

# WnM-Projekt

## Werkstoffe nach Maß *Tailor-made materials*

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GTT-Technologies

GTT User Meeting, 30.6.2016



# Outline

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



# Chemical Space

– travelling by  
trial and error



Image from NASA (Hubble telescope)



# Chemical Space

– navigating by  
thermodynamics

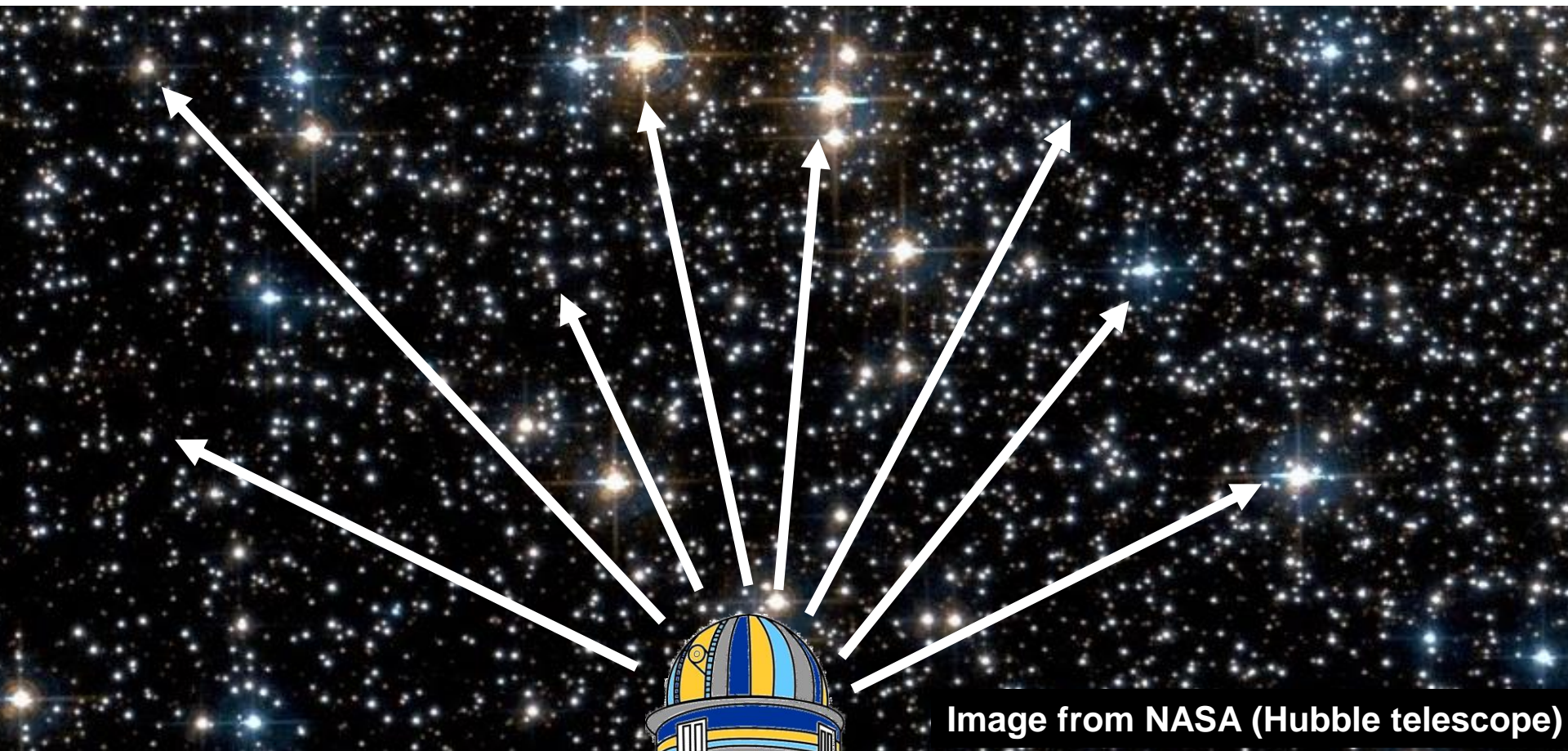


Image from NASA (Hubble telescope)



# Chemical Space

– navigating by  
thermodynamics

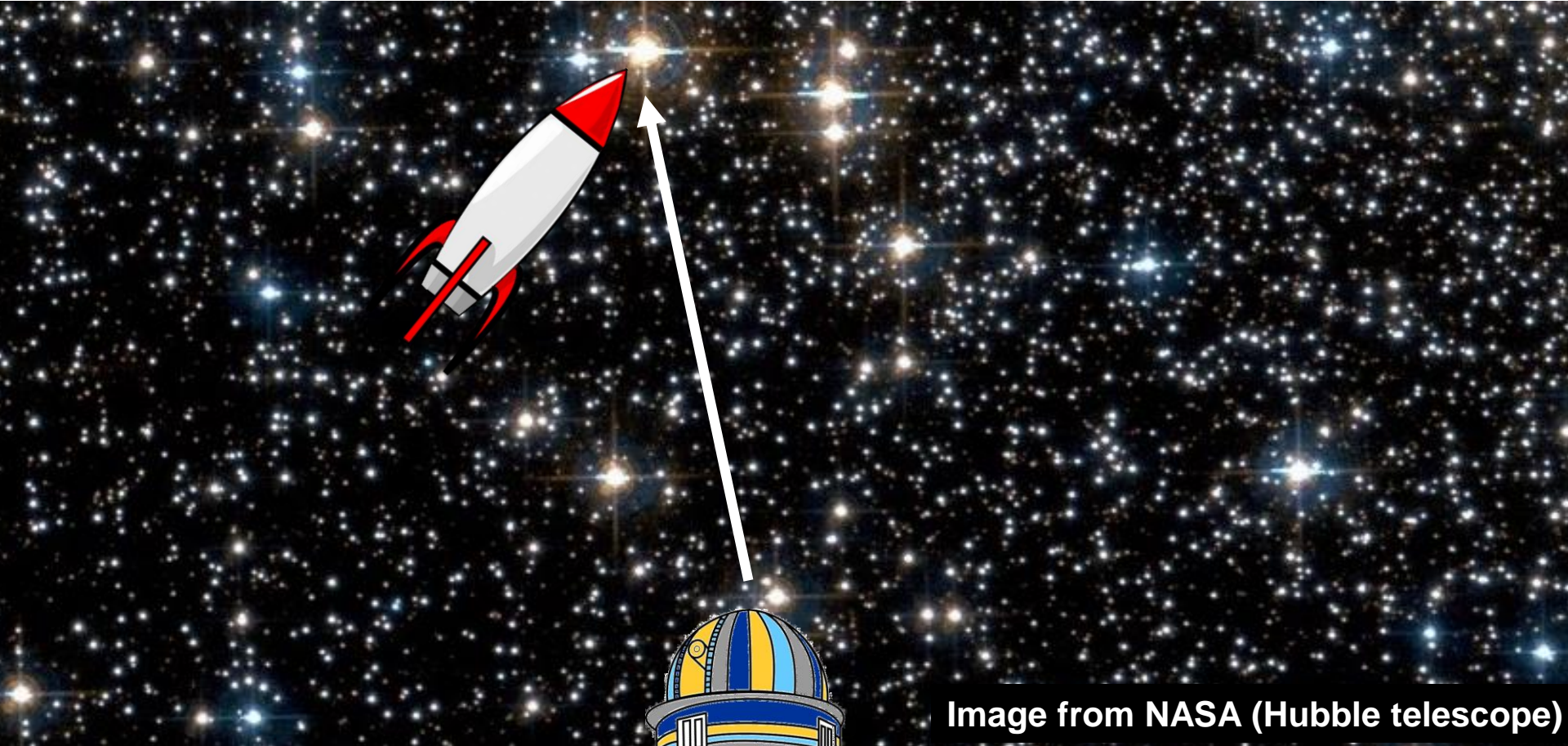


Image from NASA (Hubble telescope)





# Chemical Space

**Good and bad analogy:**

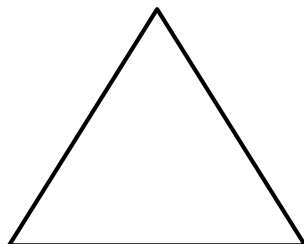
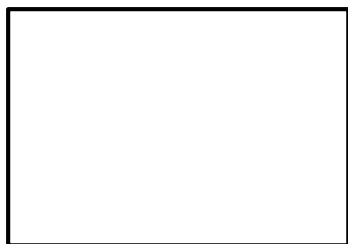
**Good: vast space**

**Bad: 3D vs 10D**

Image from NASA (Hubble telescope)



# 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



Restriction: number of solutions  $\leq 40$ .

Solution: Automated search for relevant solutions.

Equilib - Menu: WnM temp

File Units Parameters Help

T(C) P(bar) Energy(J) Mass(mol) Vol(litre)

Reactants (9)

63.2 Fe + 5 C + 0 B + 5.7 Mn + 5 Cr + 4.9 Al + 0 Ti + 10 V + 6.2 Si

Products

Compound species

gas  ideal  real 0

aqueous 0

pure liquids 0

pure solids 120

species: 120

Target

- none -

Estimate T(K): 1000

Mass(mol): 0

Solution phases

*	+	Base-Phase	Full Name
	I	SpMCBN-FCC1	FCC_A1
	I	SpMCBN-BCC1	BCC_A2
	I	SpMCBN-HCP1	HCP_A3
	+	SpMCBN-DIAM	DIAMOND_A4
	+	SpMCBN-BETA	BETA_RHOMB_BCSI
	I	SpMCBN-CBCC	CBCC_A12
	+	SpMCBN-CUB1	CUB_A13
	I	SpMCBN-SIGM	SIGMA

Legend

I - immiscible 19

J - 3-immiscible 1

+ - selected 43

Custom Solutions

fixed activities Details ...

ideal solutions

activity coefficients

Pseudonyms

apply  List ...

include molar volumes

paraequilibrium & Gmin edit

species: 820

solutions: 84

Total Species (max 3000) 940

Total Solutions (max 40) 84

Total Phases (max 1500) 204

Final Conditions

<A>	<B>	T(C)	P(bar)	Product H(J)
		300	1	

10 steps  Table 1 calculation

Equilibrium

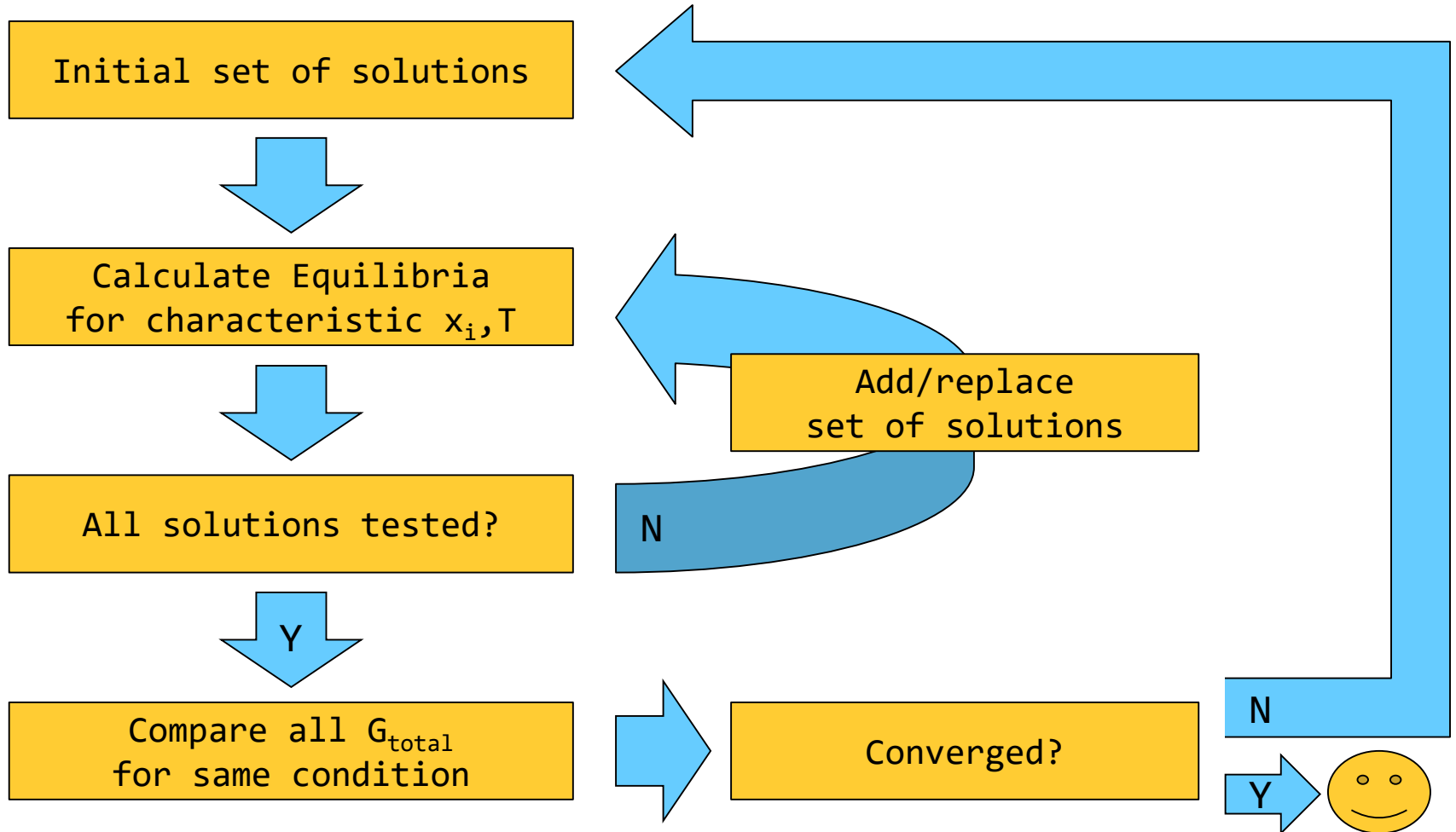
normal  normal + transitions

transitions only

open Calculate >>

FactSage 7.0 C:\FactSage70\EquiWnM\_Austenite300C.DAT

# 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:

- **martensite and ferrite**
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- **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  $\sum n_i = 100$ .

(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:  $G_{\text{FCC}}=G_{\text{BCC}}$ , @HT: FCC  
@RT:  $G_{\text{FCC}}=G_{\text{HCP}}$ , @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:  $G_{\text{FCC}}=G_{\text{BCC}}$ , @HT: FCC  
@RT:  $G_{\text{FCC}}=G_{\text{HCP}}$ , @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.



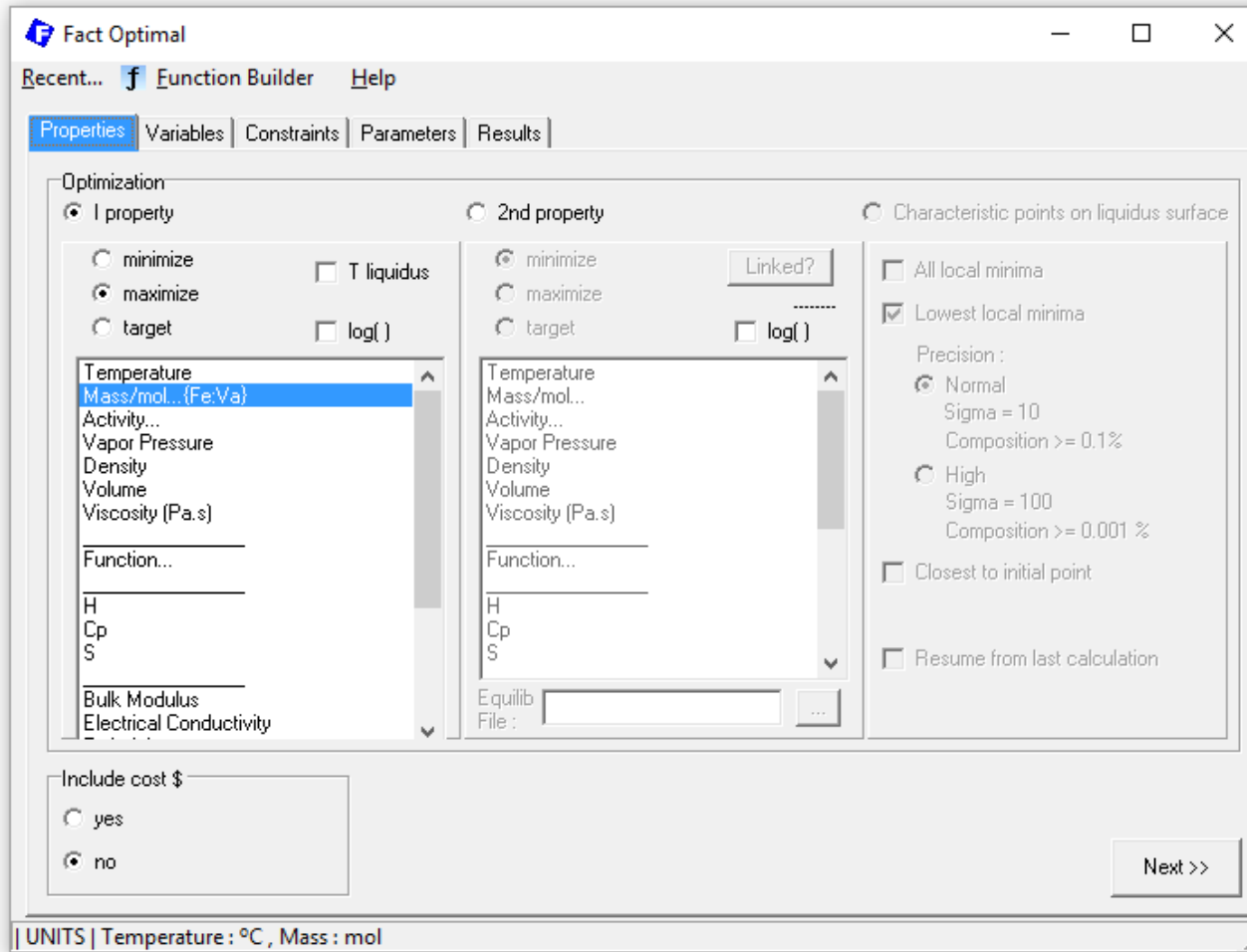
# Searching for austenite

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



- SpMCBN-FCC1\_FCC\_A1#1
- Al:Va
- Al:C
- Al:B
- Cr:Va
- Cr:C
- Cr:B
- Fe:Va
- Fe:C
- Fe:B
- Mn:Va
- Mn:C
- Mn:B
- Si:Va
- Si:C
- Si:B
- Ti:Va
- Ti:C
- Ti:B
- V:Va
- V:C
- V:B

# Fact-Optimal

Fact Optimal

Recent... f Function Builder Help

Properties Variables Constraints Parameters Results

Composition Variables

No. Species MIN ALL MAX ALL Initial Value ALL


1 Fe  Constant 0.6 0.8 0.65  Q-Random

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

Pressure MIN: 1 MAX: 10 precision: 1 Initial Value: 1 Next >>

UNITS | Temperature: °C, Mass: mol

# Fact-Optimal

 Fact Optimal

Recent... **f** Function Builder Help

Properties | Variables | Constraints | **Parameters** | Results

# of Quasi-Random calculations :

Max # of Equilib calculations :

Initial search region :   Small  Medium  Large

Precision :

Time out (minutes) :

Fact Optimal

Recent... **f** Function Builder Help

Properties Variables Constraints Parameters **Results**

Stop 0:13:56

Status : Done. Continue Run >>

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 :

```

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

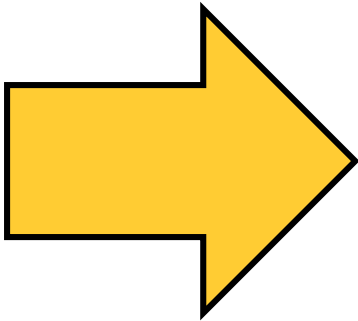
```

Results

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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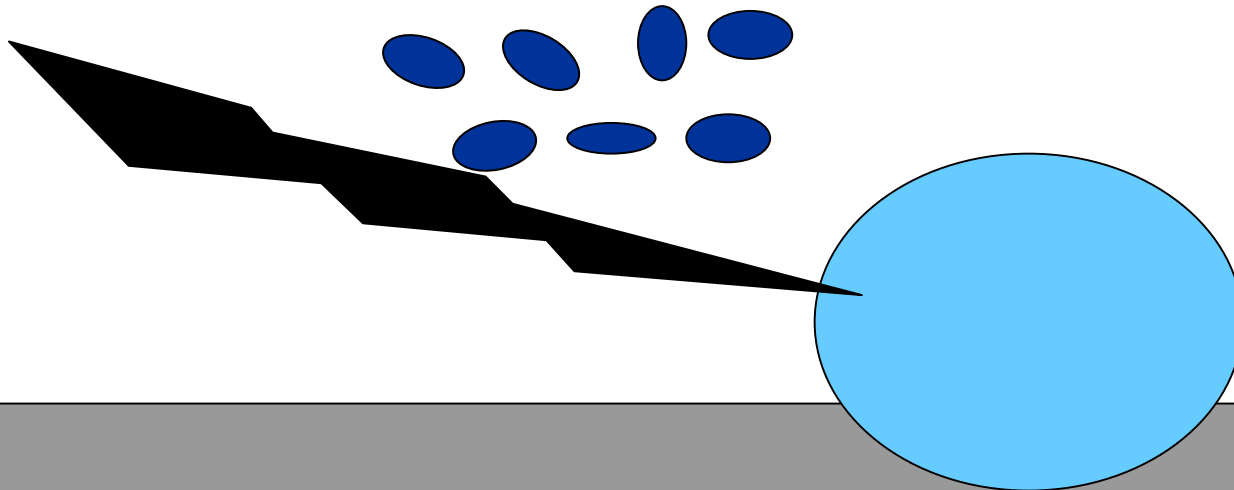


# Predicting phase formation

SiC content  $\alpha = 30\%$

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

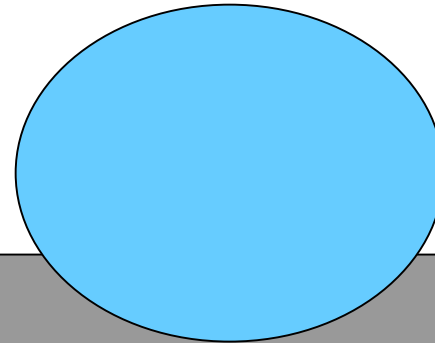
C	Si	Mn	Cr	Ni	V	Al	Fe
0.059	1.95	23.72	14.51	0.70	22.33	0.88	35.84

SiC
100

Phase formation as  $f(\alpha, \beta, T)$

$\alpha$ : SiC content

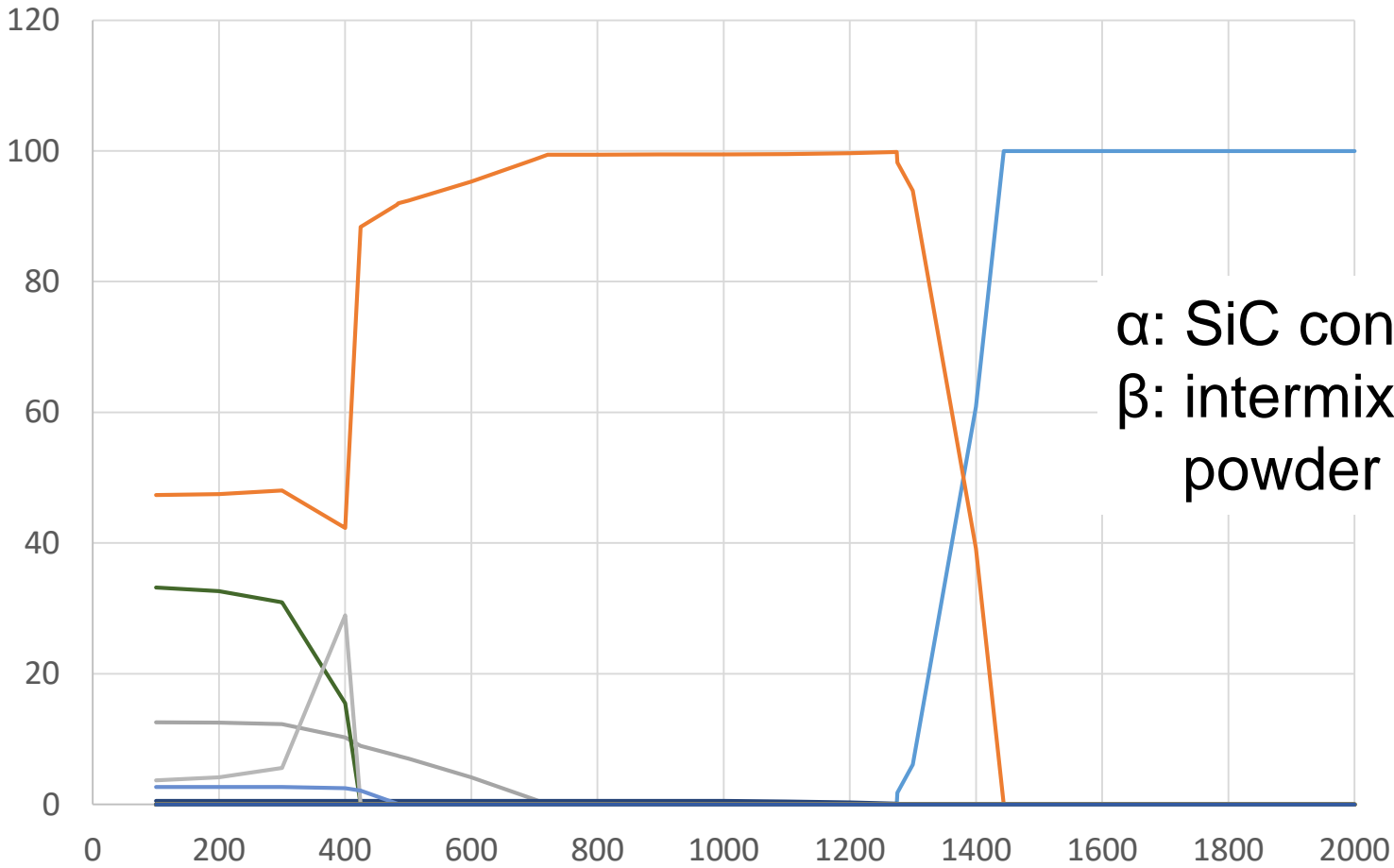
$\beta$ : intermixing between  
powder and substrate



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

$\alpha = 0$   
 $\beta = 0$

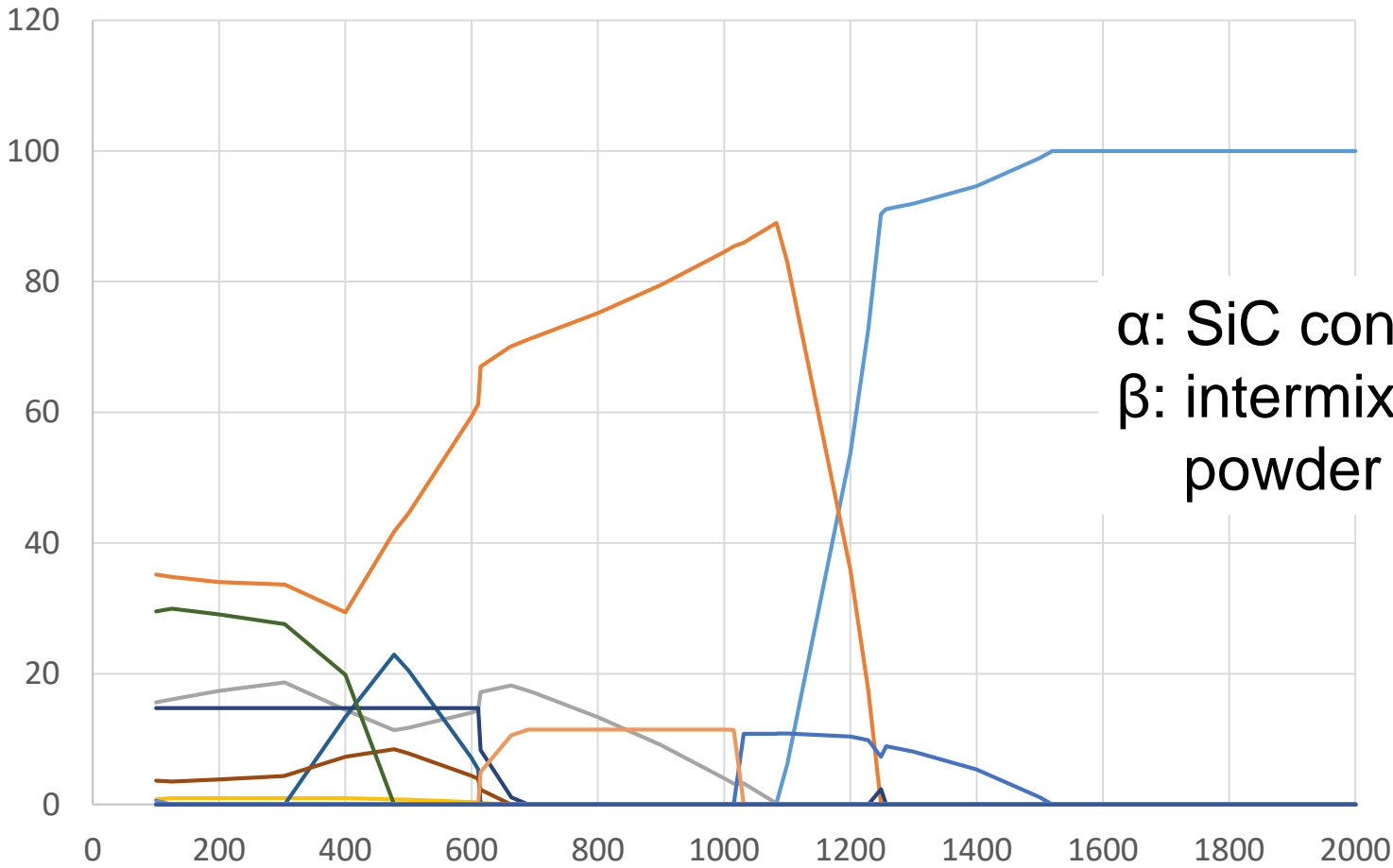
- |        |          |           |        |          |           |
|--------|----------|-----------|--------|----------|-----------|
| LIQU#1 | BCC1#1   | M3SI#1    | NiAl   | FCC1#1   | M5SI#1    |
| CUB1#1 | CR32     | D88_      | M7C3   | HCP1#1   | Cr3Mn5(s) |
| CSi(s) | V3C2     | BCC1#2    | M3C2   | Mn3Ni(s) | FCC1#2    |
| LIQU#2 | Ni2Si(s) | Ni5Si2(s) | BCC1#3 | MSI      |           |



$\alpha$ : SiC content  
 $\beta$ : intermixing between powder and substrate



- |        |          |           |        |          |           |
|--------|----------|-----------|--------|----------|-----------|
| LIQU#1 | BCC1#1   | M3SI#1    | NiAl   | FCC1#1   | M5SI#1    |
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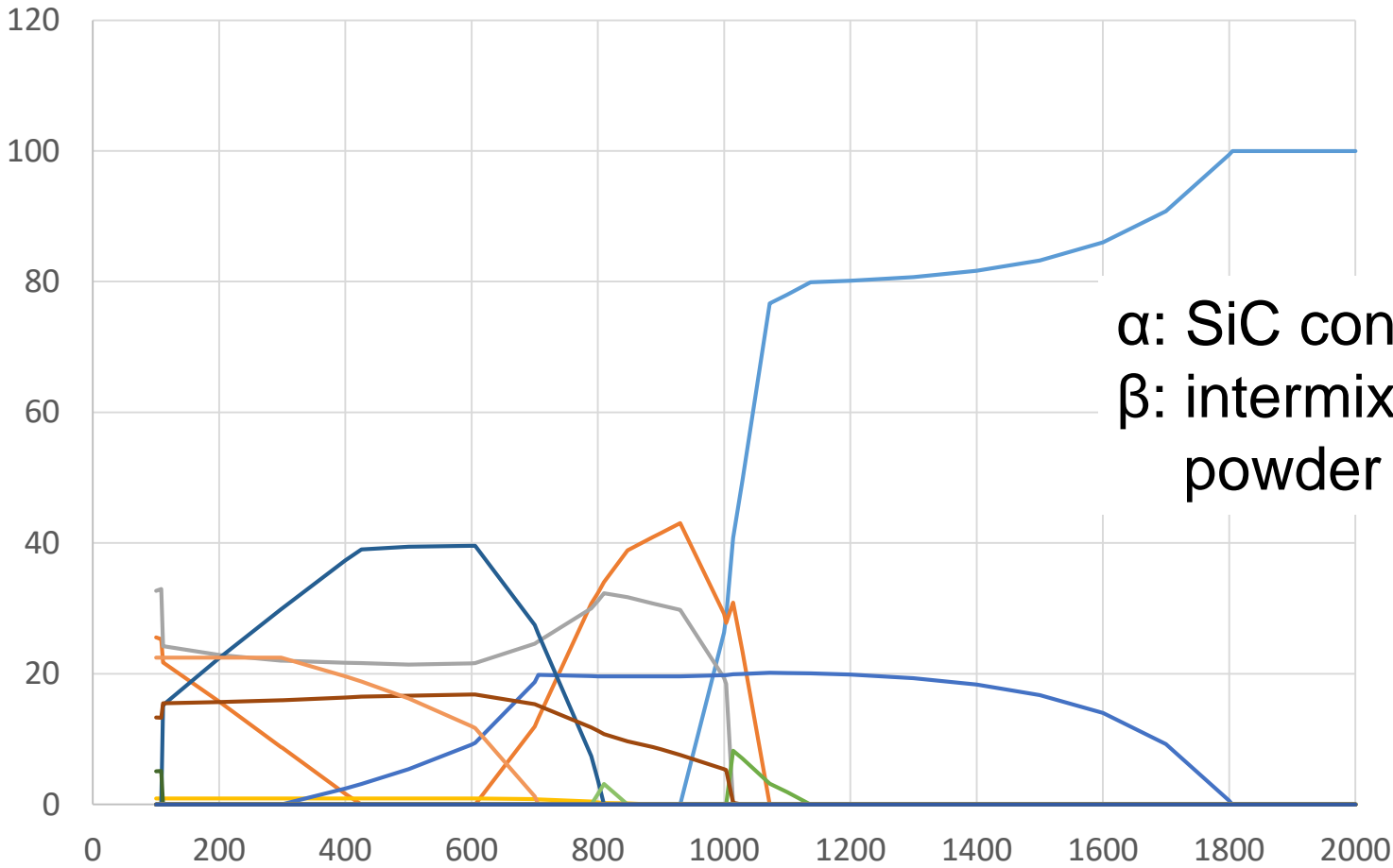
α: SiC content  
 β: intermixing between powder and substrate



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$\alpha = 0.1$   
 $\beta = 0$

- |        |          |           |        |          |           |
|--------|----------|-----------|--------|----------|-----------|
| LIQU#1 | BCC1#1   | M3SI#1    | NiAl   | FCC1#1   | M5SI#1    |
| CUB1#1 | CR32     | D88_      | M7C3   | HCP1#1   | Cr3Mn5(s) |
| CSi(s) | V3C2     | BCC1#2    | M3C2   | Mn3Ni(s) | FCC1#2    |
| LIQU#2 | Ni2Si(s) | Ni5Si2(s) | BCC1#3 | MSI      |           |

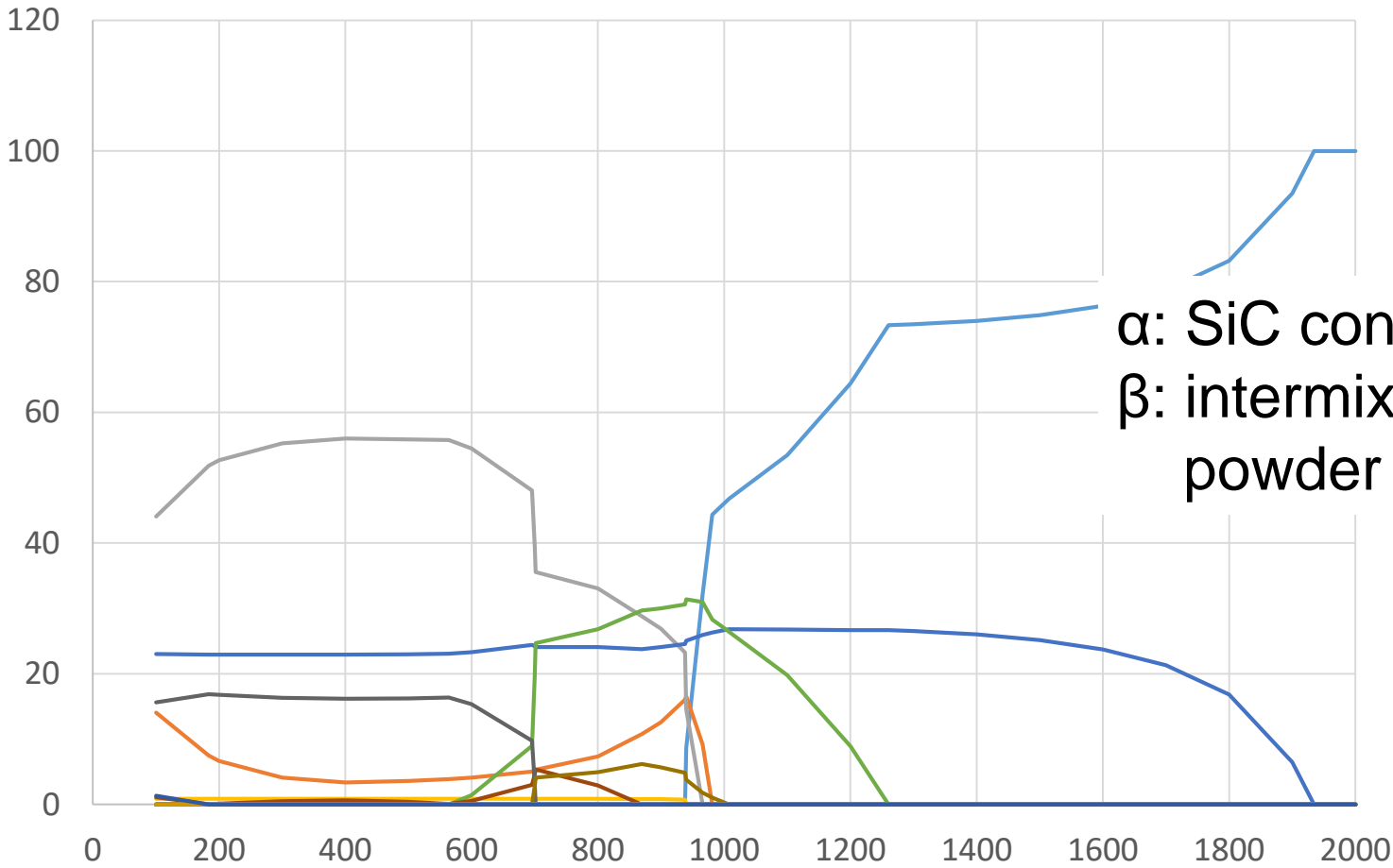


$\alpha$ : SiC content  
 $\beta$ : intermixing between powder and substrate



$\alpha = 0.15$   
 $\beta = 0$

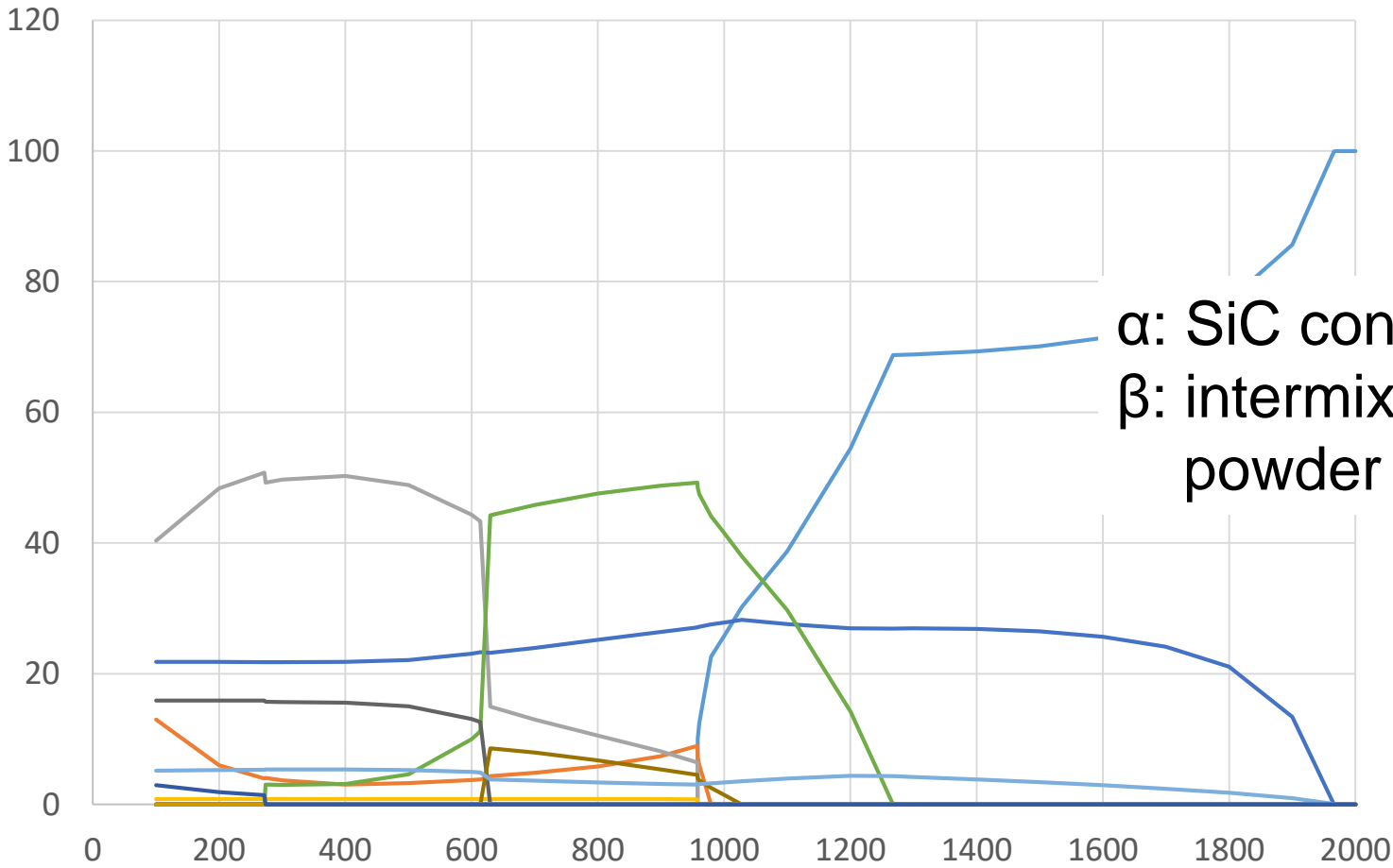
- |        |          |           |        |          |           |
|--------|----------|-----------|--------|----------|-----------|
| LIQU#1 | BCC1#1   | M3SI#1    | NiAl   | FCC1#1   | M5SI#1    |
| CUB1#1 | CR32     | D88_      | M7C3   | HCP1#1   | Cr3Mn5(s) |
| CSi(s) | V3C2     | BCC1#2    | M3C2   | Mn3Ni(s) | FCC1#2    |
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$\alpha$ : SiC content  
 $\beta$ : intermixing between powder and substrate



- |        |          |           |        |          |           |
|--------|----------|-----------|--------|----------|-----------|
| LIQU#1 | BCC1#1   | M3SI#1    | NiAl   | FCC1#1   | M5SI#1    |
| CUB1#1 | CR32     | D88_      | M7C3   | HCP1#1   | Cr3Mn5(s) |
| CSi(s) | V3C2     | BCC1#2    | M3C2   | Mn3Ni(s) | FCC1#2    |
| LIQU#2 | Ni2Si(s) | Ni5Si2(s) | BCC1#3 | MSI      |           |



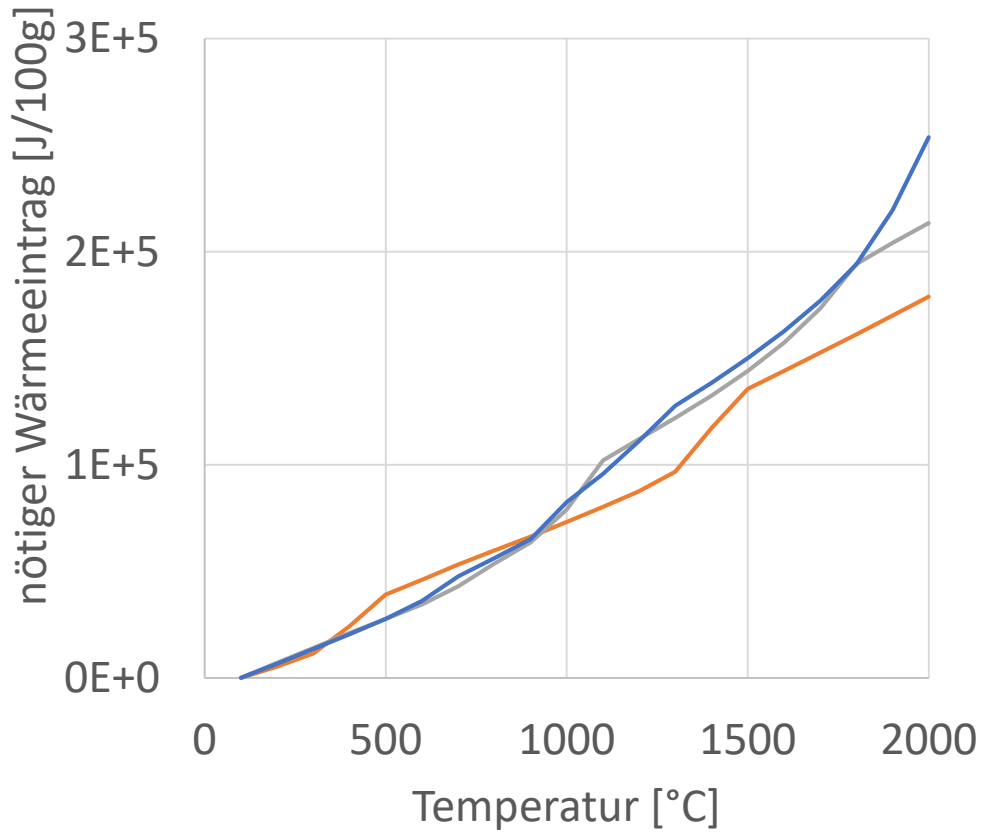
α: SiC content  
 β: intermixing between powder and substrate



# Enthalpy

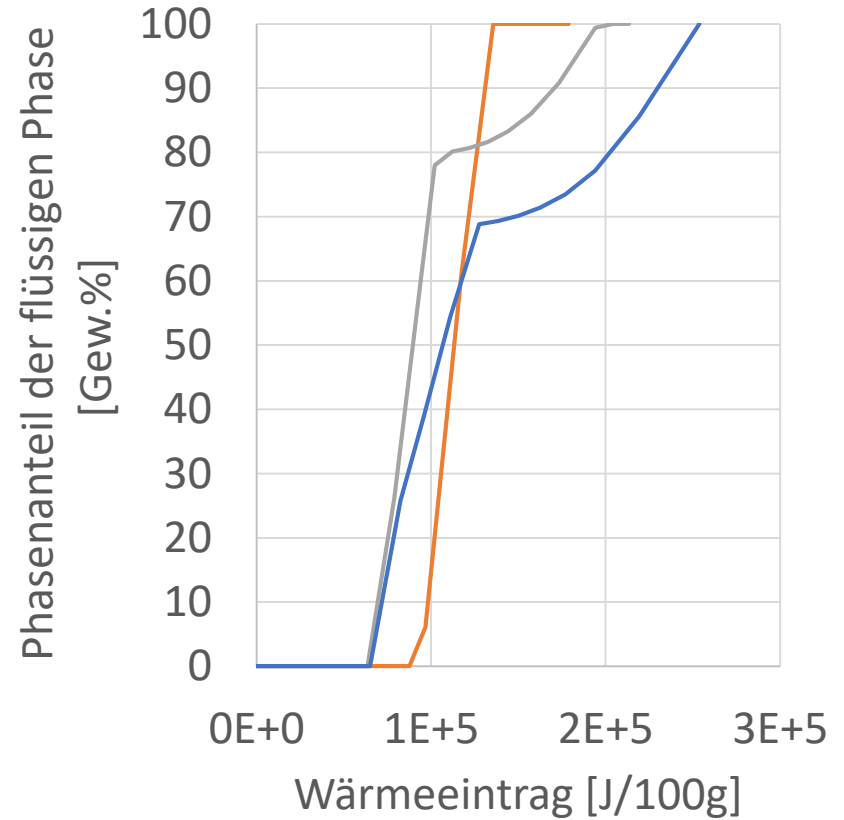
Beta = 0

Alpha 0 — Alpha 0.1 — Alpha 0.2



Beta = 0

Alpha 0 — Alpha 0.1 — Alpha 0.2





**Thank you for your attention!**

