WnM-Projekt
Werkstoffe nach Maß
Tailor-made materials

M. to Baben, K. Hack

GTT-Technologies

GTT User Meeting, 30.6.2016

Outline

- Contributing to WnM
- Using SpMCBN database
- Navigating 10-D chemical space
- Predicting phase formation

Contributing to WnM

Hard alloys based on **Fe**-Mn-Cr-Ti-V-Ni-Al-Si-C-B.

Identification of compositions for hard alloys containing:

- **martensite and ferrite**
- **austenite**
- **metastable austenite**
- **intermetallic phases stable over wide T-range**

The SpMCBN database

- Spencer Group Non-Oxide Refractories Database
- **B, C, N, Si**
- **Me = Al, Ca, Co, Cr, Fe, Hf, Mg, Mn, Mo, Nb, Ni, Re, Sc, Ta, Tc, Ti, V, W, Y, Zr**
- Assesed ternary phase diagrams consisting of
  - Two Me combined with C, B, N or Si
  - Me combined with two of C, B, N, Si
- 186 binary and 203 ternary systems (154 newly assessed)

Outline

- Contributing to WnM
- Using SpMCBN database
- **Navigating 10-D chemical space**
- Predicting phase formation

Chemical Space – travelling by trial and error

Chemical Space – navigating by thermodynamics

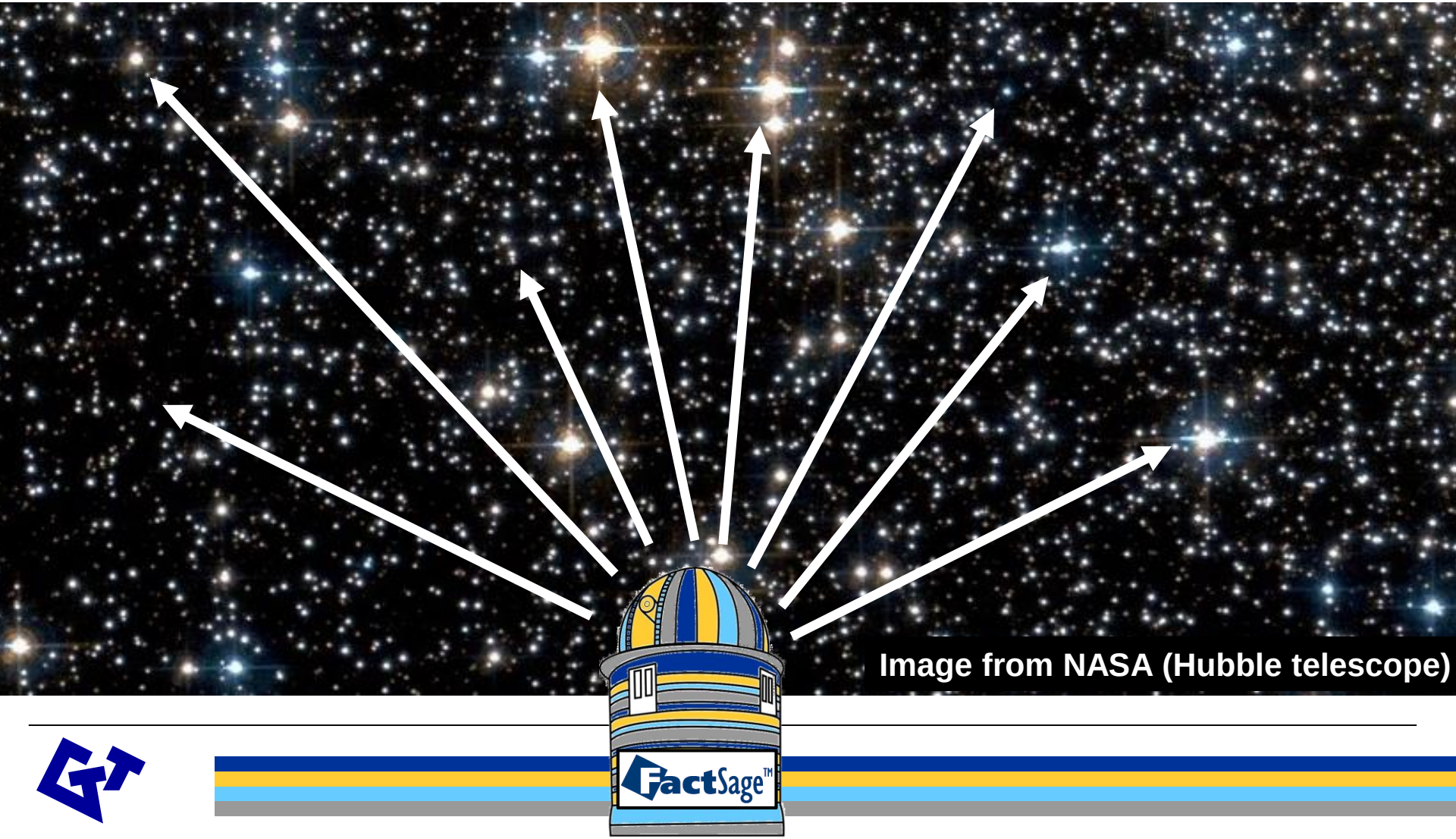


Image from NASA (Hubble telescope)

Chemical Space – navigating by thermodynamics

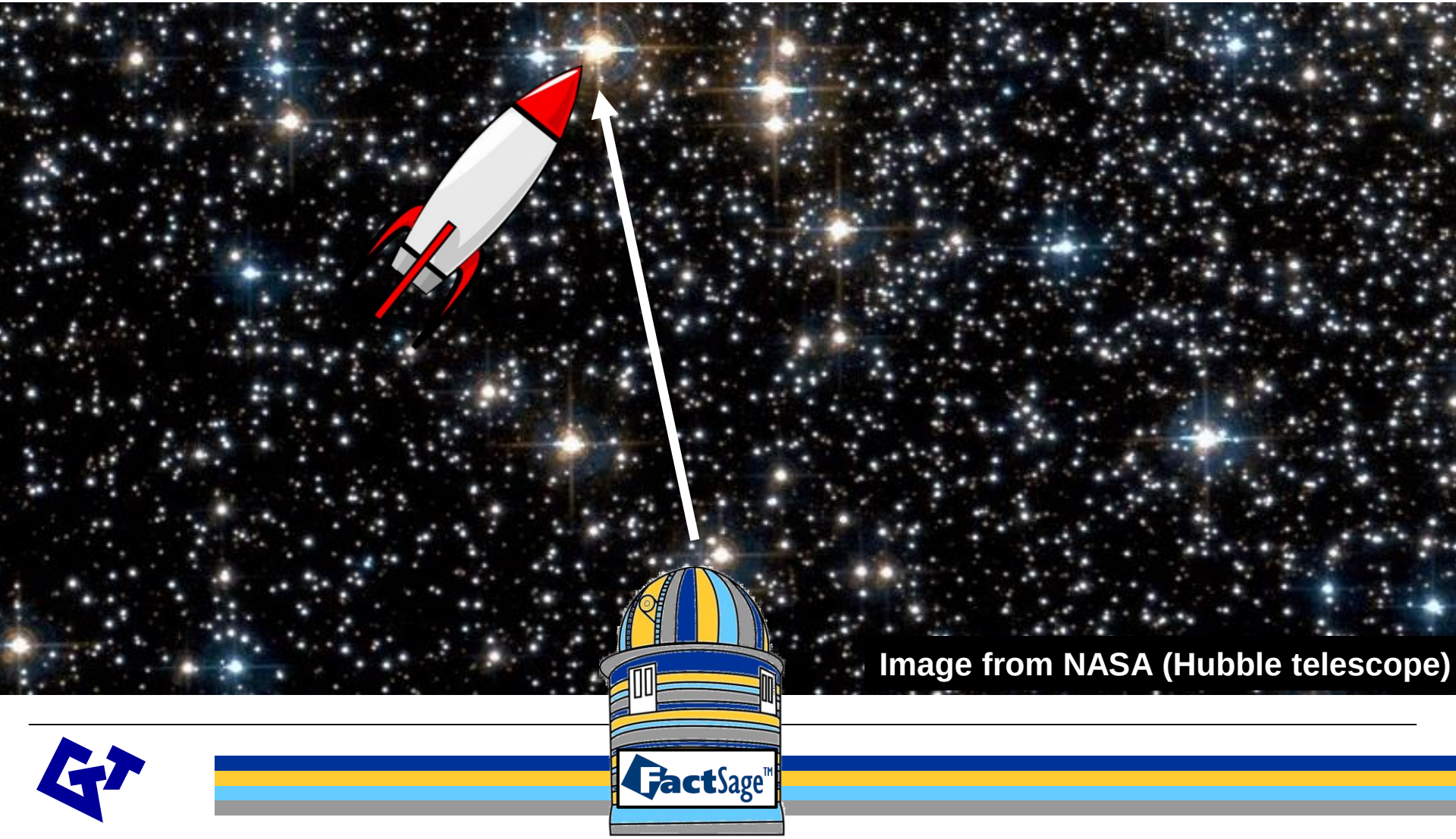
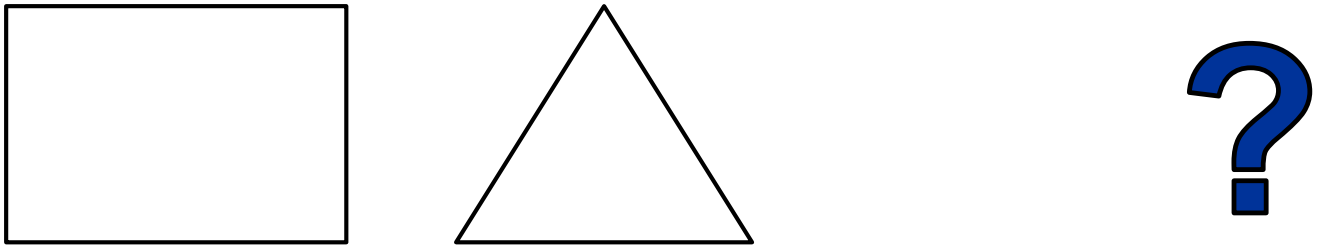


Image from NASA (Hubble telescope)

Chemical Space

Binary – Ternary – … – Denary



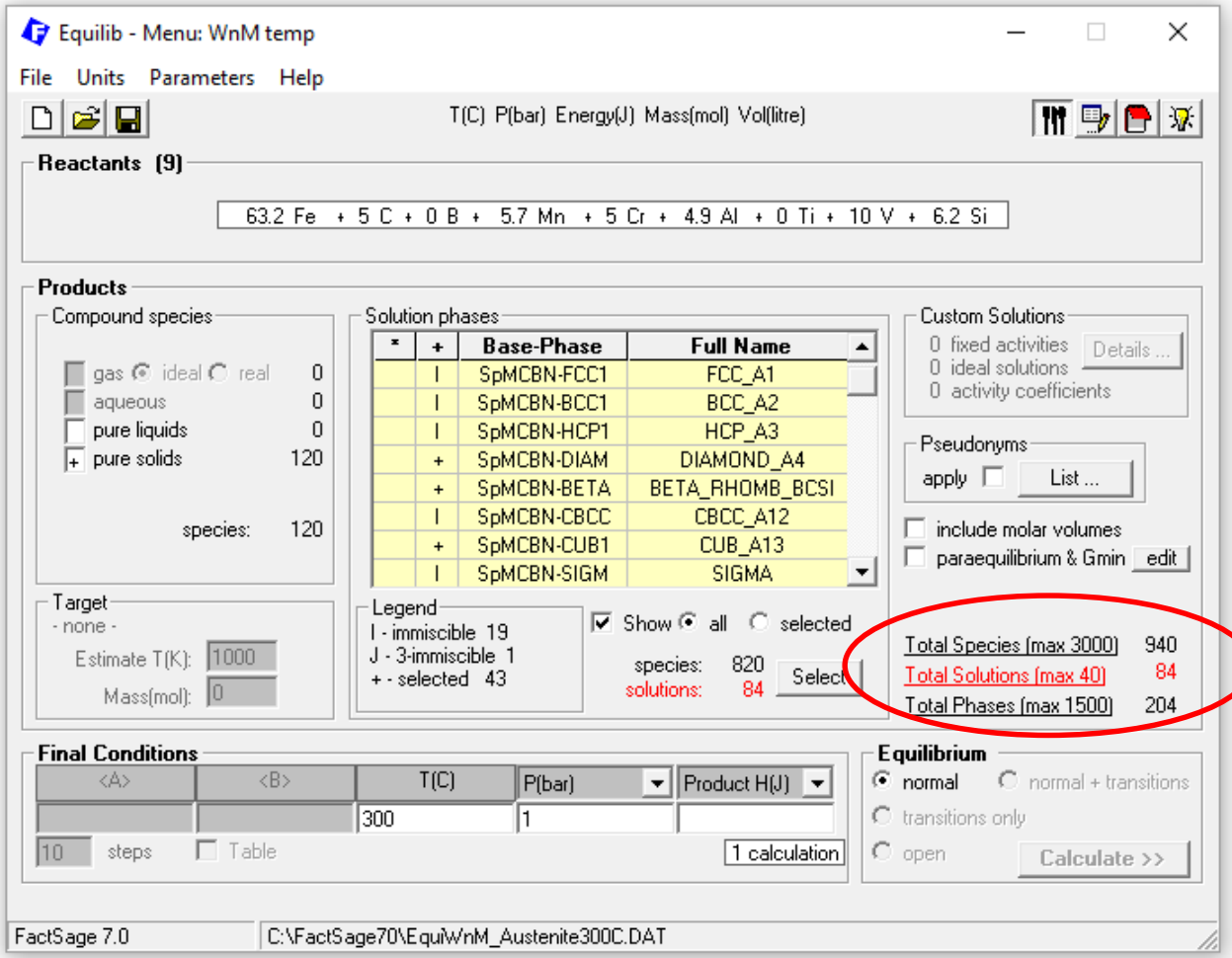
Navigating 10-dimensional chemical space

→ „Everything“ is possible to form

→ But: Nothing is possible to plot

→ Navigation using macros

Navigating 10-D chemical space

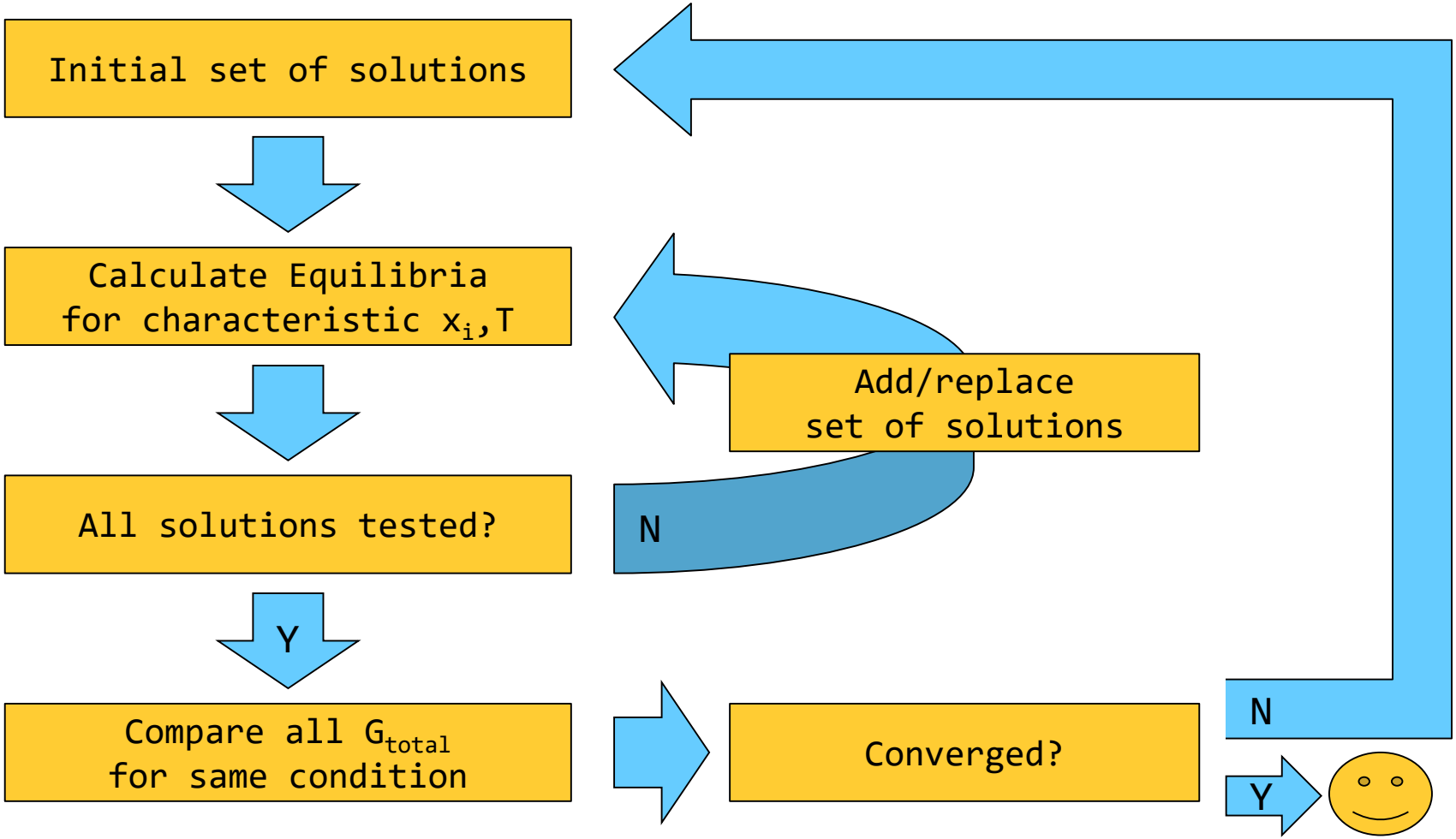


FactSage™

Restriction: number of solutions ≤ 40.

Solution: Automated search for relevant solutions.

Navigating 10-D chemical space



Navigating 10-D chemical space

Hard alloys based on **Fe**-Mn-Cr-Ti-V-Ni-Al-Si-C-B.

Identification of compositions for hard alloys containing:

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- **austenite**
- **metastable austenite**
- **intermetallic phases stable over wide T-range**

Navigating 10-D chemical space

Hard alloys based on **Fe**-Mn-Cr-Ti-V-Ni-Al-Si-C-B.

→ SEARCH MATRIX

Fe	60	70	80	
C	0	5	10	20
B	0	5	10	20
Mn	0	5	10	20
Cr	0	5	10	20
Ti	0	5	10	20
V	0	5	10	20
Al	0	5	10	20
Ni	0	10		
Si	0	10		

3277 combinations with $\Sigma n_i = 100$.

(avoid Ni to avoid cold welding)

Navigating 10-D chemical space

Hard alloys based on **Fe**-Mn-Cr-Ti-V-Ni-Al-Si-C-B.

Identification of compositions for hard alloys containing: → SEARCH CRITERIA

- **martensite and ferrite** @RT: BCC, @HT: BCC/FCC
- **austenite** @RT: FCC, @HT: FCC
- **metastable austenite** @RT: $G_{FCC}=G_{BCC}$, @HT: FCC
  @RT: $G_{FCC}=G_{HCP}$, @HT: FCC
- **intermetallic phases stable over wide T-range**
  Equilibrium @RT = Equilibrium @HT

Navigating 10-D chemical space

Hard alloys based on **Fe**-Mn-Cr-Ti-V-Ni-Al-Si-C-B.

Identification of compositions for hard alloys containing: → SEARCH CRITERIA

- **martensite and ferrite** @RT: BCC, @HT: BCC/FCC
- **austenite** **@RT: FCC, @HT: FCC**
- **metastable austenite** @RT: $G_{FCC}=G_{BCC}$, @HT: FCC
  @RT: $G_{FCC}=G_{HCP}$, @HT: FCC
- **intermetallic phases stable over wide T-range**
  Equilibrium @RT = Equilibrium @HT

Searching for austenite

3277 compositions tested @T=300, 500, 700°C.

2380 compositions without Ni.

280 compositions without BCC phase @700°C.

53 compositions without BCC phase @500°C.

5 compositions without BCC phase @300°C.

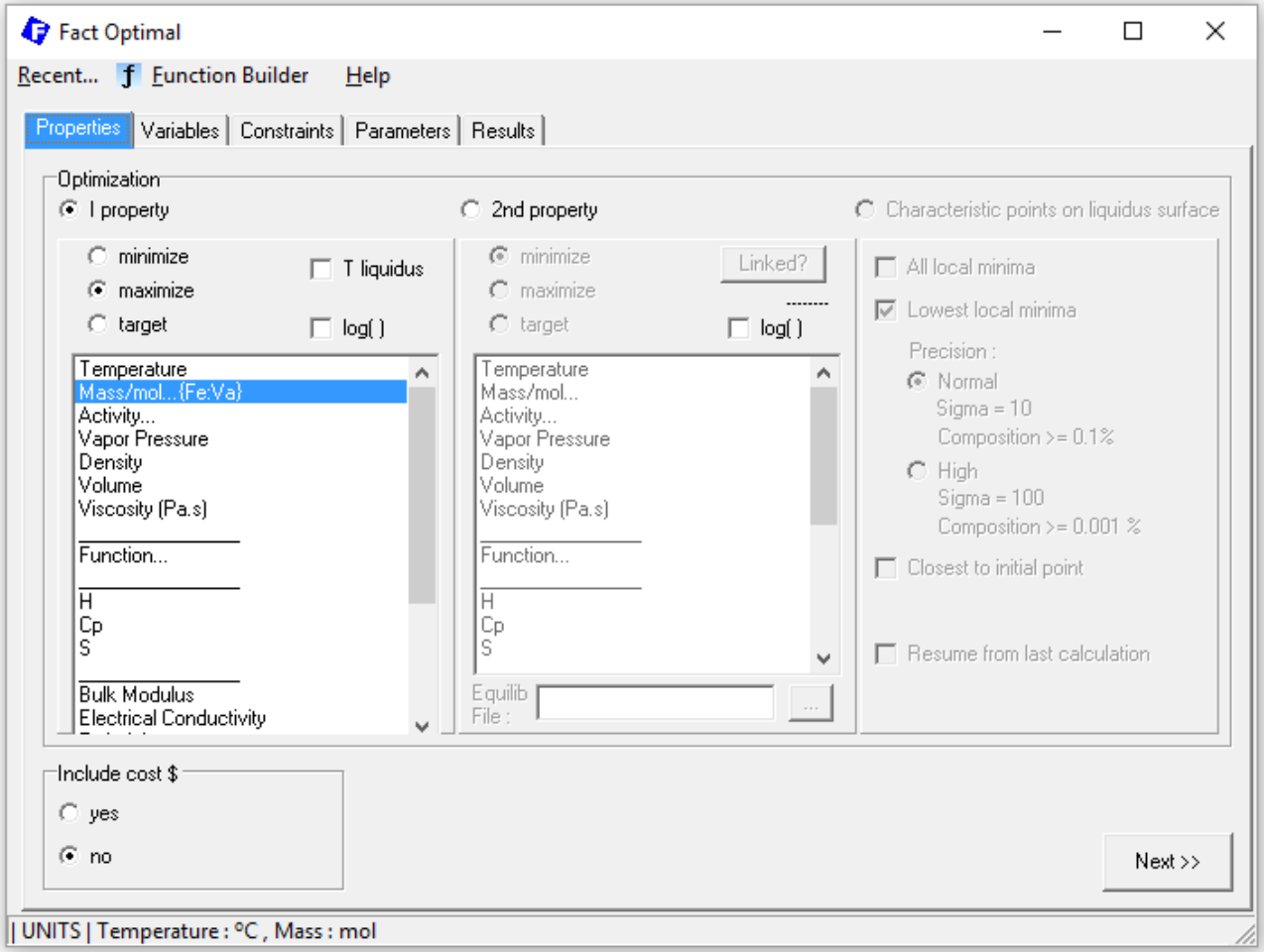
Searching for austenite

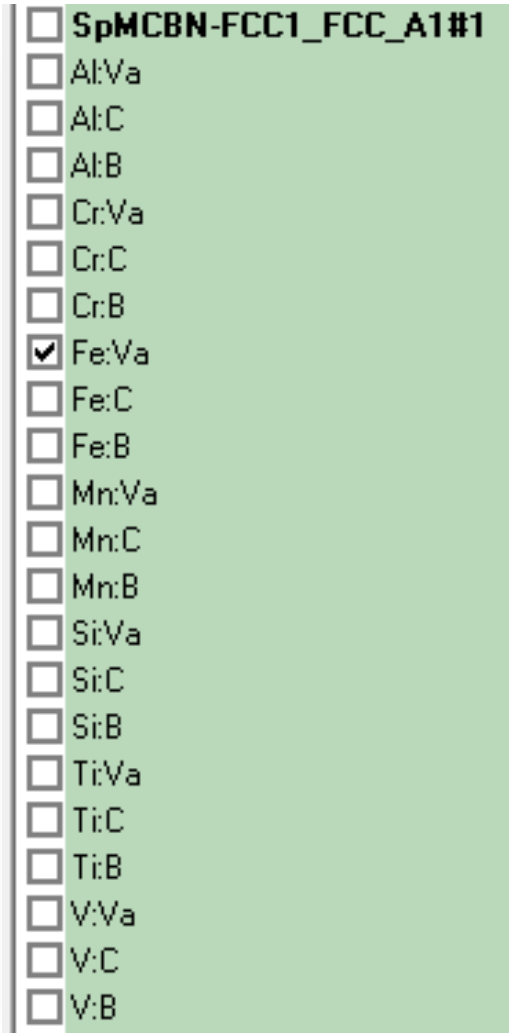
5 compositions without BCC phase @300°C:

Fe	C	B	Mn	Cr	Al	Ti	V	Si	FCC fraction
60	0	0	20	0	0	20	0	0	40%

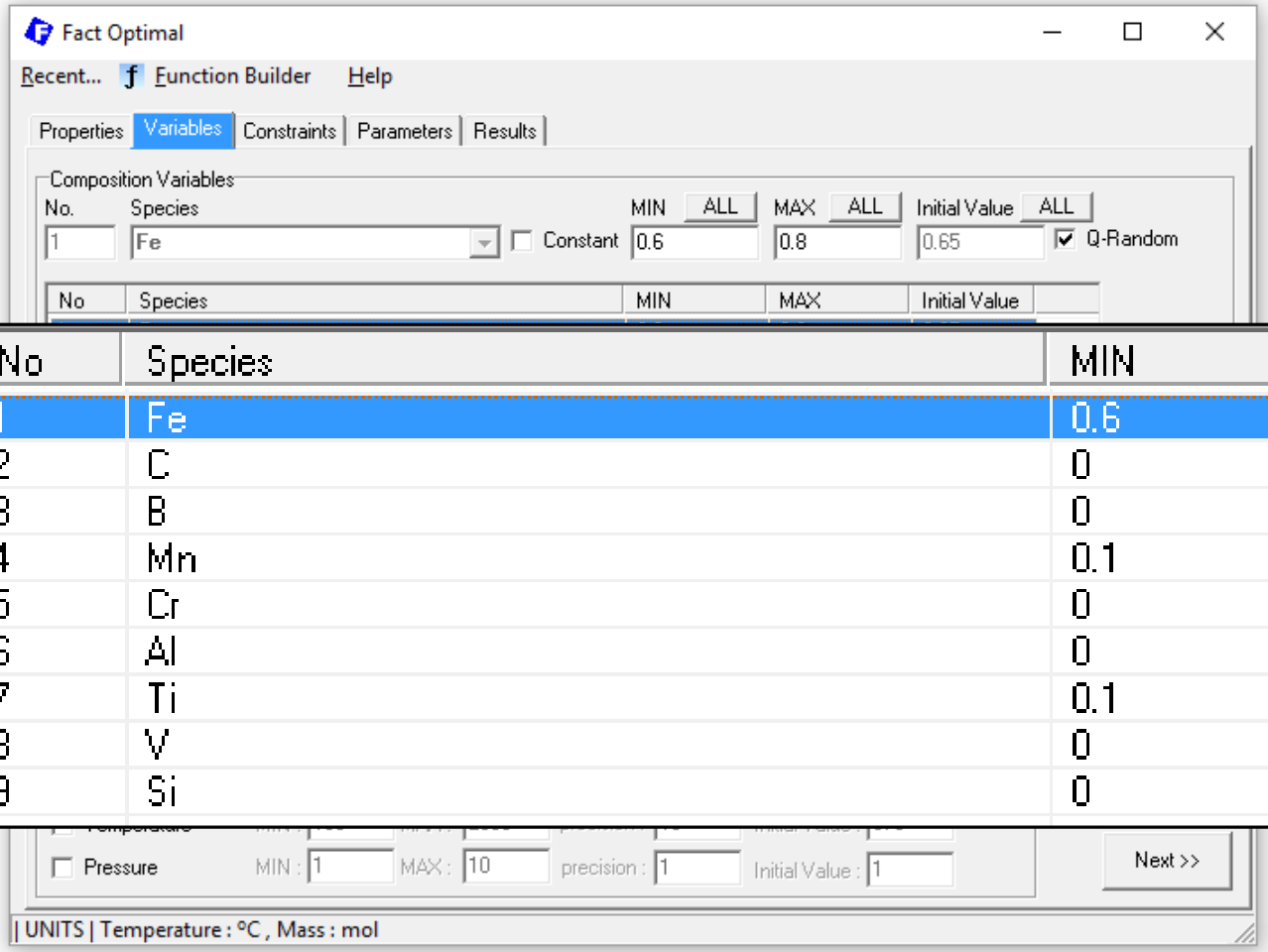
→ Input for Fact-Optimal

Fact-Optimal



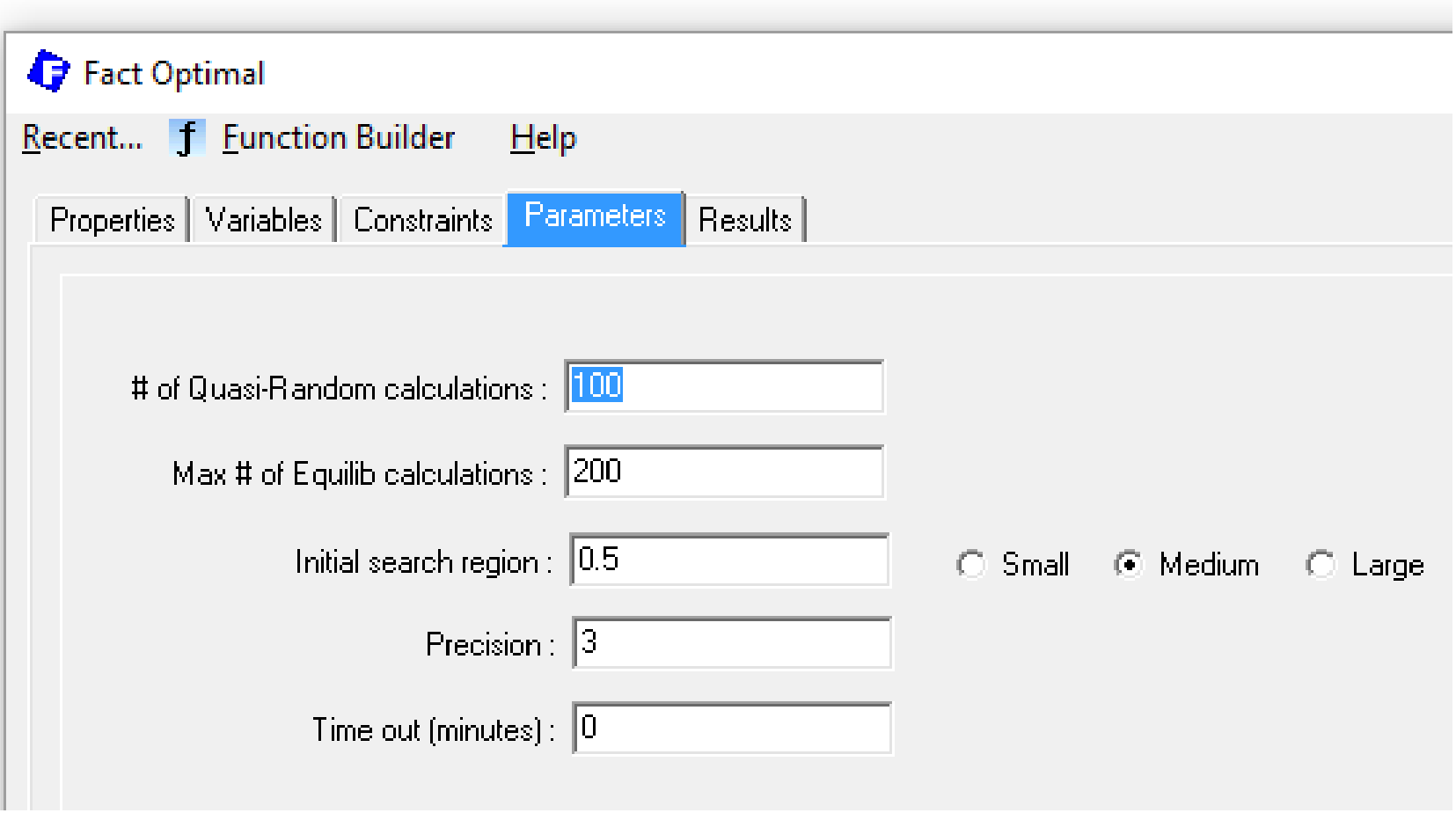


Fact-Optimal



No	Species	MIN	MAX	Initial Value
1	Fe	0.6	0.8	0.65
2	C	0	0.05	0
3	B	0	0.05	0
4	Mn	0.1	0.2	0.16
5	Cr	0	0.1	0
6	Al	0	0.1	0
7	Ti	0.1	0.2	0.19
8	V	0	0.1	0
9	Si	0	0.1	0

Fact-Optimal



Fact Optimal

Recent... Function Builder Help

Properties | Variables | Constraints | Parameters | Results

Stop

0:13:56

Status : Done.

Continue Run >>

```
600  1  0  100  0  1  100  100  23  0  −98  −1.9999
618  26  0  200  0  0  158  0  0  −999999999  2  −1
612  28  1  198  1  2  156  1  2  −0.325013000000
```

Number of Equilib calculations: 283/300

Best answer so far :

Mass/mol...{Fe:Va} : **3.390E-01**

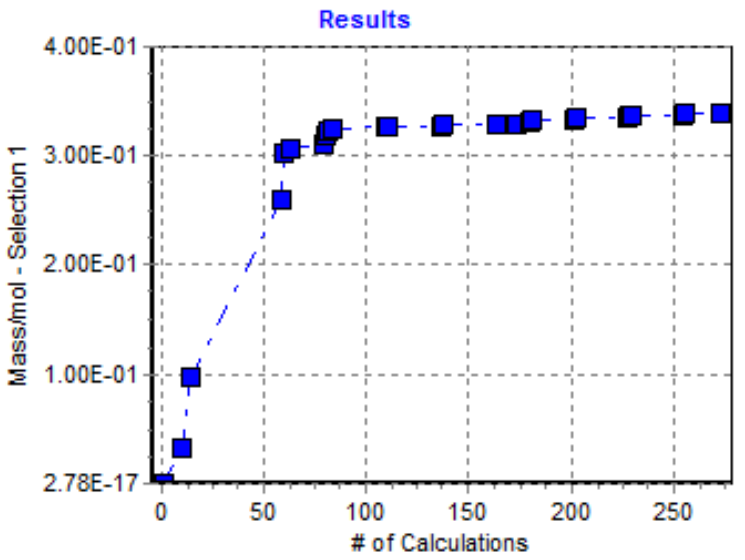
Last solution :

Species	mol
Fe	0.615
C	0.027
B	0
Mn	0.2
Cr	0
Al	0
Ti	0.157
V	0
Si	0.001

Open in Equilib

Save Pareto points

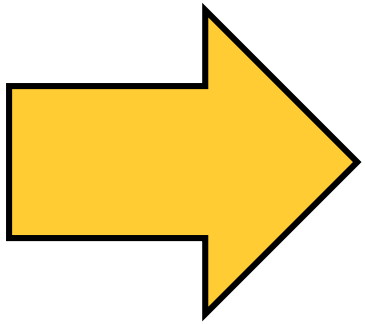
Constraints :



| UNITS | Temperature : °C , Mass : mol

Searching for austenite

Fe	C	B	Mn	Cr	Al	Ti	V	Si	FCC fraction
60	0	0	20	0	0	20	0	0	40%
61.5	2.7	0	20	0	0	15.7	0	0.1	54%



FCC_A1#1	**53.7 mol**
FCC_A1#2	**3.1 mol**
BCC_A2#1	**2.7 mol**
LAVES_C14#1	**12.5 mol**
Ti3SiC2(s)	**0.1 mol**

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- Contributing to WnM
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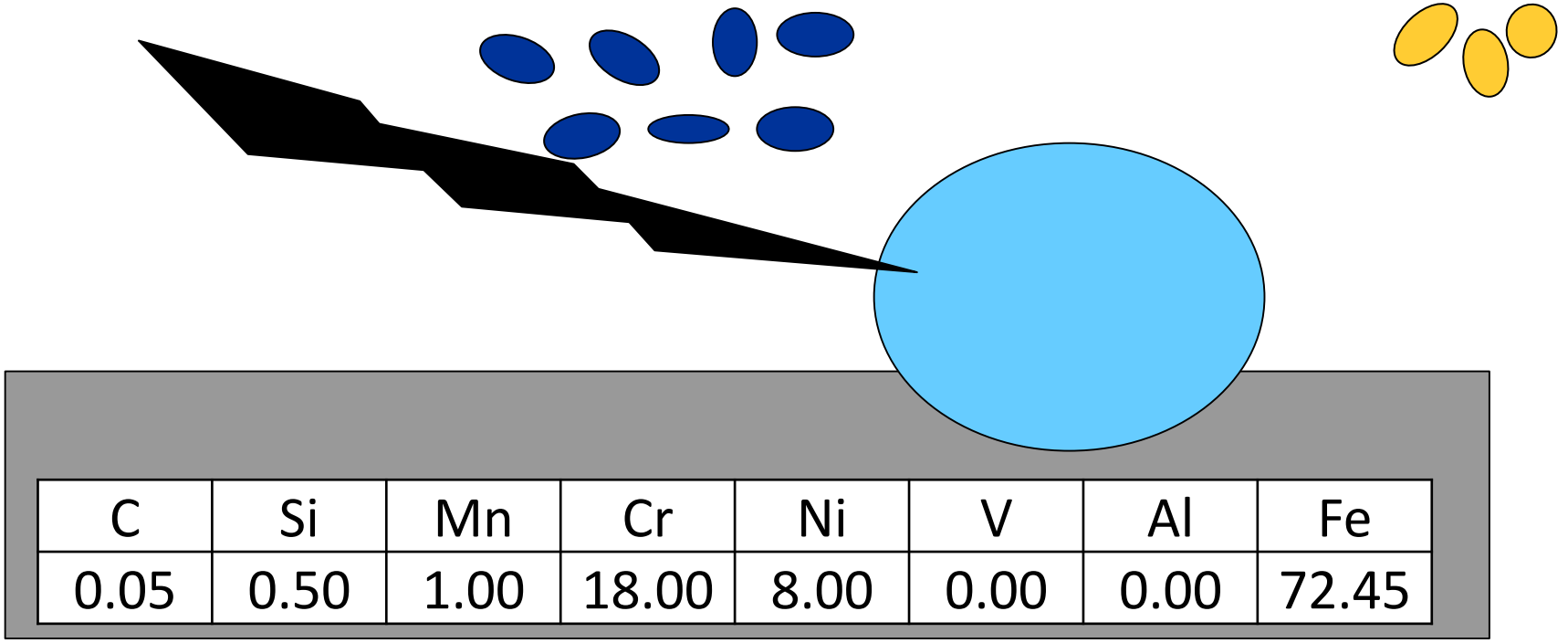
- **Predicting phase formation**

Predicting phase formation

SiC content α = 30%

C	Si	Mn	Cr	Ni	V	Al	Fe
0.059	1.95	23.72	14.51	0.70	22.33	0.88	35.84

SiC
100



C	Si	Mn	Cr	Ni	V	Al	Fe
0.05	0.50	1.00	18.00	8.00	0.00	0.00	72.45

Predicting phase formation

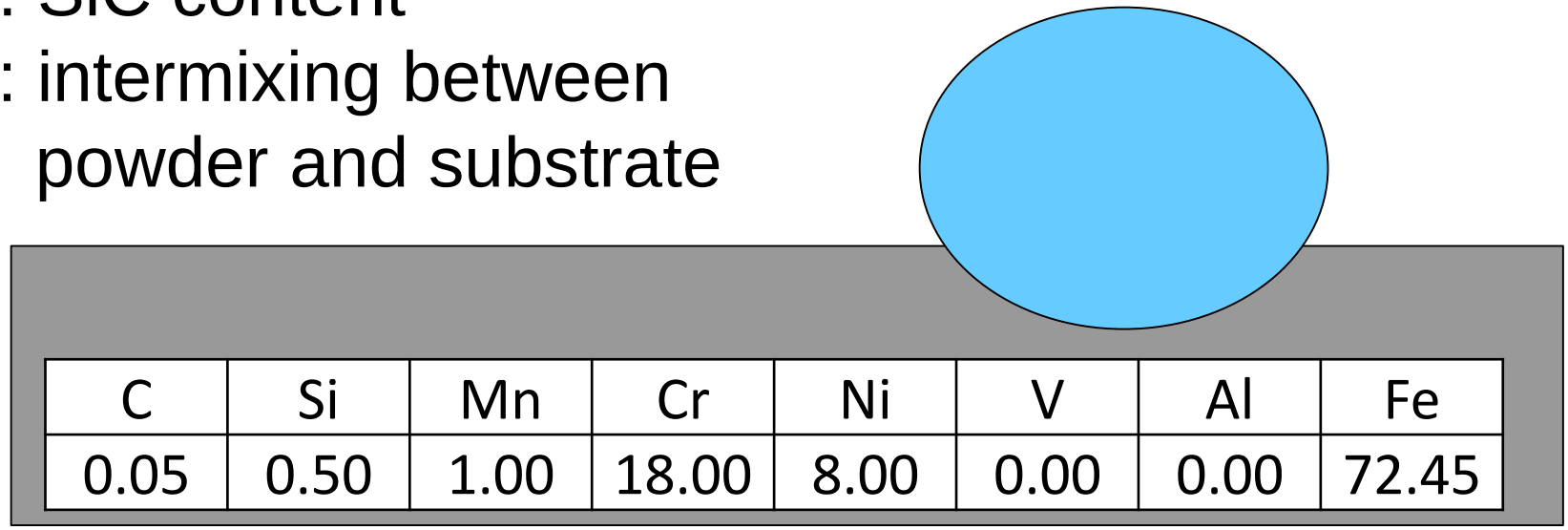
C	Si	Mn	Cr	Ni	V	Al	Fe
0.059	1.95	23.72	14.51	0.70	22.33	0.88	35.84

SiC
100

Phase formation as f(α,β,T)

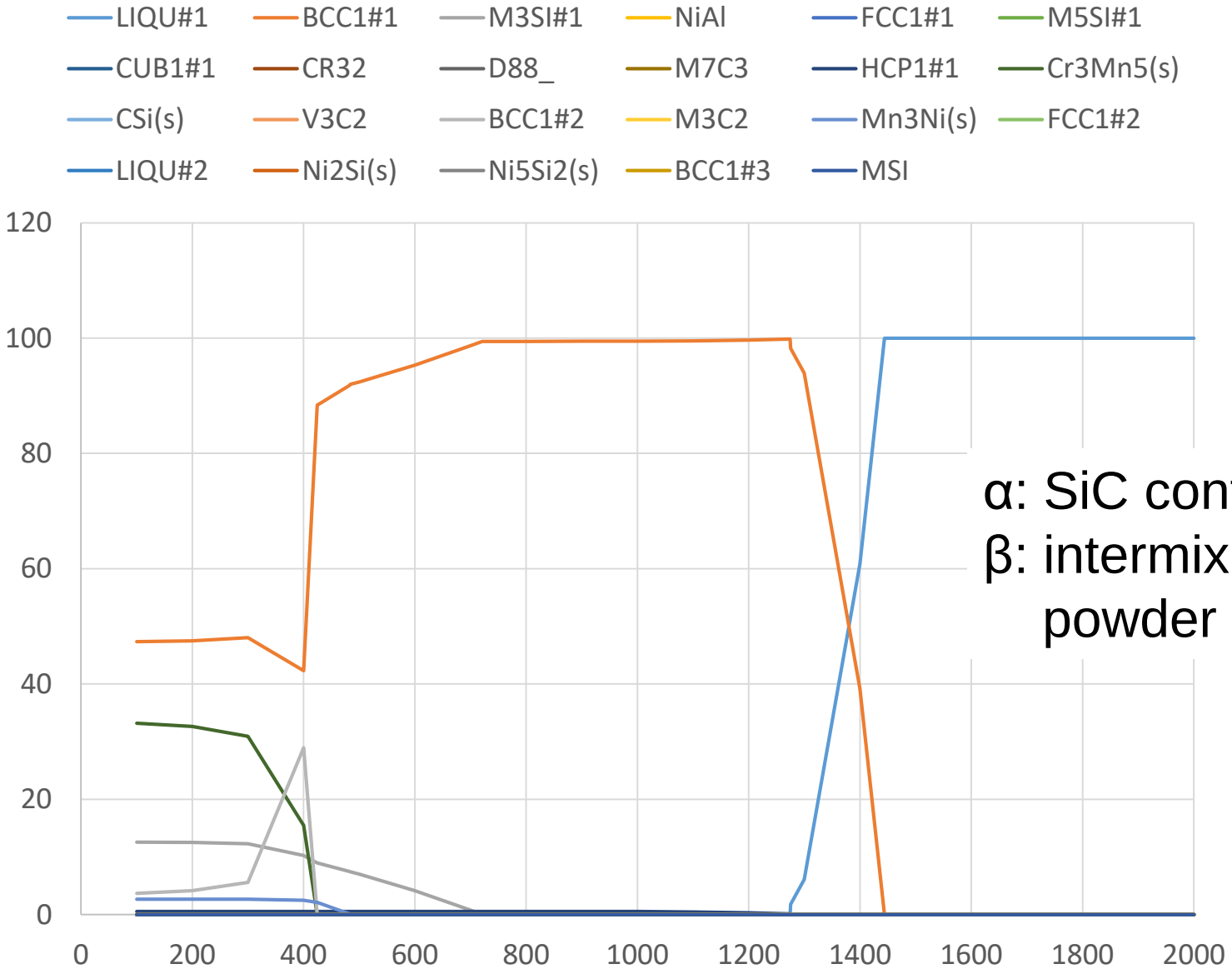
α: SiC content

β: intermixing between powder and substrate



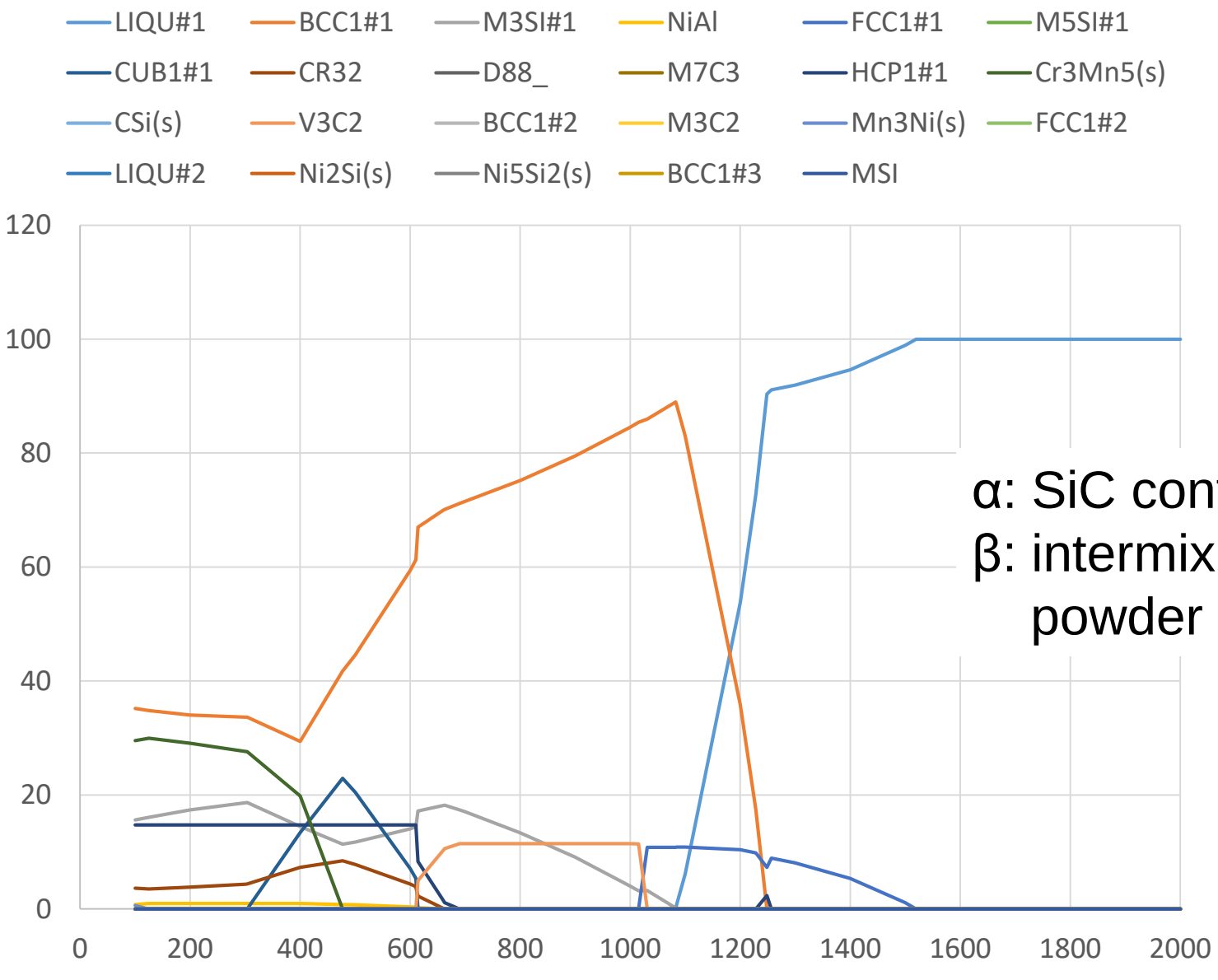
C	Si	Mn	Cr	Ni	V	Al	Fe
0.05	0.50	1.00	18.00	8.00	0.00	0.00	72.45

α = 0
β = 0



α: SiC content
β: intermixing between powder and substrate

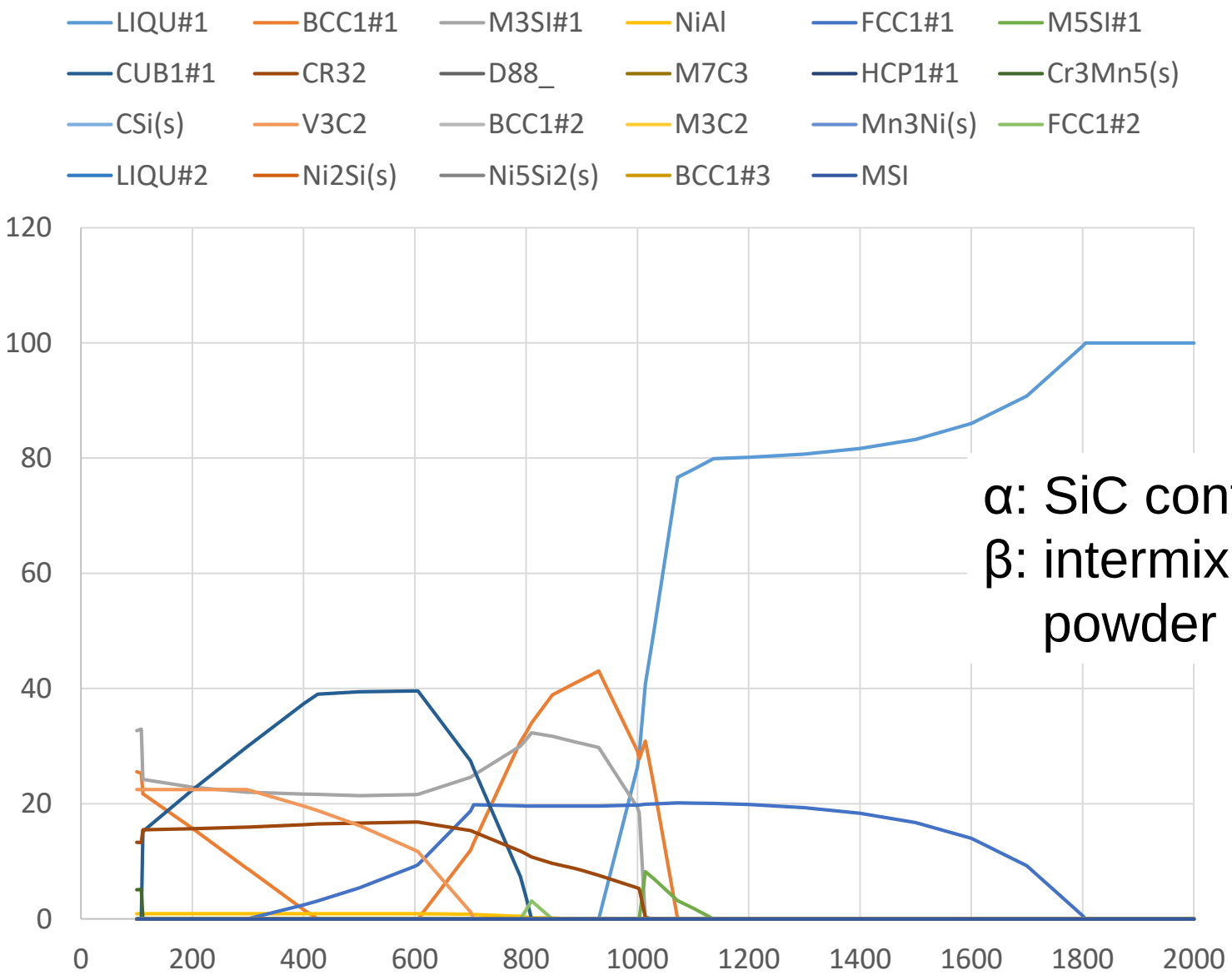
α = 0.05
β = 0



α: SiC content

β: intermixing between powder and substrate

α = 0.1
β = 0



α: SiC content

β: intermixing between powder and substrate

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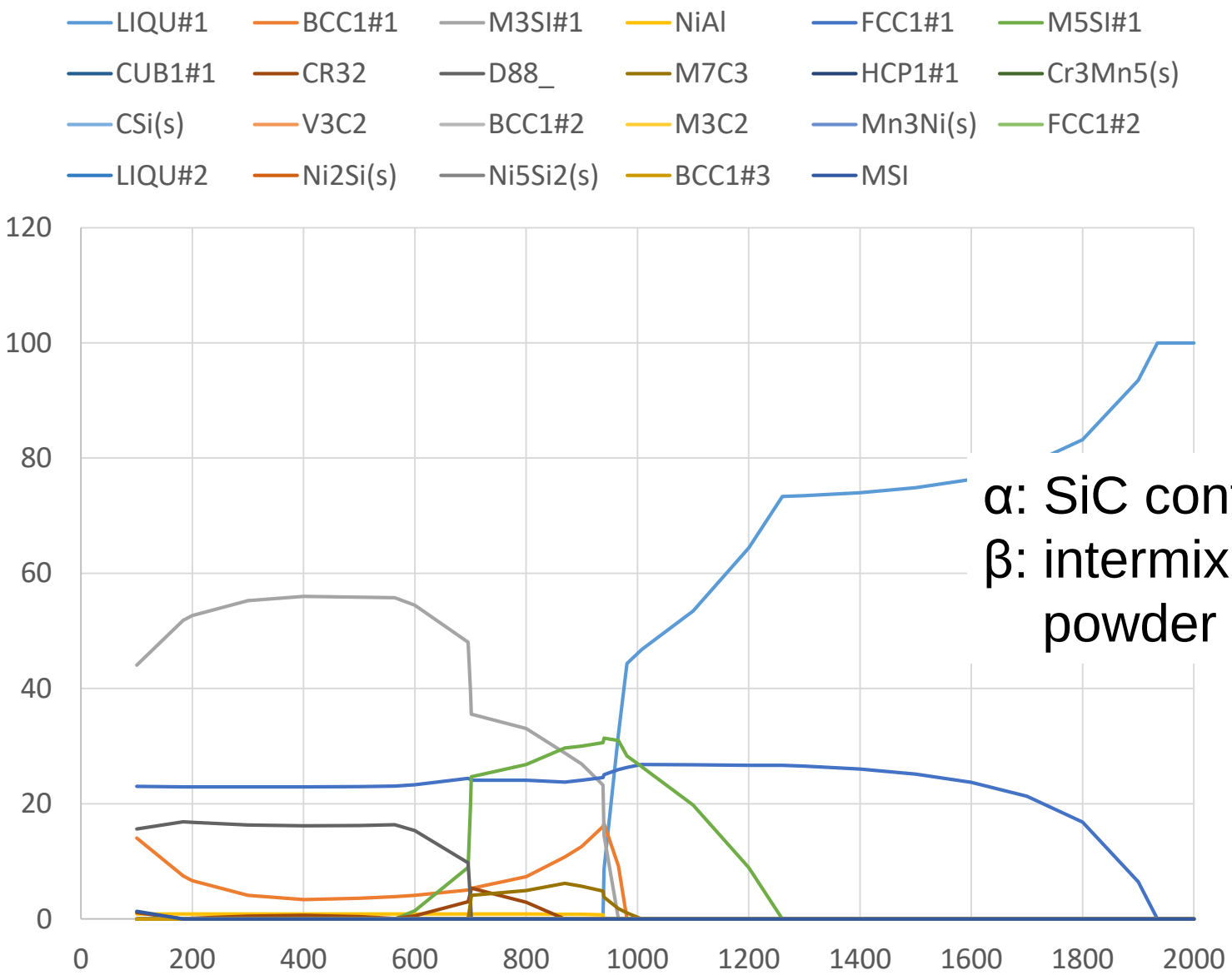
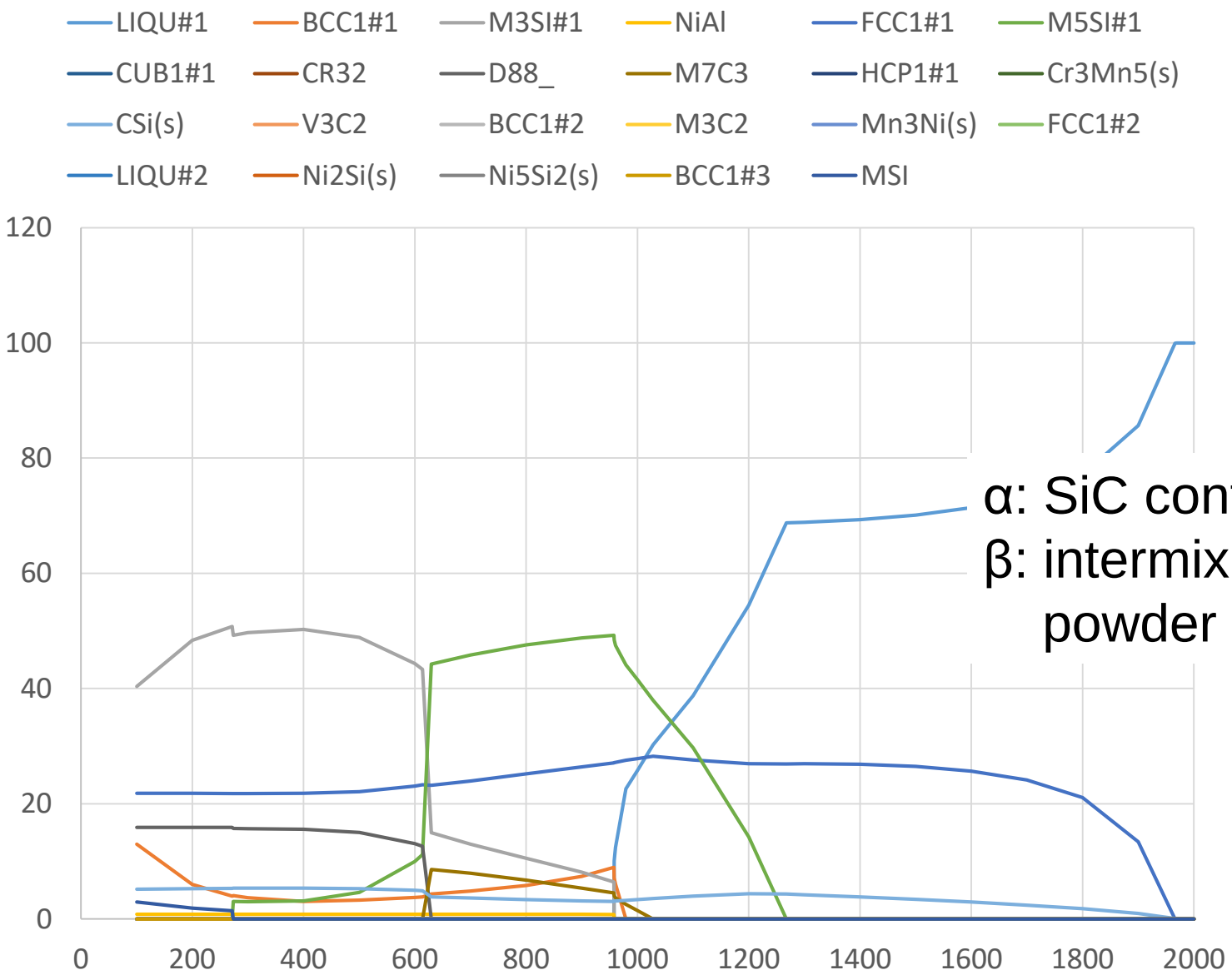
α = 0.15
β = 0



α: SiC content

β: intermixing between powder and substrate

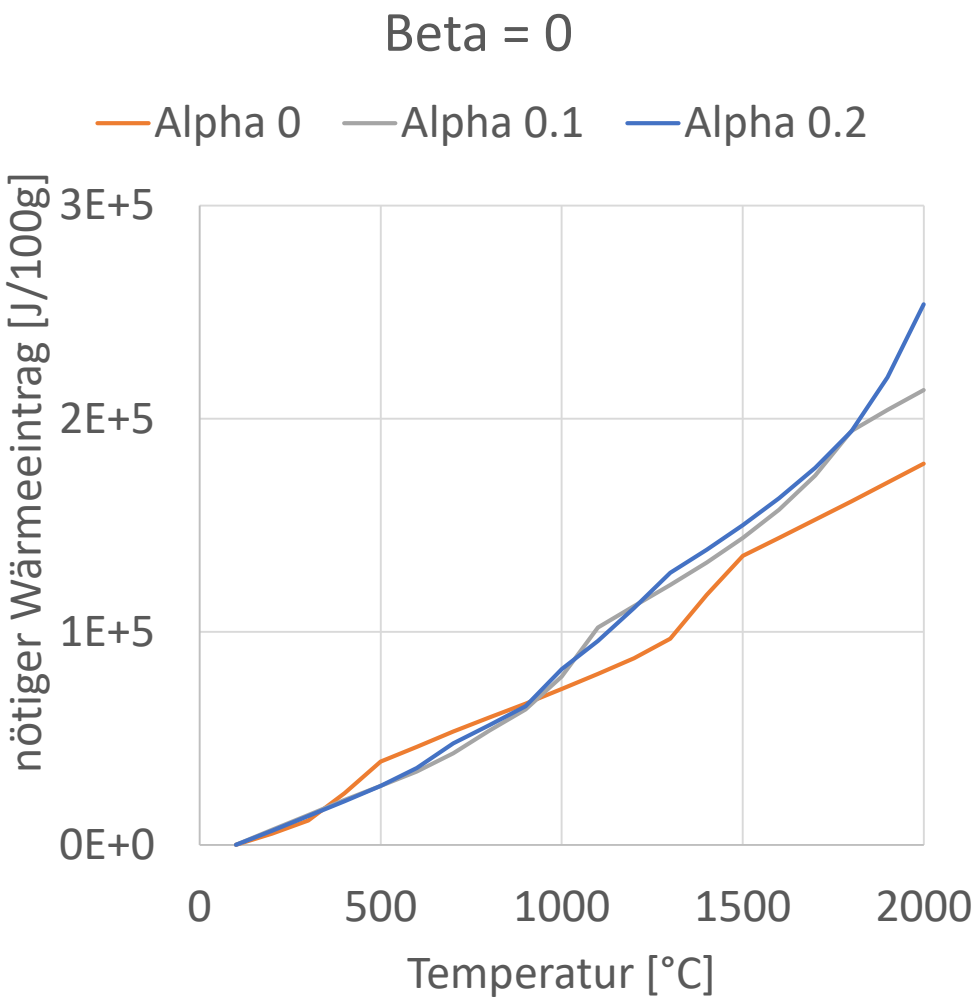
α = 0.2
β = 0

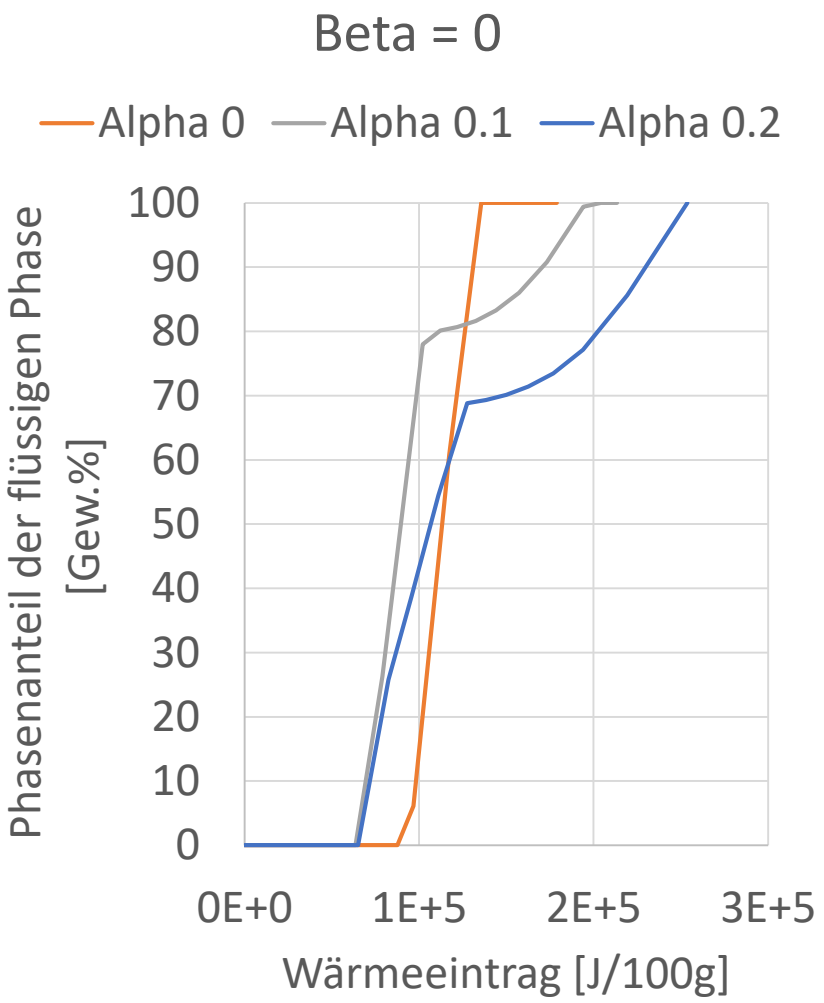


α: SiC content

β: intermixing between powder and substrate

Enthalpy


Beta = 0
Alpha 0
Alpha 0.1
Alpha 0.2
nötiger Wärmeeintrag [J/100g]
3E+5
2E+5
1E+5
0E+0
0
500
1000
1500
2000
Temperatur [°C]


Beta = 0
Alpha 0
Alpha 0.1
Alpha 0.2
Phasenanteil der flüssigen Phase [Gew.%]
100
90
80
70
60
50
40
30
20
10
0
0E+0
1E+5
2E+5
3E+5
Wärmeeintrag [J/100g]

Thank you for your attention!