MatCalc
Engineering

Phase description with sublattice concept

MatCalc 6.03.1000

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Sublattice represenation

- Idea behind: To reflect the effect of crystal structure on the thermodynamic functions of the given phase.
- Realization: Distinguish sublattices (crystal sites) according to the elements that occupy these.
- Notation (in MatCalc):

  :elements on sublattice 0:elements on sublattice 1: **…** ***:elements on last sublattice:***

  (Sublattices are separated with a colon ":". Stoichiometric ratios of the sublattices are not expressed)

Sublattice representation - examples

- Liquid phase in system Al-Cr-Cu-Fe-Mn-Ni-Si-Ti-Y

  Representation - :Al,Cr,Cu,Fe,Mn,Ni,Si,Ti,Y:

  Comments:

  - 1 sublattice
  - All elements can occur on sublattice 0 (sublattice indexing starts from zero)

Sublattice representation - examples

- FCC_A1 phase in unary system Ni

  Representation - :Ni:Va:

  Comments:

  - 2 sublattices
  - Ni can occur only on sublattice 0
  - Va (element “Vacuum” representing vacancies) can occur only on sublattice 1.

Sublattice representation - examples

- Cementite phase in system Fe-C

  Representation - :Fe:C:

  Comments:

  - 2 sublattices
  - Fe can occur only on sublattice 0
  - C can occur only on sublattice 1
  - Va is not given in the description so it is not allowed to occur on any sublattice. The sublattices are completely filled with atoms

Sublattice representation - examples

- Theta_DP_GPB phase in Al-Cu-Mg-Si system

  Representation - :Al,Mg,Si:Al,Mg,Si:Al:Cu,Mg,Si:Cu,Mg,Si:

  Comments:

  - 5 sublattices
  - Al can occur on sublattices 0, 1 and 2
  - Cu can occur on sublattices 3 and 4
  - Mg and Si can occur on sublattices 0, 1, 3 and 4
  - Al, Mg and Si can coexist on sublattice 0 and 1
  - Cu, Mg and Si can coexist on sublattice 3 and 4

Sublattice representation - examples

- AlN phase in Fe-Mn-Si-Al-C-N system

  Representation - :Al:N:

  Comment:

  - 2 sublattices
  - Al can occur on sublattice 0
  - N can occur on sublattice 1
  - Fe, Mn, Si and C cannot occur on any sublattice (-> there is no solubility of these elements in AlN phase)

Site fraction, y_i^j

- Describes the molar content of a given element i on a given sublattice j referred to this sublattice j.
- Has a value in 0 – 1 range.
- Site fractions for all elements on the given sublattice j sum up to unity.
- Does not carry any information on the stoichiometry of the phase.

$$\sum_i y_i^j = 1$$

Site fraction, y_i^j - examples

- :Fe:C,Va:

  y_{Fe}^0 = 1

  y_C^1 = 0,019; y_{Va}^1 = 0,981

For sublattices filled with only one element, the relevant site fractions have to be unity

- :Cr,Fe,Mn:Cr,Fe,Mn:C:

  y_{Cr}^0 = 0,6; y_{Fe}^0 = 0,1; y_{Mn}^0 = 0,3

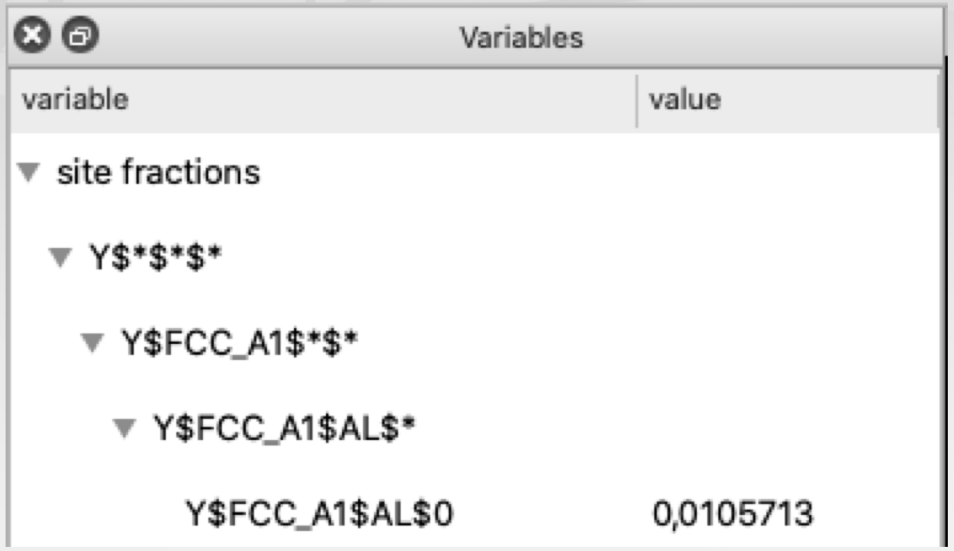
  y_{Cr}^1 = 0,45; y_{Fe}^1 = 0,15; y_{Mn}^1 = 0,4

  y_C^2 = 1

Site fractions of the same element on various sublattices can (and usually do) have different values

Site fraction, y_i^j - MatCalc representation

- MatCalc built-in variable: *Y$#Phase$#Element$#Sublattice_index*
- Examples: *Y$LIQUID$CR$0* ; *Y$THETA_DP_GPBCU3*
- GUI: “Variables” window -> “site fractions” section



Mole fraction on sublattice, x_i^j

- Describe the molar content of a given element i on a given sublattice j referred to all sublattices in the phase.
- Have a value in 0 – 1 range.
- Site fractions for all elements on all sublattices sum up to unity.
- Carries any information on the stoichiometry of the phase.
- “Vacuum” contents are not accounted in the balance ($i \neq Va$).

$$\sum_i \sum_j x_i^j = 1$$

Mole fraction on sublattice, x_i^j - examples

- :Fe:C,Va:

x_{Fe}^0 = 0,982

x_C^1 = 0,018

$x_{Fe}^0 + x_C^1 = 1$

Vacuum is not accounted in the mole fraction balance

- :Cr,Fe,Mn:Cr,Fe,Mn:C:

x_{Cr}^0 = 0,4138; x_{Fe}^0 = 0,0690; x_{Mn}^0 = 0,2069; $\sum_i x_i^0$=0,6897

x_{Cr}^1 = 0,0517; x_{Fe}^1 = 0,0103 x_{Mn}^1 = 0,0414; $\sum_i x_i^1$=0,1034

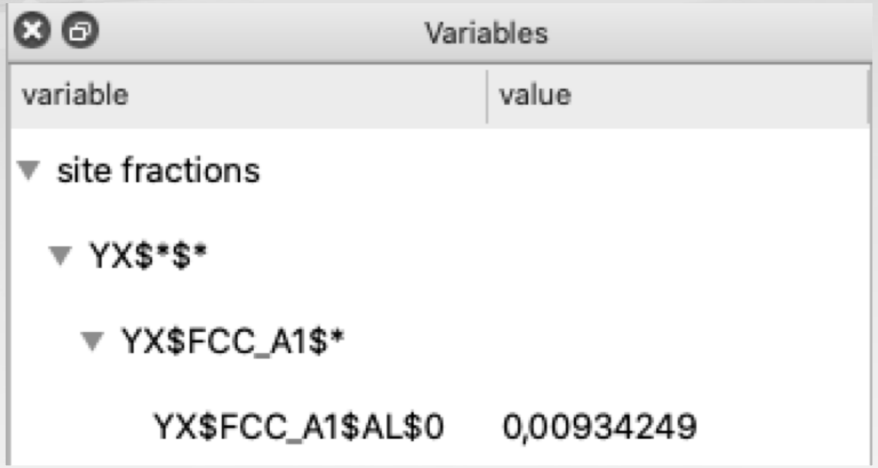
x_C^2 = 0,2069; $\sum_i x_i^2$=0,2069

$\sum_i x_i^0 : \sum_i x_i^1 : \sum_i x_i^2$ = 20:3:6

$\sum_i x_i^0 + \sum_i x_i^1 + \sum_i x_i^2 = 1$

Mole fraction on sublattice, x_i^j - MatCalc representation

- MatCalc built-in variable: *YX$#Phase$#Element$#Sublattice_index*
- Examples: *YX$LIQUID$CR$0* ; *YX$THETA_DP_GPBCU3*
- GUI: “Variables” window -> “site fractions” section

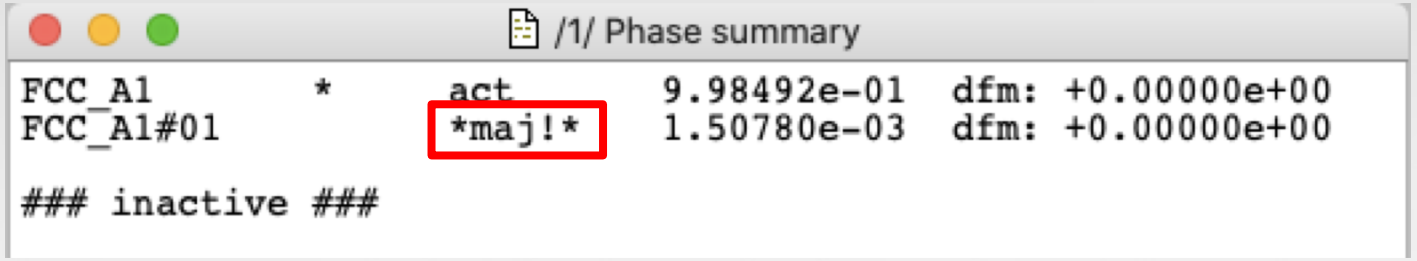


Major constitutents of phase

- Some elements on the sublattice might be specified as major constituents.
- MatCalc representation: “**%**” (percent sign) after the relevant element.
- On the phase initialization (after reading the database), the site fraction values of major constituents are much greater than the ones of the other elements on the relevant sublattice.

Major constitutents of phase

- In equilibrium state, the site fraction values of major constituents are also **not** expected to become less than the ones of the other elements on the relevant sublattice.
  - However, if this happens, MatCalc will display a warning "**maj!**" in "Phase summary" window at the relevant phase.



Major constitutents of phase - examples

- FCC-phase - :Fe%,Nb:C,Va%:
  - Major constituents: Fe on sublattice 0, Va on sublattice 1.
  - Comment: This phase is expected to depict austenite. Some Nb and C can dissolve in it, on the relevant sublattices.
- FCC-phase - :Fe,Nb%:C%,Va:
  - Major constituents: Nb on sublattice 0, C on sublattice 1.
  - Comment: This phase is expected to depict NbC phase (MX carbide). Some Fe can dissolve in it, some sites on sublattice 1 remain empty (Va presence).

Where does MatCalc know it all from?

- Sublattice representation (=distribution of elements among sublattices) and the major constituent settings for the phases are defined by default in thermodynamic database.

/Applications/MatCalc_6_dev/database/thermodynamic/mc_ni.tdb

```
$
$##########################################################################
$                    THERMODYNAMIC PARAMETERS: GAMMA_PRIME
$##########################################################################
$
 PHASE GAMMA_PRIME % 2 0.25 0.75 >
Cubic Ni3Al-type, L12-structure; simplified description
as solid solution phase consisting of two substitutional sublattices
>> 6 !
    CONST GAMMA_PRIME : AL%,CO,CR,FE,HF,MO,NB%,NI,SI,TI%,W,ZR : AL,
    CO,CR,FE,HF,MO,NB,NI%,SI,TI,W,ZR : !
PARAMETER G(GAMMA_PRIME,AL:AL:0) 273.00 +GHSERAL#+5000; 6000.00  N
```

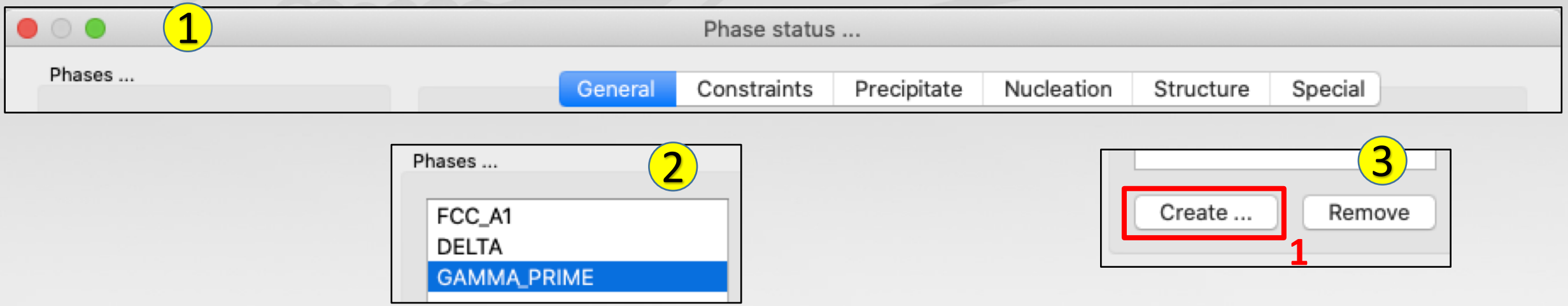
- Number of sublattices
- Stoichiometric indices of the sublattices
- Element distribution and major constituent definition

User settings – Elements presence on sublattices

- If a user wants to restrict some sublattices of the phase to the presence of some elements, a “composition set” for this phase has to be created.
- In a composition set, a user can restrict the default settings (from the database) of the element presence on a given sublattice.
- At least one element has to be present on each sublattice.

User settings – Elements presence on sublattices

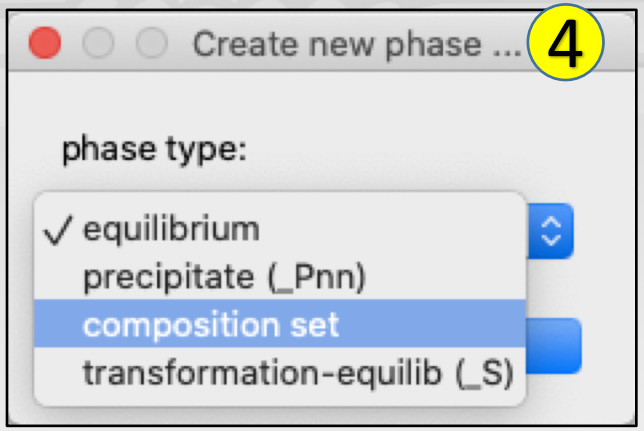
1. In “Phase status” window, select “General” tab.
2. In “Phases” field select the relvant parent phase.
3. Click on “Create” button.

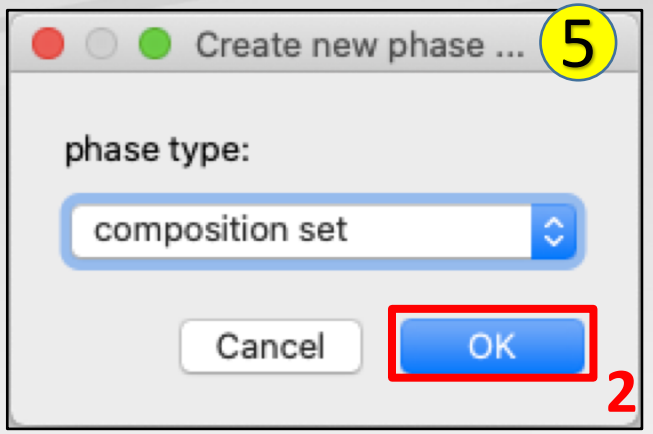


User settings – elements on sublattices

4. In a newly created window “Create new phase”, select “composition set”.

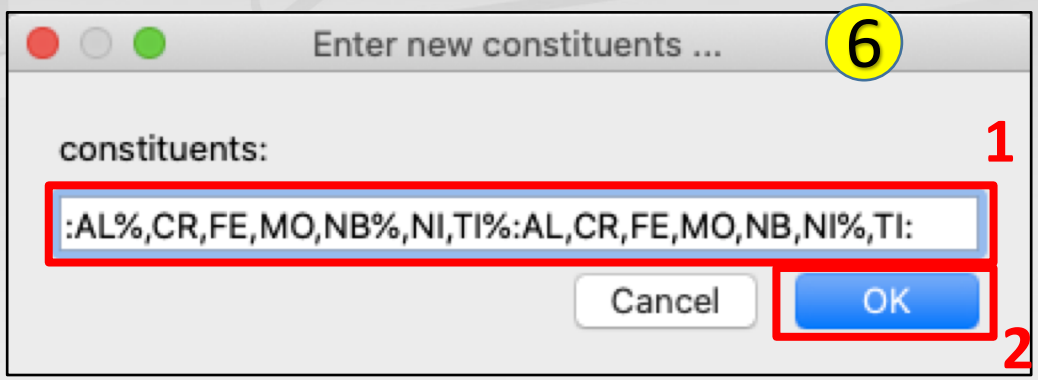
5. Confirm the selection with a click on “OK” button.





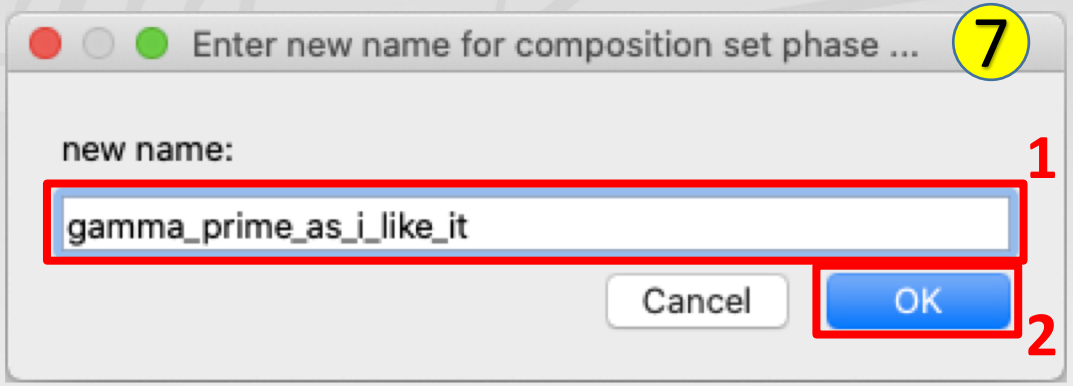
User settings – elements on sublattices

6. In a newly created window “Enter new constituents”, modify the default settings of the sublattices (elements presence, major constituents). Confirm the modification with a click on “OK” button.



User settings – elements on sublattices

7. In a newly created window “Enter new name for composition set phase”, name the newly created phase. Confirm the name with a click on “OK” button.

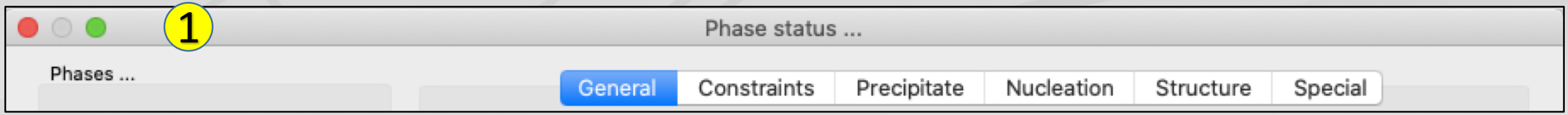


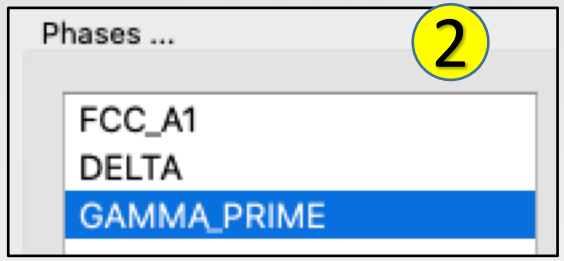
User settings – major constituents

- Default settings (from the database) of the major constituents on various sublattices can be modified within the phase → there is no need to create a new phase for this purpose.
- Specification of major constituents is not mandatory (e.g., the setting ":::" indicates the presence of 3 sublattices without any specification of major constituents for these).

User settings – major constituents

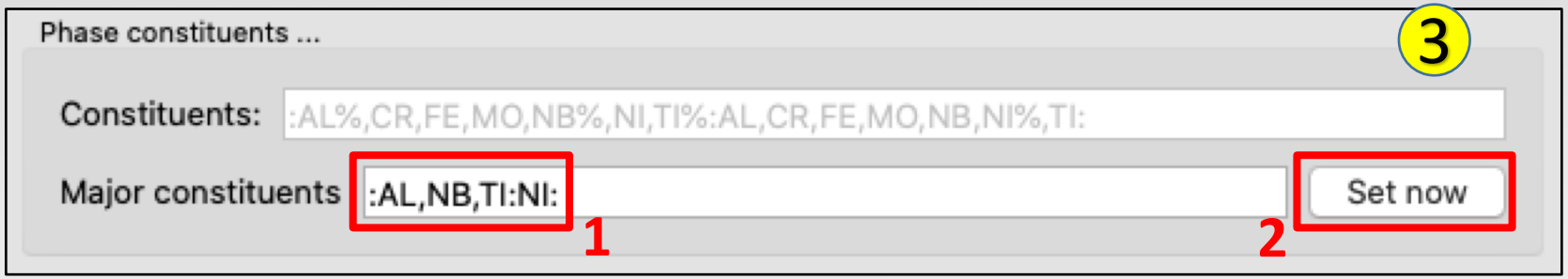
1. In “Phase status” window, select “General” tab.
2. In “Phases” field select the relvant parent phase.





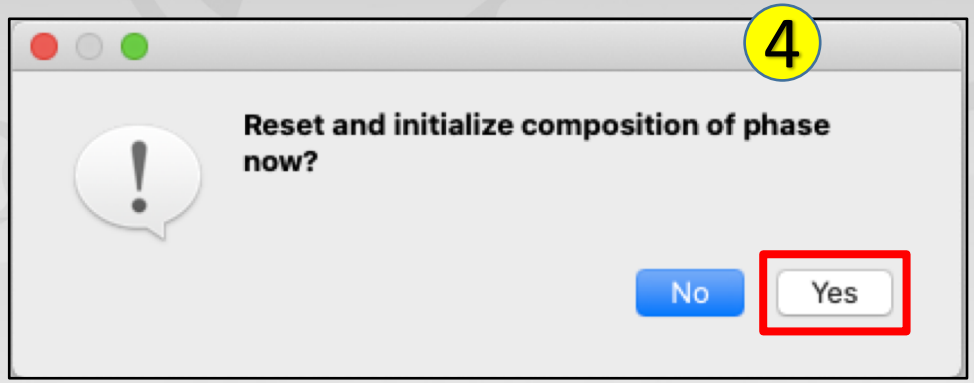
User settings – major constituents

3. In “Phase constituents” area, type in the major constituent elements for the relevant sublattices in the “major constituents area”. Confirm the specification with a click on “OK” button.



User settings – major constituents

4. In a newly created window, confirm the specification with a click on “Yes” button.



User settings – site fractions & mole fractions on sublattices

- Site fractions and mole fractions on sublattices cannot be set by the user - these are evaluated during MatCalc calculations. No restrictions can be imposed here.

„Automatic“ creation of additional phases

- On some occasions, MatCalc creates additional equilibrium phases to the selected ones when reading the data from the database.
- Example:
  - Fe-Nb-C system
    - FCC_A1 selected in database, obtains major constituent setting “:Fe:Va:”
    - FCC_A1#01 created by MatCalc, obtains major constitutents setting “:Nb:C:”

„Automatic“ creation of additional phases

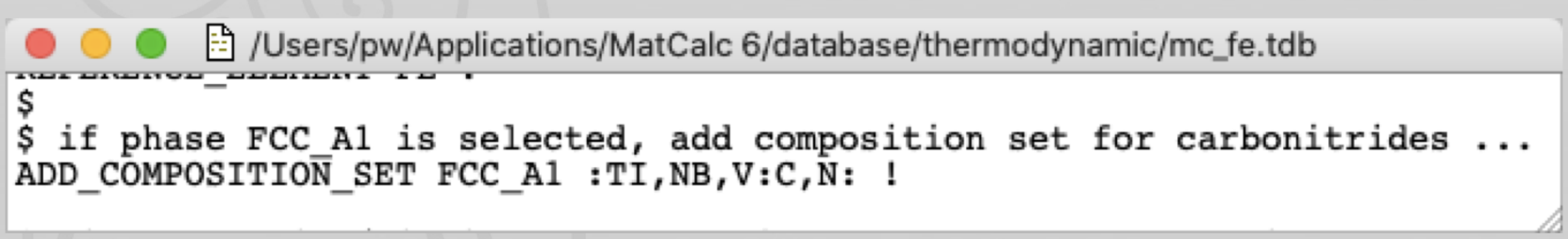
- Creation of the additional phases is governed by command “*add_composition_set*” included in database.

/Users/pw/Applications/MatCalc 6/database/thermodynamic/mc_fe.tdb

```
$
$ if phase FCC_A1 is selected, add composition set for carbonitrides ...
ADD_COMPOSITION_SET FCC_A1 :TI,NB,V:C,N: !

$ simple carbide/nitride phases derived from parent are defined
$ by MatCalc syntax (5.44.0.008)
$ CREATE_NEW_PHASE parent_phase_name c :El1,El2,...:El3,El4,...: new_name
$
$ if phase HCP_A3 is selected, add composition set for carbides and nitrides
ADD_COMPOSITION_SET HCP_A3 :CR:N: !
ADD_COMPOSITION_SET HCP_A3 :MO:C: !
ADD_COMPOSITION_SET HCP_A3 :CR,V:C: !
$
$ if phase M6C is selected, add composition set for eta-nitride Cr3Ni2SiN
ADD_COMPOSITION_SET M6C :CR:NI:SI:N: !
$
$ MatCalc syntax (MatCalc 5.23.1036) for split model of ordered phases
```

„Automatic“ creation of additional phases



- Interpretation of “*ADD_COMPOSITION_SET FCC_A1 :TI,NB,V:C,N:*” :
  - Additional equilibrium phase (named “*FCC_A1#01*”) is created if both of the following conditions are fulfilled:
    - “FCC_A1” phase is selected in database
    - For all sublattices, at least one element on the given sublattice is selected in database

„Automatic“ creation of additional phases

/Users/pw/Applications/MatCalc 6/database/thermodynamic/mc_fe.tdb

```
$
$ if phase FCC_A1 is selected, add composition set for carbonitrides ...
ADD_COMPOSITION_SET FCC_A1 :TI,NB,V:C,N: !
```

- Examples:
  - Fe-C system with FCC_A1 phase: FCC_A1#01 **not created**, as neither of elements needed on sublattice 0 (Nb, Ti, V) is selected.
  - Fe-Nb system with FCC_A1 phase: FCC_A1#01 **not created**, as neither of elements needed on sublattice 1 (C, N) is selected.
  - Fe-Ti-V-N system with FCC_A1 phase: FCC_A1#01 **created** with major constituent setting “*:Ti,V:N:*”.

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Thank you for

your attention!