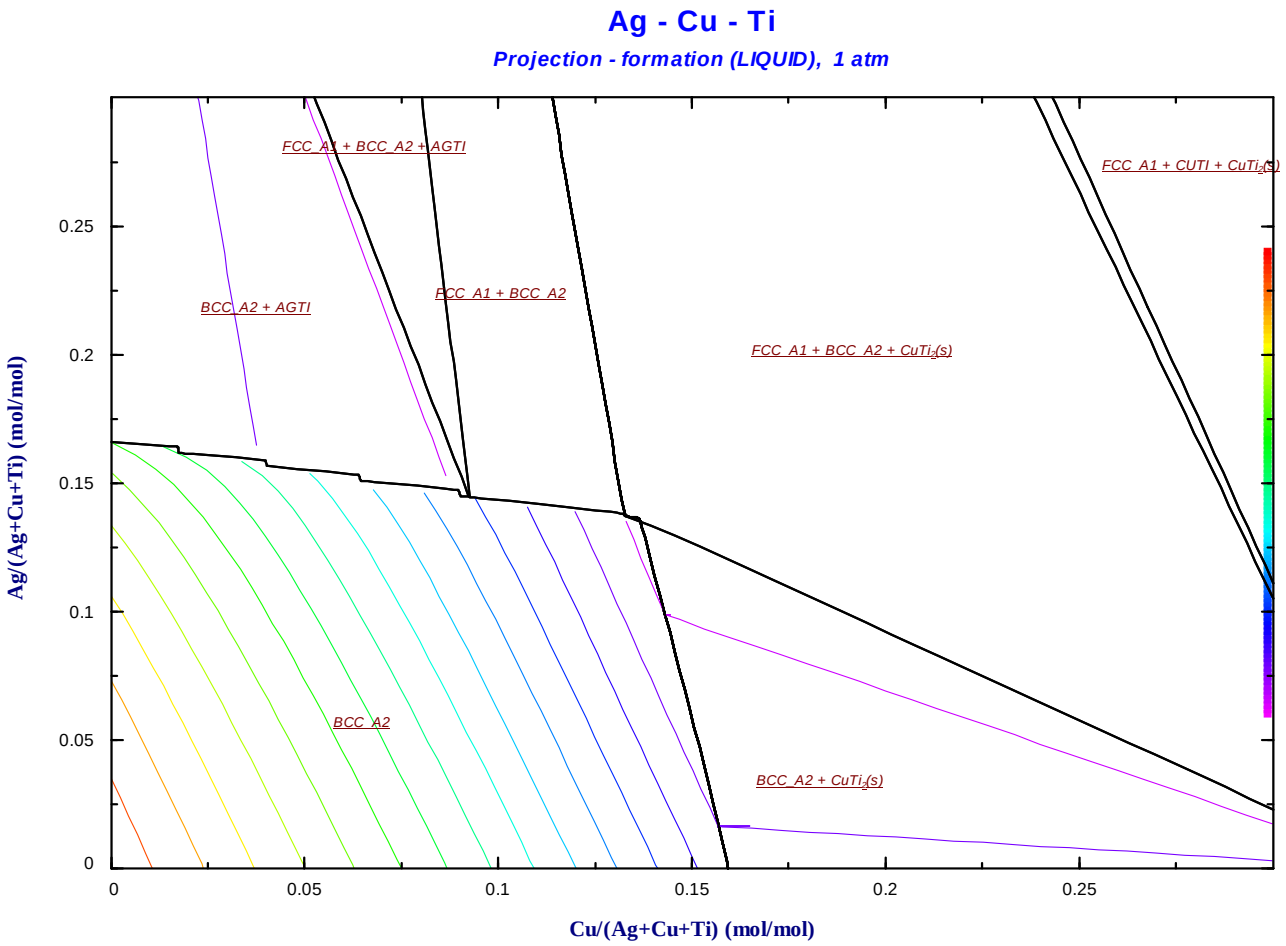
The catatectic system Ce-Mn

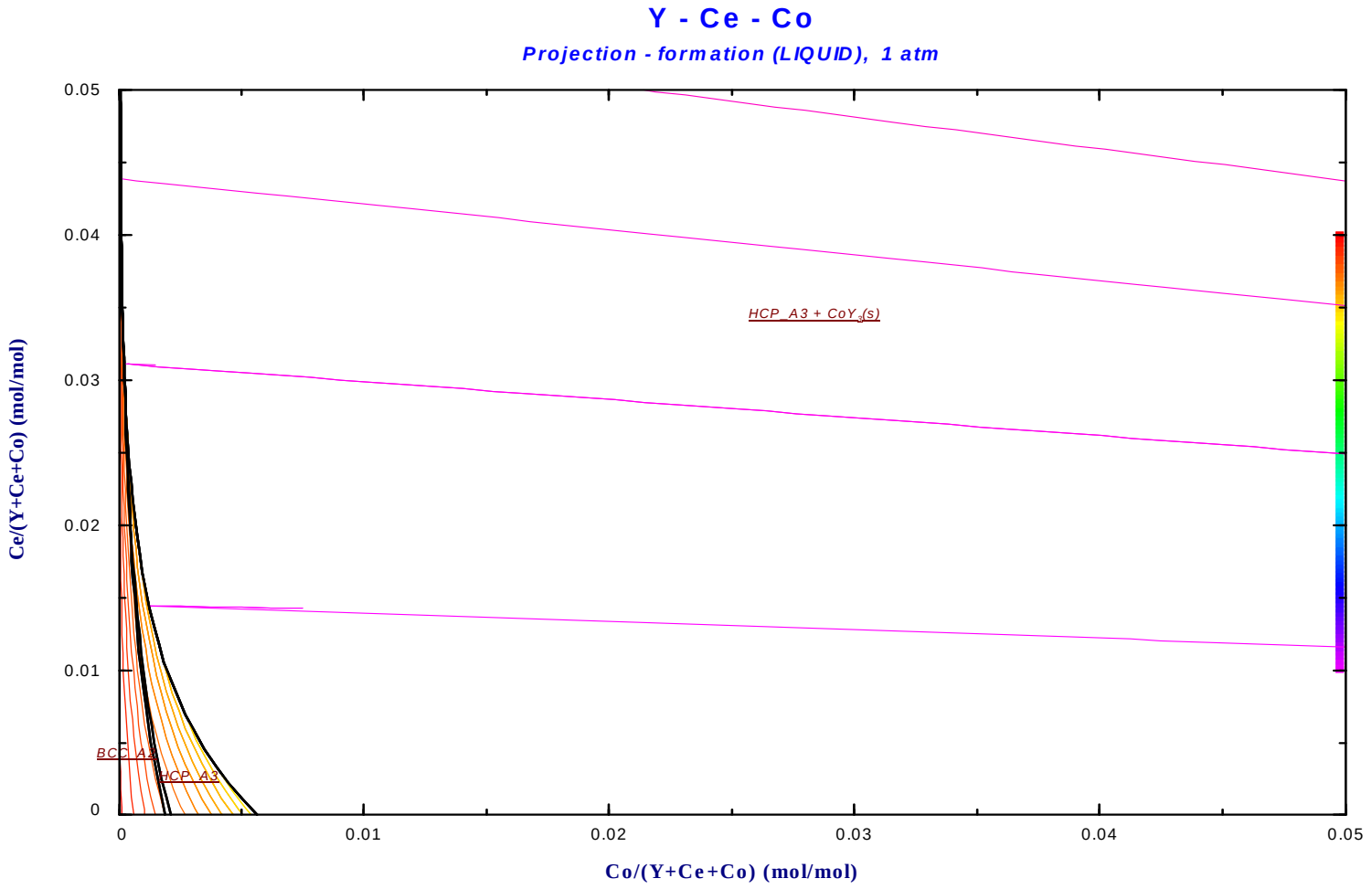


The catatectic system Ce-Ag

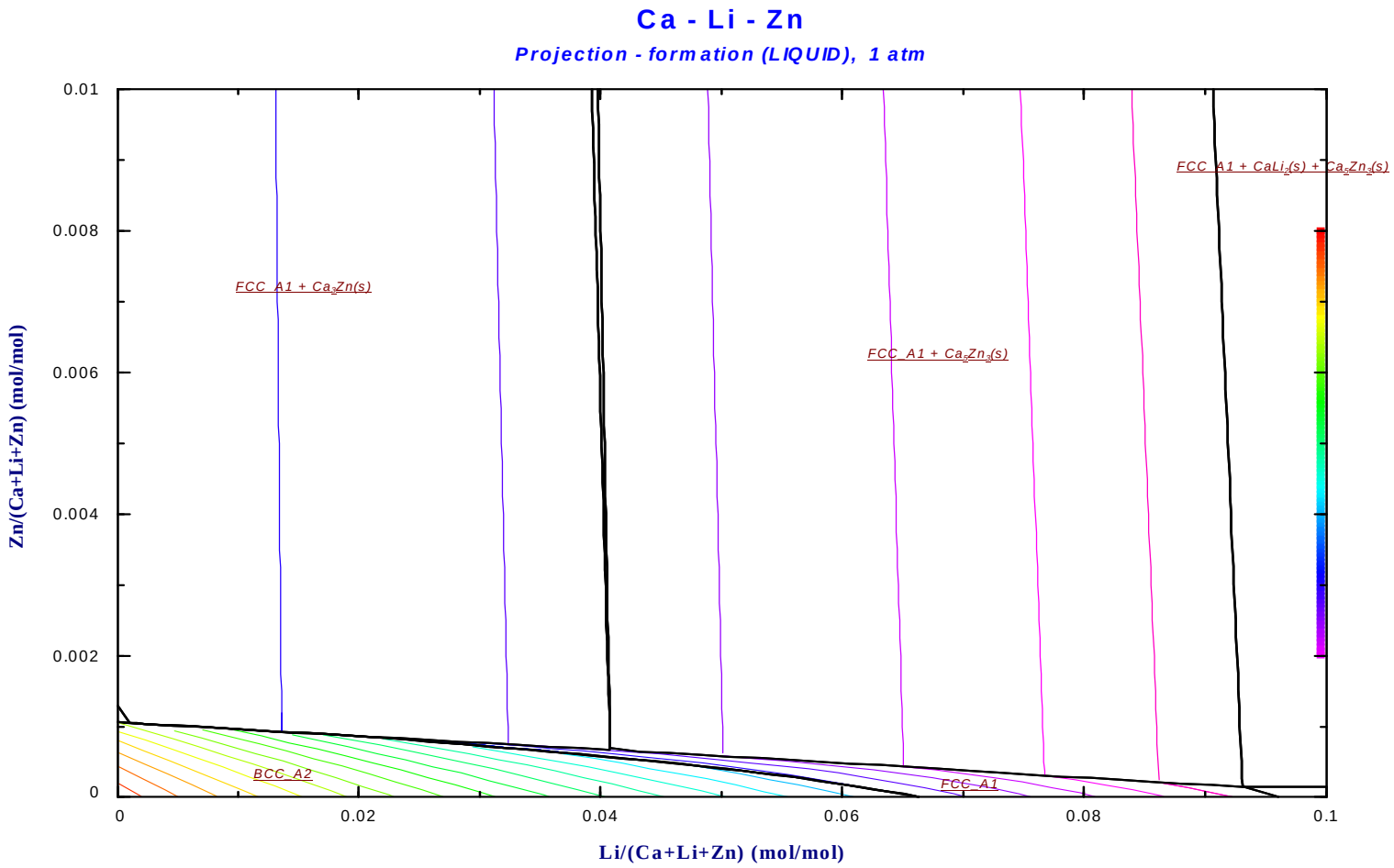


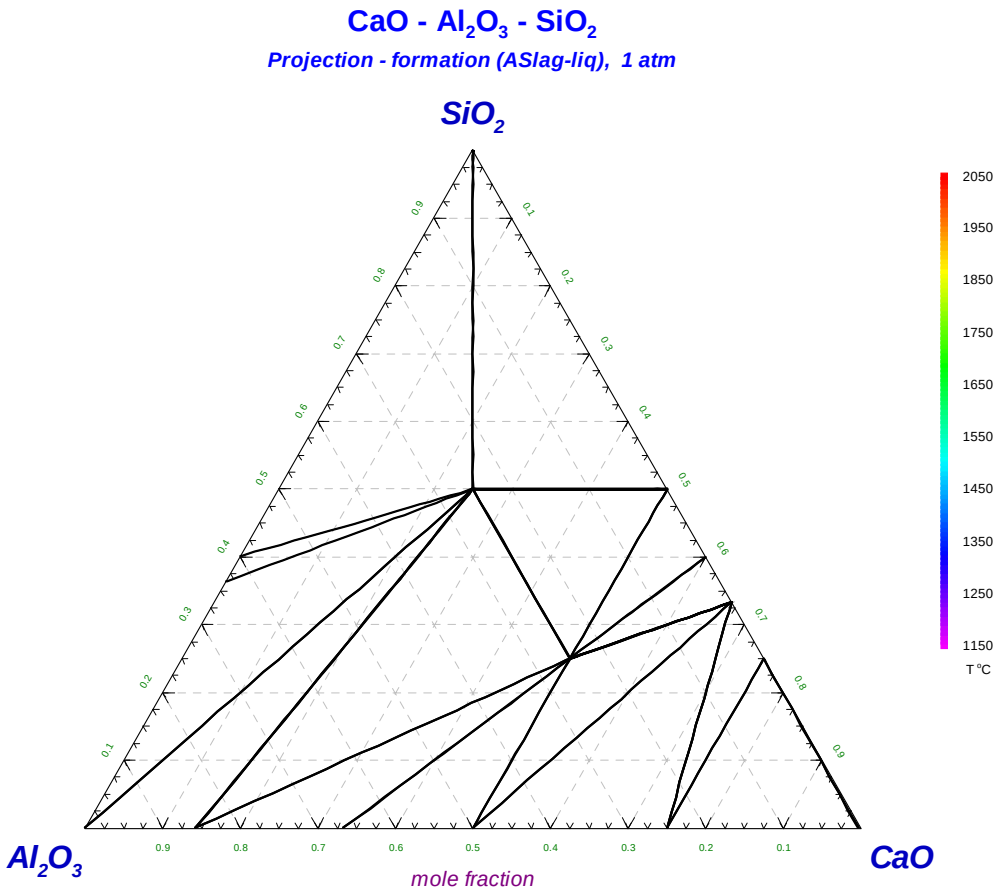

Ag - Mn - Ce
Projection - formation (LIQUID), 1 atm
FCC_A1 + Mn(s) + AgCe(s)
FCC_A1 + AgCe(s)
FCC_A1
FCC_A1 + Mn(s)
BCC_A2
Ag/(Ag+Mn+Ce) (mol/mol)
Mn/(Ag+Mn+Ce) (mol/mol)
0
0.01
0.02
0.03
0.04
0.05
0.06

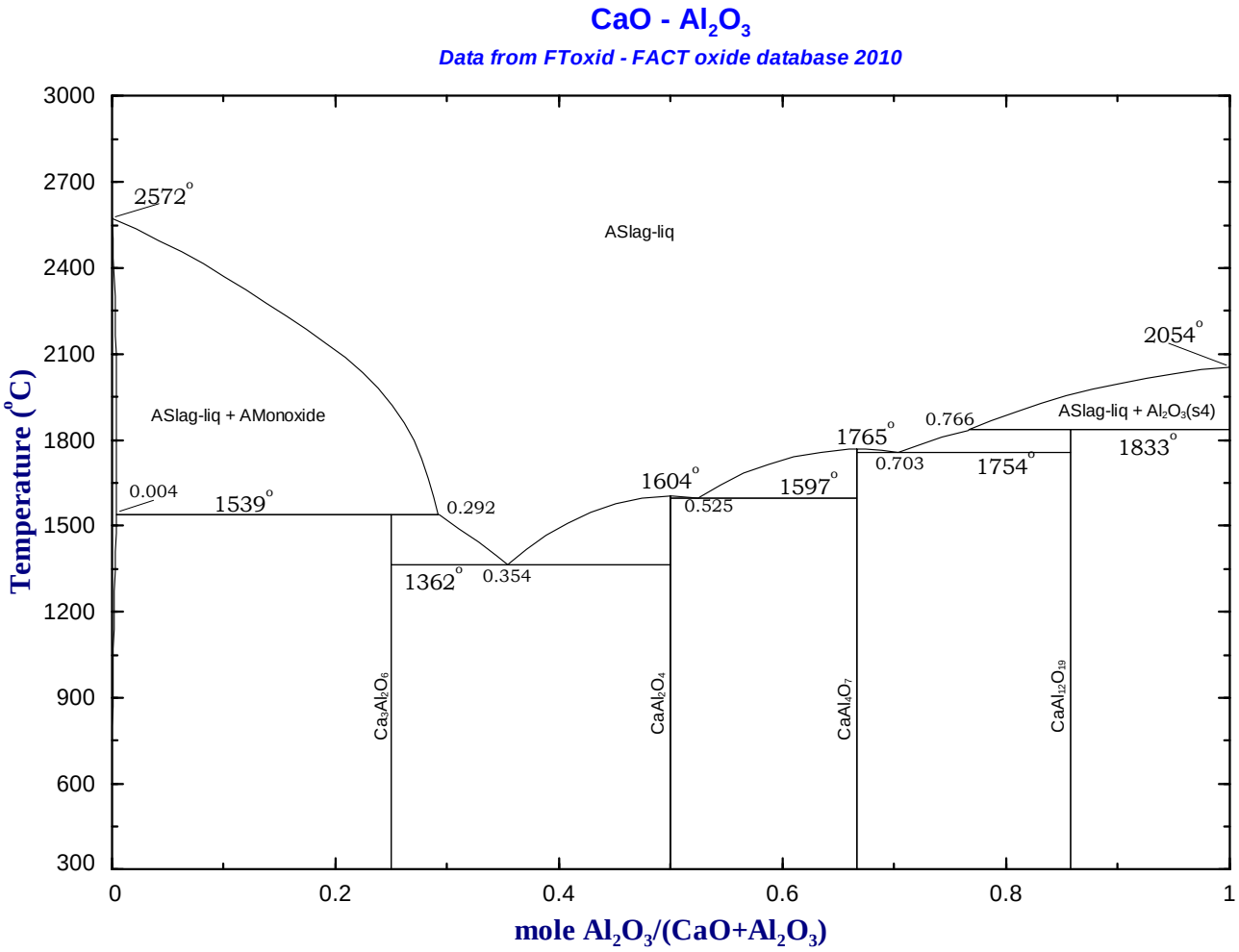

Ag - Cu - Ti
Projection - formation (LIQUID), 1 atm
FCC_A1 + BCC_A2 + AGTI
FCC_A1 + CUTI + CuTi2(s)
BCC_A2 + AGTI
FCC_A1 + BCC_A2
FCC_A1 + BCC_A2 + CuTi2(s)
BCC_A2
BCC_A2 + CuTi2(s)
Ag/(Ag+Cu+Ti) (mol/mol)
Cu/(Ag+Cu+Ti) (mol/mol)
0
0.05
0.1
0.15
0.2
0.25

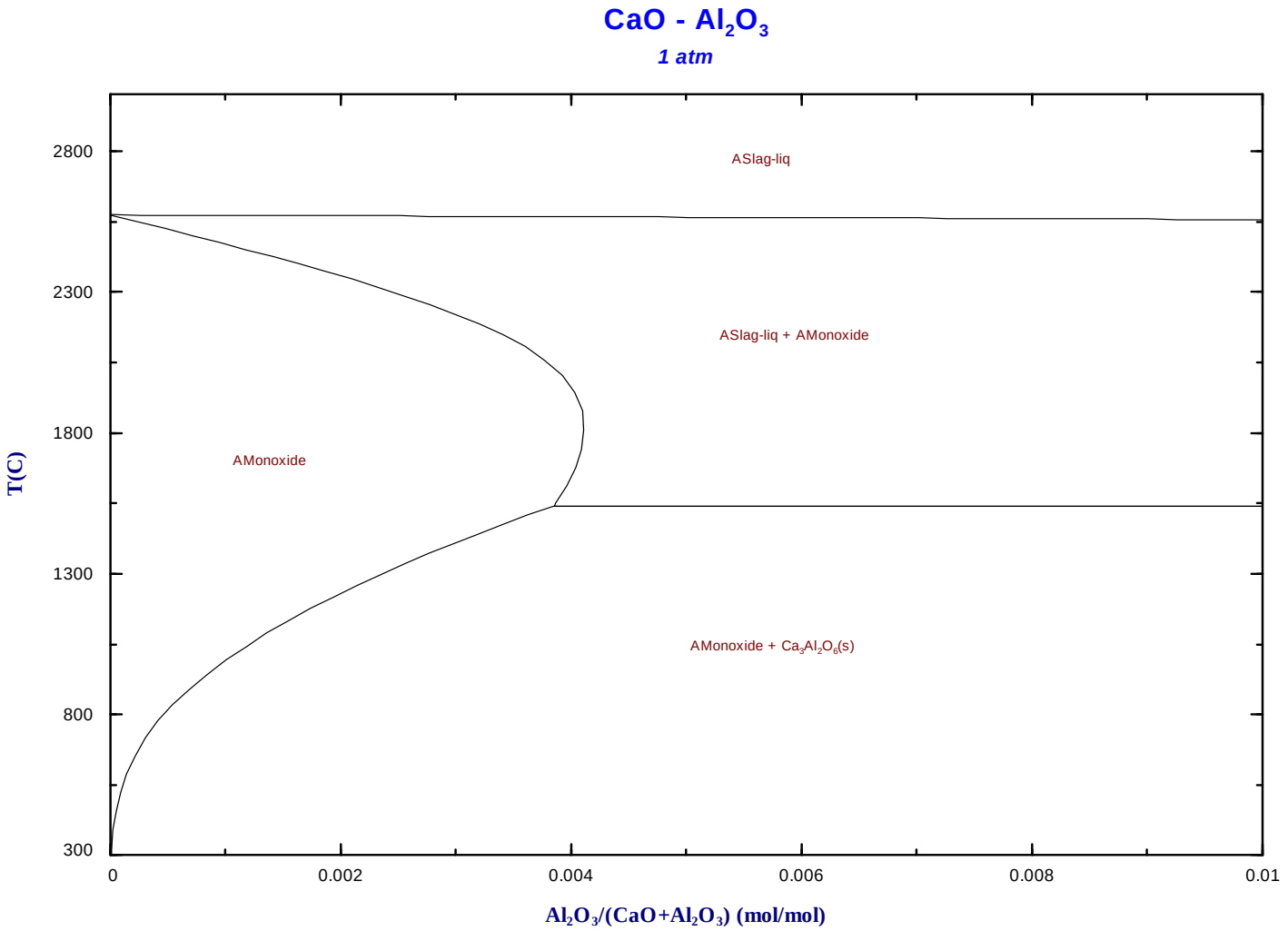

Y - Ce - Co
Projection - formation (LIQUID), 1 atm
Ce/(Y+Ce+Co) (mol/mol)
Co/(Y+Ce+Co) (mol/mol)
0.05
0.04
0.03
0.02
0.01
0
0
0.01
0.02
0.03
0.04
0.05
HCP_A3 + CoY3(s)
BCC_A2
HCP_A3

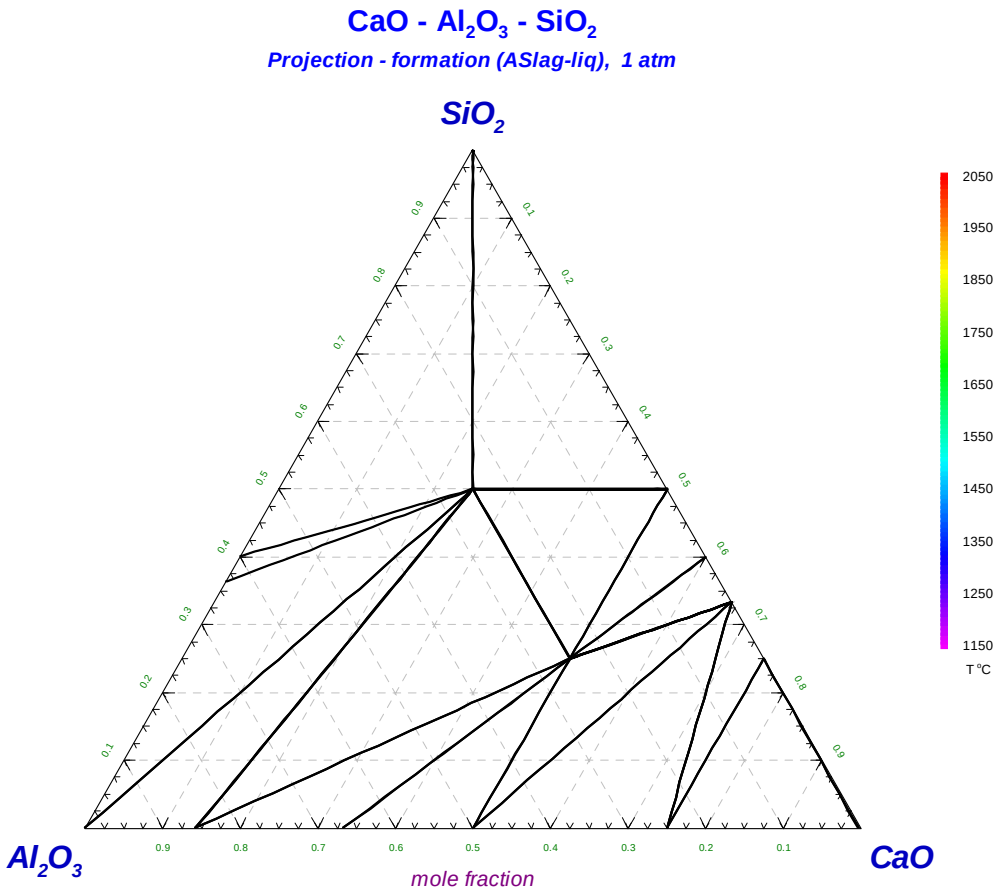
Ca-Zn: retrograde solubility
Ca-Li: catatectics
Li-Zn: not evaluated




CaO - Al2O3 - SiO2
Projection - formation (ASlag-liq), 1 atm
SiO2
Al2O3
CaO
mole fraction
2050
1950
1850
1750
1650
1550
1450
1350
1250
1150
T °C


CaO - Al2O3
Data from FToxid - FACT oxide database 2010
Temperature (°C)
mole Al2O3/(CaO+Al2O3)
ASlag-liq
ASlag-liq + AMonoxide
ASlag-liq + Al2O3(s4)
2572°
2054°
1539°
1362°
1604°
1597°
1765°
1754°
1833°
0.004
0.292
0.354
0.525
0.703
0.766
Ca3Al2O6
CaAl2O4
CaAl4O7
CaAl12O19
3000
2700
2400
2100
1800
1500
1200
900
600
300
0
0.2
0.4
0.6
0.8
1


CaO - Al2O3
1 atm
ASlag-liq
ASlag-liq + AMonoxide
AMonoxide
AMonoxide + Ca3Al2O6(s)
T(C)
2800
2300
1800
1300
800
300
0
0.002
0.004
0.006
0.008
0.01
Al2O3/(CaO+Al2O3) (mol/mol)


CaO - Al2O3 - SiO2
Projection - formation (ASlag-liq), 1 atm
SiO2
Al2O3
CaO
mole fraction
2050
1950
1850
1750
1650
1550
1450
1350
1250
1150
T °C

State-of-the-art solidus vs. first-melting-temperature projection

- Solidus projection works acceptably with FactSage 6.3.
- For solidus projection in FactSage 6.4, temperature would have to be scanned along the phase diagram axes to explore whether or not the system to be calculated exhibits retrograde solubilities or catatectics. When this is found to be the case, a first-melting-temperature projection would have to be executed.

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Thank you for your kind attention!