geochemical society

The P-T-t Trajectory of Metamorphic Processes

Applications of equilibrium thermodynamics using the Theriak/Domino software

Fred Gaidies, Carleton U. (fred.gaidies@carleton.ca)

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https://titan.minpet.unibas.ch/minpet/theriak/theruser.html

What is Theriak-Domino?

THERIAK-DOMINO is a program collection developed by **Christian de Capitani** (Basel, Switzerland) to calculate and plot thermodynamic functions, equilibrium assemblages and equilibrium assemblage diagrams

Theriak: stable phase assemblages and phase compositions for a given bulk composition at specified P-T

Domino: equilibrium assemblage diagrams [P, T, a, ln(a)]; pseudo-binary or pseudo-ternary phase diagrams; isopleths, density or volume distributions; and more

Therbin,Therter:
binary and ternary phase diagrams

Thalia,Thermo:
thermodynamic functions (T, P or composition)

Guzzler, Explot, Makemap:
transform graphics information into .ps and .svg files

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Guzzler, **Explot**, Makemap:
transform graphics information into .ps and .svg files

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
25
     O          AL         BA          C          CA         CL         CO
     CU         F          FE          H          K          MN         MG
     NA         NI         P           S          SI         SR         TI
     ZN         ZR         B           E
  15.99940   26.98154  137.32700   12.01100   40.07800   35.45270   58.93320
  63.54600   18.99840   55.84700    1.00794   39.09830   54.93085   24.30500
  22.98977   58.69000   30.97362   32.06600   28.08550   87.62000   47.88000
  65.39000   91.22400   10.81000    1.00000
   0.0        1.5        1.0         2.0        1.0        0.0        1.0
   1.0        0.0        1.0         0.5        0.5        1.0        1.0
   0.5        1.0        1.0         0.0        2.0        1.0        2.0
   1.0        2.0        0.0         0.0
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
25
     O          AL         BA          C          CA         CL         CO
     CU         F          FE          H          K          MN         MG
     NA         NI         P           S          SI         SR         TI
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  15.99940   26.98154  137.32700   12.01100   40.07800   35.45270   58.93320
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  22.98977   58.69000   30.97362   32.06600   28.08550   87.62000   47.88000
  65.39000   91.22400   10.81000    1.00000
   0.0         1.5        1.0         2.0        1.0        0.0        1.0
   1.0         0.0        1.0         0.5        0.5        1.0        1.0
   0.5         1.0        1.0         0.0        2.0        1.0        2.0
   1.0         2.0        0.0         0.0


*** ... MINERAL DATA ...
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
25
     O          AL         BA          C          CA         CL         CO
     CU         F          FE          H          K          MN         MG
     NA         NI         P           S          SI         SR         TI
     ZN         ZR         B           E
  15.99940   26.98154  137.32700   12.01100   40.07800   35.45270   58.93320
  63.54600   18.99840   55.84700    1.00794   39.09830   54.93085   24.30500
  22.98977   58.69000   30.97362   32.06600   28.08550   87.62000   47.88000
  65.39000   91.22400   10.81000    1.00000
   0.0        1.5        1.0         2.0        1.0        0.0        1.0
   1.0        0.0        1.0         0.5        0.5        1.0        1.0
   0.5        1.0        1.0         0.0        2.0        1.0        2.0
   1.0        2.0        0.0         0.0


*** ... MINERAL DATA ...


*** ... GAS DATA ...
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
25
     O          AL         BA          C          CA         CL         CO
     CU         F          FE          H          K          MN         MG
     NA         NI         P           S          SI         SR         TI
     ZN         ZR         B           E
  15.99940   26.98154  137.32700   12.01100   40.07800   35.45270   58.93320
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  22.98977   58.69000   30.97362   32.06600   28.08550   87.62000   47.88000
  65.39000   91.22400   10.81000    1.00000
   0.0        1.5        1.0         2.0        1.0        0.0        1.0
   1.0        0.0        1.0         0.5        0.5        1.0        1.0
   0.5        1.0        1.0         0.0        2.0        1.0        2.0
   1.0        2.0        0.0         0.0


*** ... MINERAL DATA ...

*** ... GAS DATA ...

*** ... SOLUTION DATA ...
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
25
     O          AL         BA          C          CA         CL         CO
     CU         F          FE          H          K          MN         MG
     NA         NI         P           S          SI         SR         TI
     ZN         ZR         B           E
  15.99940   26.98154  137.32700   12.01100   40.07800   35.45270   58.93320
  63.54600   18.99840   55.84700    1.00794   39.09830   54.93085   24.30500
  22.98977   58.69000   30.97362   32.06600   28.08550   87.62000   47.88000
  65.39000   91.22400   10.81000    1.00000
   0.0         1.5        1.0         2.0        1.0        0.0        1.0
   1.0         0.0        1.0         0.5        0.5        1.0        1.0
   0.5         1.0        1.0         0.0        2.0        1.0        2.0
   1.0         2.0        0.0         0.0


*** ... MINERAL DATA ...

*** ... GAS DATA ...

*** ... SOLUTION DATA ...

*** ... MARGULES ...
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
****MINERAL DATA*****    from Holland and Powell (1998+)
pyrope               SI(3)AL(2)MG(3)O(12)    py            3nh
 ST              0.0   -6284720.000       266.3000       11.3180
 C3        633.50000      0.0000000     -5196100.0      -4315.200          0.00
 VHP     0.000043600         1737.0          0.0000           0.00       0.00000
 VH2         10.0000         4.0000   -0.000260550
almandine            SI(3)AL(2)FE(3)O(12)    alm           3nh
 ST              0.0   -5263520.000       340.0000       11.5110
 C3        677.30000      0.0000000     -3772700.0      -5044.000          0.00
 VHP     0.000040300         1690.0          0.0000           0.00       0.00000
 VH2         10.0000         4.0000   -0.000253500
spessartine          SI(3)AL(2)MN(3)O(12)    spss          3nh
 ST              0.0   -5646400.000       367.0000       11.7920
 C3        584.60000     -0.0015930     -7516700.0      -2750.100          0.00
 VHP     0.000046200         1790.0          0.0000           0.00       0.00000
 VH2         10.0000         4.0000   -0.000268500
grossular            SI(3)AL(2)CA(3)O(12)    gr            3nh
 ST              0.0   -6644150.000       255.0000       12.5350!
 C3        626.00000      0.0000000     -5779200.0      -4002.900          0.00
 VHP     0.000039300         1680.0          0.0000           0.00       0.00000
 VH2         10.0000         4.0000   -0.000252000
..
..
..
..
..
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
****MINERAL DATA*****    from Holland and Powell (1998+)
pyrope               SI(3)AL(2)MG(3)O(12)    py            3nh


 ST              0.0   -6284720.000       266.3000        11.3180


 C3        633.50000      0.0000000     -5196100.0      -4315.200           0.00
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
****MINERAL DATA*****     from Holland and Powell (1998+)
pyrope                SI(3)AL(2)MG(3)O(12)     py              3nh
```

name **formula** **abbrev** **code**

```
 ST              0.0    -6284720.000        266.3000         11.3180


 C3         633.50000       0.0000000     -5196100.0       -4315.200              0.00
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
****MINERAL DATA*****    from Holland and Powell (1998+)
pyrope                SI(3)AL(2)MG(3)O(12)    py              3nh
```

name **formula** **abbrev** **code**

```
ST              0.0    -6284720.000        266.3000        11.3180
```

$\Delta_f G^o$ $\Delta_f H^o$ S^o V^o

```
C3        633.50000       0.0000000     -5196100.0       -4315.200            0.00
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
****MINERAL DATA*****     from Holland and Powell (1998+)
pyrope                SI(3)AL(2)MG(3)O(12)     py              3nh
```

name **formula** **abbrev** **code**

```
ST              0.0    -6284720.000        266.3000         11.3180
```

$\Delta_f G^o$ $\Delta_f H^o$ S^o V^o

```
C3         633.50000       0.0000000    -5196100.0       -4315.200          0.00
```

a b c d

$$c_p = a + \frac{b}{\sqrt{T}} + \frac{c}{T^2} + \frac{d}{T^3}$$

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
****MINERAL DATA*****    from Holland and Powell (1998+)
pyrope                SI(3)AL(2)MG(3)O(12)    py              3nh
```

name **formula** **abbrev** **code**

```
ST              0.0    -6284720.000        266.3000        11.3180
```

$\Delta_f G^o$ $\Delta_f H^o$ S^o V^o

```
C3         633.50000       0.0000000    -5196100.0      -4315.200          0.00
```

a b c d

$$c_p = a + \frac{b}{\sqrt{T}} + \frac{c}{T^2} + \frac{d}{T^3}$$

```
COM       BRUCITE[1] PERICLASE[-1]
```

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
****MINERAL DATA*****     from Holland and Powell (1998+)
pyrope                SI(3)AL(2)MG(3)O(12)     py              3nh
```

name **formula** **abbrev** **code**

```
ST              0.0    -6284720.000        266.3000        11.3180
```

$\Delta_f G^o$ $\Delta_f H^o$ S^o V^o

```
C3         633.50000       0.0000000    -5196100.0      -4315.200          0.00
```

a b c d

$$c_p = a + \frac{b}{\sqrt{T}} + \frac{c}{T^2} + \frac{d}{T^3}$$

```
COM     BRUCITE[1] PERICLASE[-1]
```

combination of phases

Input Files: thermodynamic database, bulk composition

Thermodynamic database (e.g., ds5_5.txt update to HP98)

```
*****  SOLUTION DATA  *****
GARNET    (MARGULES,IDEAL)3   M(3):Ca,Mg,Fe,Mn
   grossular      Ca,Ca,Ca - Al,Al
   pyrope         Mg,Mg,Mg - Al,Al
   almandine      Fe,Fe,Fe - Al,Al
   spessartine    Mn,Mn,Mn - Al,Al
!
*****  MARGULES PARAMETER  *****
pyrope - grossular
12     33000.    0.00    0.00
pyrope - almandine
12     2500.     0.00    0.00
pyrope - spessartine
12     4500.     0.00    0.00
almandine - spessartine
12      240.     0.00    0.00
..
..
..
..
..
..
..
..
```

Input Files: thermodynamic database, bulk composition

Bulk composition (THERIN.txt)

```
! ----------> don't forget: at least two blanks between items!!! <----------
!             element bulk composition in moles!
!
!
!
!
!-------------------------------------------------------------------------------
    600    9500
0   AL(2)SI(1)O(5)      * my first test run
```

Input Files: thermodynamic database, bulk composition

Bulk composition (THERIN.txt)

```
! ----------> don't forget: at least two blanks between items!!! <----------
!             element bulk composition in moles!
!
!
!
!
!-------------------------------------------------------------------------------
    600    9500
0   AL(2)SI(1)O(5)      * my first test run
```

Temperature (C)

Pressure (bar)

*

0: short output (stable assemblage)

1: long output (composition, considered phases, solution models, stable assemblage, activities of all considered phases, etc.)

Theriak: my first test run

THERIN.txt:

```
     600   9500
0    AL(2)SI(1)O(5)     * my first test run
```

Theriak: my first test run

Mac, Linux:

(1) Open Terminal

(2) Enter:
`cd /Users/fredsmacbookpro/TheriakDominoMAC/GeochemSoc2020/Working`
or enter (if you followed the installation instructions):
`dom`

replace with your Home Directory

(3) Enter:
`theriak`

Windows:

(1) Use File Explorer and navigate to
C:\TheriakDominoWIN\GeochemSoc2020\Working

(2) Double-click start.bat (opens Command Prompt)

(3) Enter:
`theriak`

Theriak: my first test run

```
--------------------
database definition
--------------------
Enter [ "?" | CR | "files" | database filename ] < >?
```

Theriak: my first test run

```
-------------------
database definition
-------------------
Enter [ "?" | CR | "files" | database filename ] < >?
ds5_5.txt

database for this run: ds5_5.txt


Input from file THERIN.txt
--------------------------
T =  600.00 C      P =  9500.00 Bar
0   AL(2)SI(1)O(5)      * my first test run

----------------------------
define type of calculations
----------------------------
Enter [ "?" | CR | "no" | "bin" | "loop" | filename ] <no>?
```

Theriak: my first test run

```
 ---------------------------
 define type of calculations
 ---------------------------
 Enter [ "?" | CR | "no" | "bin" | "loop" | filename ] <no>?
loop
…
…
 -------------------------------
 define Temperature and Pressure
 -------------------------------
 Enter [ "?" | CR | "end" | T(C)  P(bar) ]:
300  2000
```

at least two spaces!!

Theriak: my first test run

```
 ----------------------------
 define type of calculations
 ----------------------------
 Enter [ "?" | CR | "no" | "bin" | "loop" | filename ] <no>?
loop
…
…
 ------------------------------
 define Temperature and Pressure
 ------------------------------
 Enter [ "?" | CR | "end" | T(C)  P(bar) ]:
300   2000
300   10000
800   10000
800   2000
500   3000
```

Theriak: my first test run

```
 ---------------------------
 define type of calculations
 ---------------------------
 Enter [ "?" | CR | "no" | "bin" | "loop" | filename ] <no>?
loop
…
…
 -------------------------------
 define Temperature and Pressure
 -------------------------------
 Enter [ "?" | CR | "end" | T(C)  P(bar) ]:
300   2000
300   10000
800   10000
800   2000
500   3000
…
…
end
```

Domino

Mac, Linux:

(1) Enter:
`domino`

Windows:

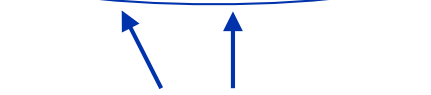
(1) Enter:
`domino`

Domino

```
--------------------
database definition
--------------------
Enter [ "?" | CR | "files" | "script" | database filename ] < >?
ds5_5.txt
```

Domino

```
--------------------
definition of X-axis
--------------------

X-variable may be: TC, TK, P, A(abc), LNA(abc), LOGA(abc), BIN, TER

Enter [ "?" | "list" | CR | X-variable  X-min  X-max  (X-Grid)  (width)  (ptdist)] < >?
TC   300    800
```



at least two spaces!!

Domino

```
--------------------
definition of X-axis
--------------------

X-variable may be: TC, TK, P, A(abc), LNA(abc), LOGA(abc), BIN, TER

Enter [ "?" | "list" | CR | X-variable  X-min  X-max  (X-Grid)  (width)  (ptdist)] < >?
TC   300    800

--------------------
definition of Y-axis
--------------------

Y-variable may be: TC, TK, P, PT, THG, A(abc), LNA(abc), LOGA(abc), BIN

Enter [ "?" | CR | "list" | Y-variable  Y-min  Y-max  (Y-Grid)  (height)] < >?
P    2000    10000
```

Domino

```
-----------------------------
definition of calculation type
-----------------------------

to calculate                          enter
------------                          -----
equilibrium phase diagram              "." (dot)
isolines:
   special functions:                          Key       min  max  step
   non-solution phases:                Name    Key       min  max  step
   solution phases:                    Name    Key  Nr   min  max  step

For help with isoline definition type "i".


Enter [  "?"  | CR | "point" | "list" | "i" | "." |
      | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] < >?
.
```

Domino

```
-----------------------------
definition of calculation type
-----------------------------

to calculate                              enter
------------                              -----
equilibrium phase diagram                  "." (dot)
isolines:
   special functions:                              Key       min   max   step
   non-solution phases:                  Name      Key       min   max   step
   solution phases:                      Name      Key   Nr  min   max   step

For help with isoline definition type "i".


Enter [  "?"  | CR | "point" | "list" | "i" | "." |
      | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] < >?
.

--------------------
labeling of reactions
--------------------

Labels: 1=assemblages, 2=new phases, 3=reactions, -1=special

Enter [ "?" | CR | Label (prec  smooth) ] < >?
1
```

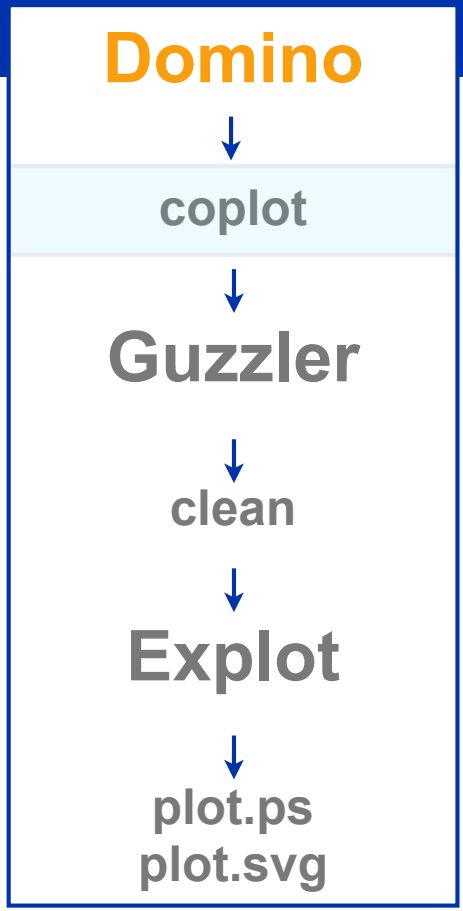
Domino

```
....
....
 LEVEL:  4   SQUARE: ( 80 , 49 ) LINE     1   REACTION    1: OPEN END
     10   389  Y =  4425.0000 ,      2 REACTIONS:    1    2
      6   395  X =   548.4375 ,      1 REACTIONS:    1
 NUMBER OF LINES:   3    NUMBER OF POINTS:  30    max.ph.    9
 LEVEL:  5   SQUARE: (160 , 98 ) LINE     1   REACTION    1: OPEN END
      6   401  Y =  4437.5000 ,      1 REACTIONS:    3
      5   406  X =   549.2188 ,      1 REACTIONS:    1
 NUMBER OF LINES:   3    NUMBER OF POINTS:  32    max.ph.    9
 LEVEL:  0   SQUARE: (  6 ,  4 ) LINE     3   REACTION    3: BUMP
     11   417  Y =  4800.0000 ,      1 REACTIONS:    3
     10   427  X =   575.0000 ,      1 REACTIONS:    3
 NUMBER OF LINES:   3    NUMBER OF POINTS:  34    max.ph.    9

exit DOMINO
CPU time:    0h 00m 00.03s
```

Creates file “**coplot**” in working directory

Domino

```
....
....
 LEVEL:  4   SQUARE: ( 80 , 49 ) LINE     1   REACTION    1: OPEN END
     10   389  Y =  4425.0000 ,      2 REACTIONS:    1    2
      6   395  X =   548.4375 ,      1 REACTIONS:    1
 NUMBER OF LINES:   3    NUMBER OF POINTS:  30    max.ph.    9
 LEVEL:  5   SQUARE: (160 , 98 ) LINE     1   REACTION    1: OPEN END
      6   401  Y =  4437.5000 ,      1 REACTIONS:    3
      5   406  X =   549.2188 ,      1 REACTIONS:    1
 NUMBER OF LINES:   3    NUMBER OF POINTS:  32    max.ph.    9
 LEVEL:  0   SQUARE: (  6 ,  4 ) LINE     3   REACTION    3: BUMP
     11   417  Y =  4800.0000 ,      1 REACTIONS:    3
     10   427  X =   575.0000 ,      1 REACTIONS:    3
 NUMBER OF LINES:   3    NUMBER OF POINTS:  34    max.ph.    9

exit DOMINO
CPU time:    0h 00m 00.03s
```



Creates file “**coplot**” in working directory

Guzzler

Mac, Linux:

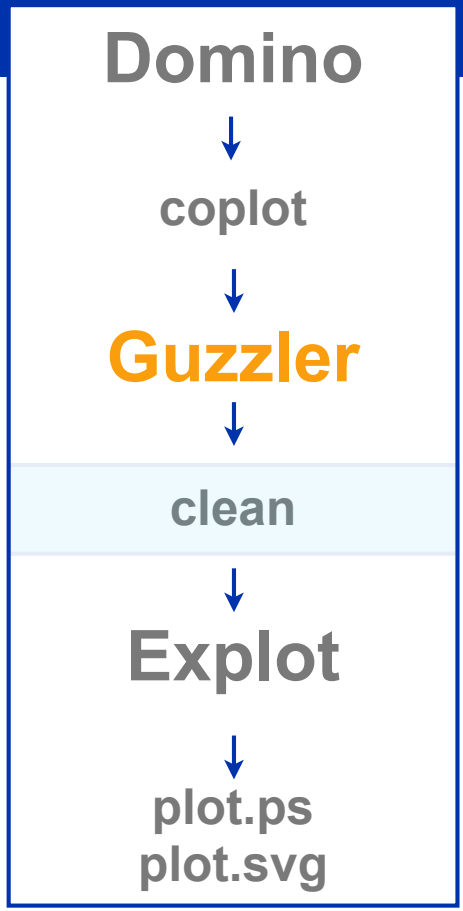
(1) Enter:

```
guzzler
```

Windows:

(1) Enter:

```
guzzler
```

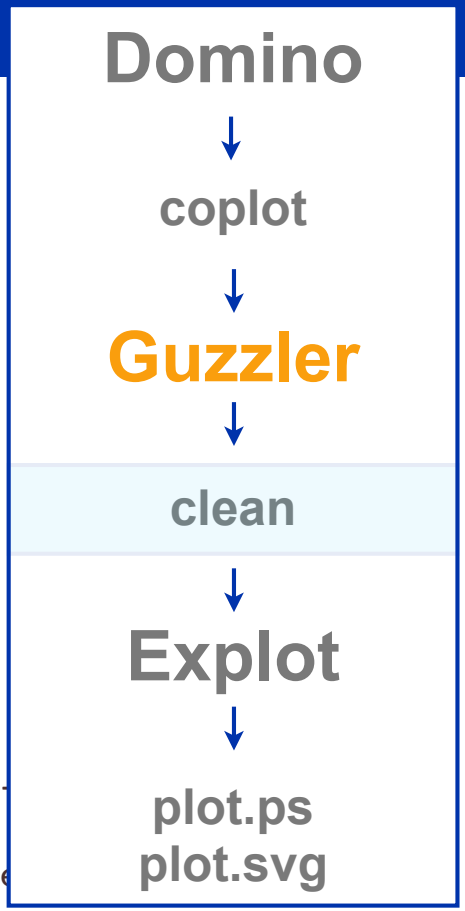


Guzzler

```
Enter [ "?" | CR | graphics file name ] < >?
coplot

working directory: .....

Enter [ "?" | CR | size of labels ] <0.2>?

   1):  ky = and
   2):  and = sill
   3):  ky = sill

 ---------------------------------------------------------------------
 Most important options for labeling:
  -3: automatic (default)      0: no labels or numbers      5: no offse

 Enter [ "?" | CR | option  (min_length)] <-3  0.020>?


exit GUZZLER
```

accept this
(hit return)

accept this also
(hit return again)



Creates file “**clean**” in working directory

Explot

Mac, Linux:

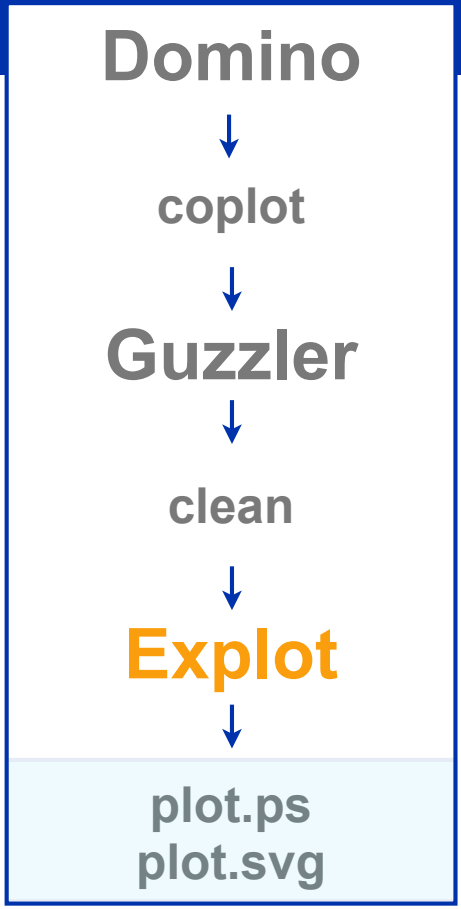
(1) Enter:

```
explot
```

Windows:

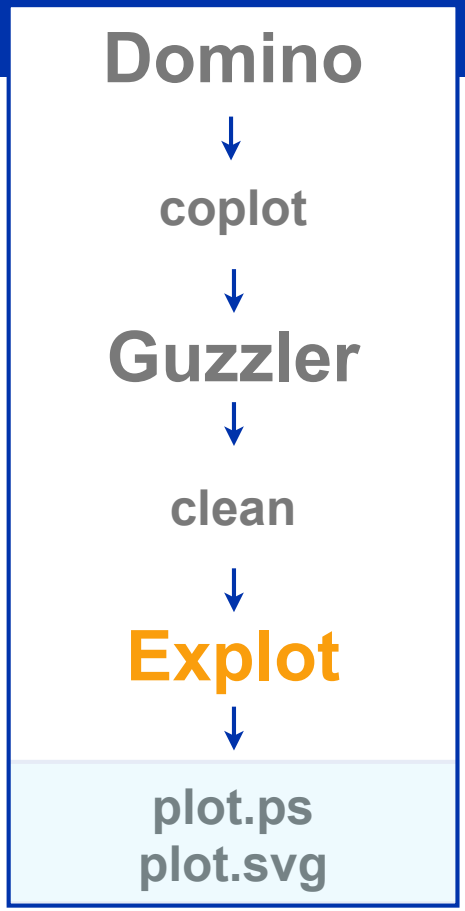
(1) Enter:

```
explot
```

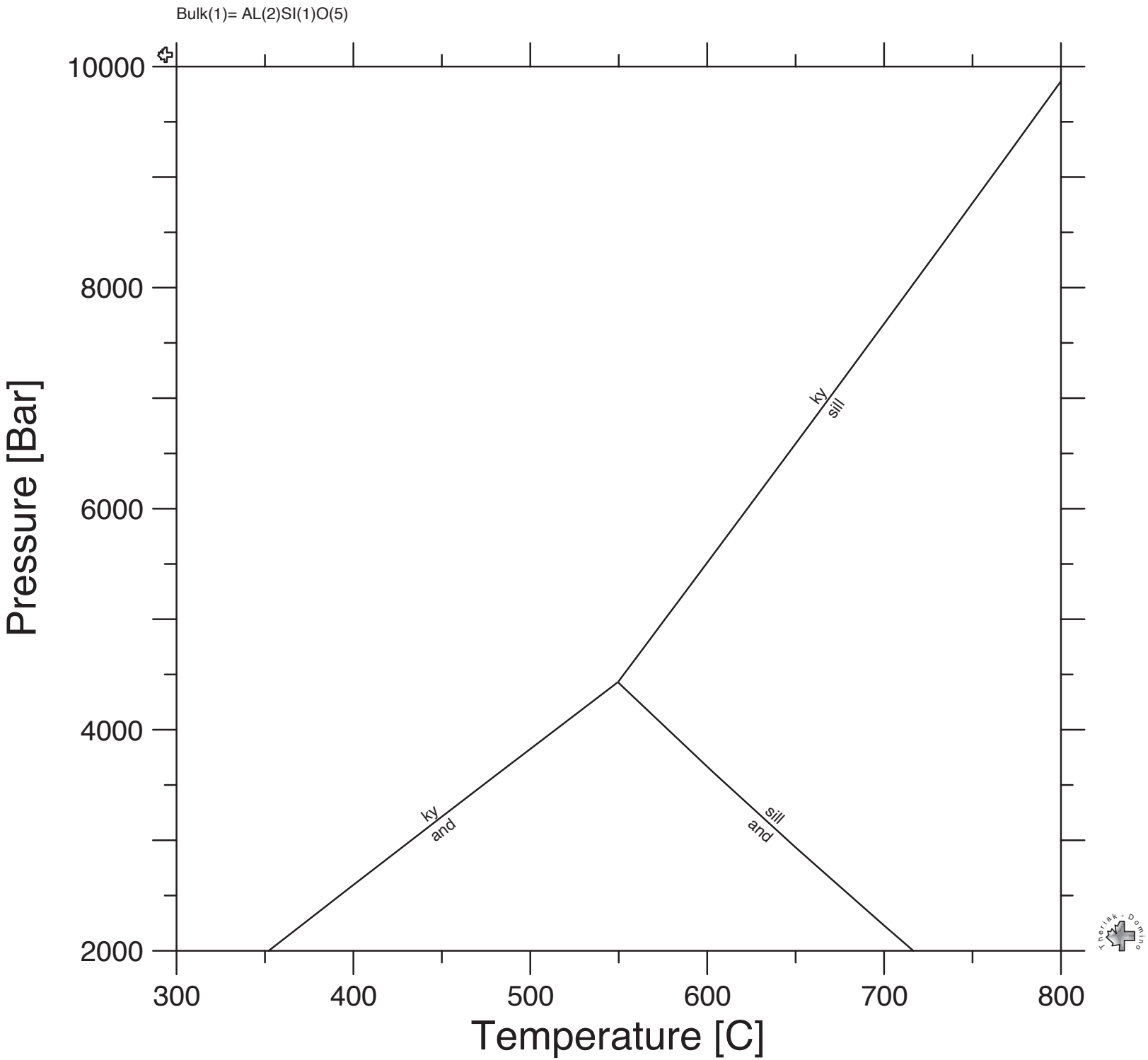


Explot

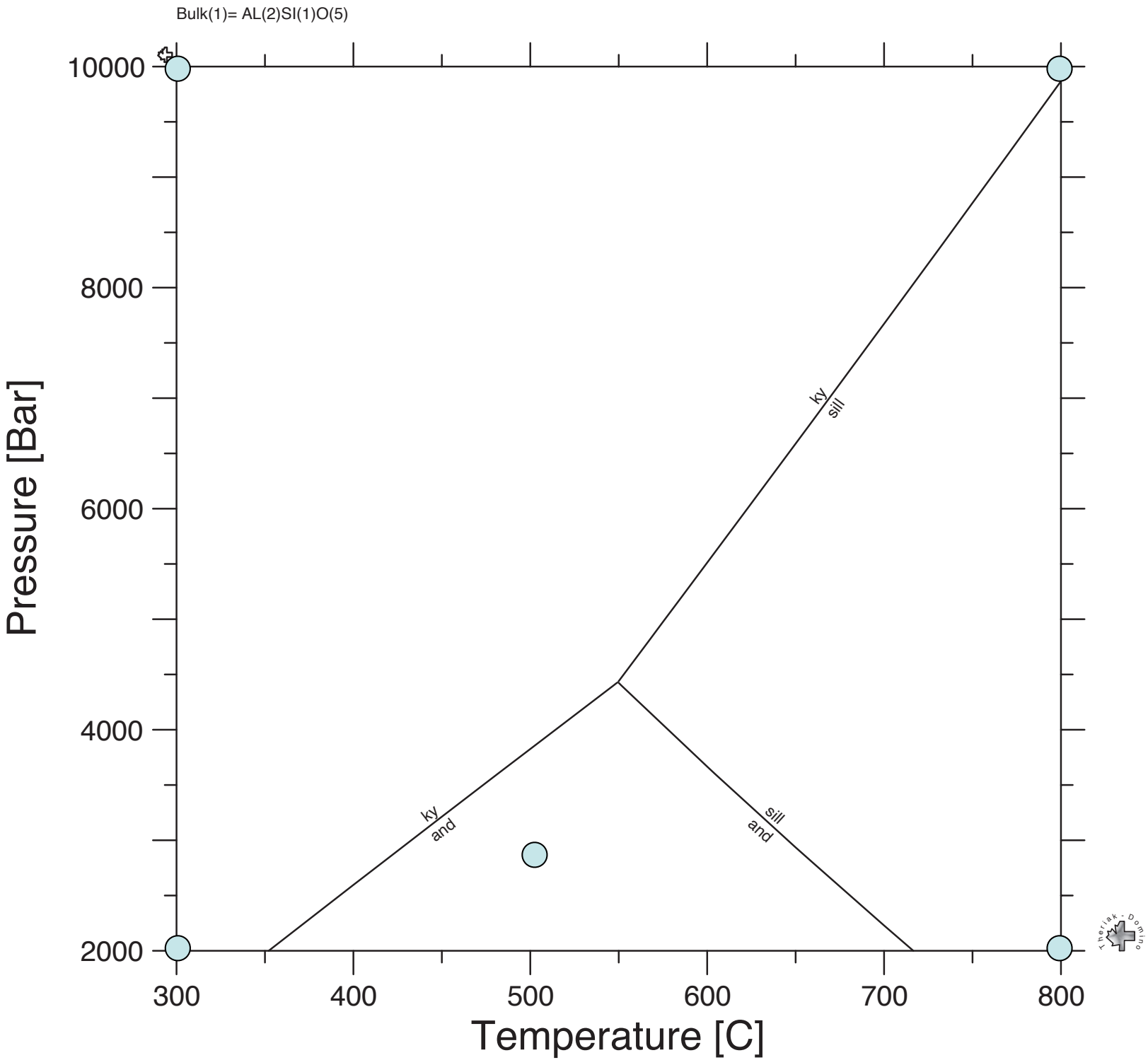
```
Enter [ "?" | CR | graphics file name ] < >?
clean

working directory: ........

exit EXPLOT
```



Creates files “**plot.ps**” and “**plot.svg**” in working directory



CPU time: 0h 00m 00.03s



CPU time: 0h 00m 00.03s

Domino

Mac, Linux:

(1) Enter:
`domino`

Windows:

(1) Enter:
`domino`

Domino

```
--------------------
database definition
--------------------
Enter [ "?" | CR | "files" | "script" | database filename ] <ds5_5.txt>?


---------------------
definition of X-axis
---------------------

X-variable may be: TC, TK, P, A(abc), LNA(abc), LOGA(abc), BIN, TER

Enter [ "?" | "list" | CR | X-variable  X-min  X-max  (X-Grid)  (width)  (ptdist)] <TC   300    800>?


---------------------
definition of Y-axis
---------------------

Y-variable may be: TC, TK, P, PT, THG, A(abc), LNA(abc), LOGA(abc), BIN

Enter [ "?" | CR | "list" | Y-variable  Y-min  Y-max  (Y-Grid)  (height)] <P    2000    10000>?
```

accept these
(previous input)

Domino

```
------------------------------
definition of calculation type
------------------------------

to calculate                          enter
------------                          -----
equilibrium phase diagram              "." (dot)
isolines:
   special funtions:                          Key       min  max  step
   non-solution phases:                Name   Key       min  max  step
   solution phases:                    Name   Key  Nr   min  max  step

For help with isoline definition type "i".


Enter [  "?"  | CR | "point" | "list" | "i" | "." |
      | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
?
```

Domino

```
(i) --------------------------------
(i) Help: calculation type ($DOM-ISO)
(i) --------------------------------
(i) Enter
(i)
(i)      "list"  : to list names for phases, endmembers and solutions
(i)                in the database.
(i)
(i)      "point" : Allows to calculate equilibria for individual x-y-values.
(i)                (seful when x or y is "BIN", LOGA(..) etc.)
(i)
(i)      "."     : to calculate an equilibrium phase diagram.
(i)
(i) For isopleths calculation, input of the following forms must be entered.
(i)
(i)       Key              min  max  step     (Form 1 for bulk rock properties)
(i)      Name  key         min  max  step     (Form 2 for non-solution phases)
(i)       Name  Key  Nr    min  max  step     (Form 3 for solution phases)
(i)
(i) where
(i)
(i)     Name          : Is the name of a pure endmember or solution phase.
(i)                     You may list the valid names by entering "list".
(i)
(i)     Key           : Is one of the keywords listed below.
(i)
(i)     min max step  : Is the minimum, maximum and step values for the isolines.
(i)                     The maximum number of isopleths calculated is 50.
(i)
(i)     Nr            : If more than one phase of the same solution is stable, the
(i)                     phase with the highest "Key"-value is numbered 1, the next
(i)                     lower is numbered 2 and so on.
(i)
(i) Note: All input arguments must be delimited by at least 2 spaces.

 Press the RETURN-key to continue!
```

Domino

```
(i) ISOPLETH KEYWORDS
(i) ================
(i)
(i)    Bulk rock properties (Form 1:              "Key          min   max   step")
(i)    ____________________________________________________________________________
(i)
(i)       Volume of solids [ccm]                : "volsol"
(i)       Weight of solids [g]                  : "wtsol"
(i)       Density of solids [g/ccm]             : "rhosol"
(i)       Total Gibbs Free Energy [J]           : "gtot"
(i)       Wt% of H2O in solids                  : "%h2o.sol"
(i)
(i)    Non-solution phase properties (Form 2:   "Name   Key     min   max   step")
(i)    ____________________________________________________________________________
(i)
(i)       Amount of phase abc [mol]             : abc    "mol"
(i)       Volume of phase abc [ccm]             : abc    "vol"
(i)       Molar volume of phase abc [ccm/mol]   : abc    "mvol"
(i)       Weight of phase abc [g]               : abc    "wt"
(i)       Molar weight of phase abc [g/mol]     : abc    "mwt"
(i)       Density of phase abc [g/ccm]          : abc    "rho"
(i)       Volume% of phase abc (% of solids)    : abc    "vol%"
(i)
(i)    Solution phase properties (Form 3:        "Name   Key          Nr   min   max   step")
(i)    ____________________________________________________________________________
(i)
(i)       Isopleths [mol fractions]             : abc    species     Nr
(i)       Site occupancies                      : abc    El(site)    Nr
(i)       Amount of phase abc [mol]             : abc    "mol"       Nr
(i)       Volume of phase abc [ccm]             : abc    "vol"       Nr
(i)       Molar volume of abc phase [g/mol]     : abc    "mvol"      Nr
(i)       Weight of phase abc [g]               : abc    "wt"        Nr
(i)       Molar weight of phase abc [g/mol]     : abc    "mwt"       Nr
(i)       Density of phase abc [g/ccm]          : abc    "rho"       Nr
(i)       Ratio Mg/(Mg+Fe) of phase abc         : abc    "Mg#"       Nr
(i)       Volume% of phase abc (% of solids)    : abc    "vol%"      Nr
(i)
(i) Note: abc and species are case sensitive names or abbreviations of phases and endmembers
```

Domino

```
Press the RETURN-key to continue!

 (i)
 (i) Summary
 (i) =======
 (i)
 (i) To calculate                          enter
 (i) ------------                          -----
 (i) An equilibrium phase diagram          "." (dot)
 (i)
 (i) Property isopleths of
 (i)    Bulk rock                                  Key       min   max   step
 (i)    Non-solution phases:                Name   Key       min   max   step
 (i)    Solution phases:                    Name   Key   Nr  min   max   step
 (i)
 (i) Examples for isopleths:
 (i) -----------------------
 (i) To plot grossular isopleths in garnet between 0.3 and 0.6 in steps of 0.02
 (i)
 (i)                  GARNET  Grs  1   0.3  0.6  0.02
 (i)
 (i) To plot iso-density lines of quartz (non-solution phase)
 (i) between 2.5 and 2.7 in steps of 0.02
 (i)
 (i)                  A-QUARTZ  rho   2.5   2.7   0.02
 (i)
 (i) To plot iso-density lines of feldspar (solution phase)
 (i) between 2.5 and 2.7 in steps of 0.02
 (i)
 (i)                  FSP  rho   1  2.5   2.7   0.02
 (i)
 (i) To plot Wt% of H2O in solids between 0 and 10 in steps of 0.5
 (i)
 (i)                  %h2o.sol    0   10   0.5
 (i) ------------------------------------------------------------------------

 Press the RETURN-key to continue!
```

Domino

```
 Enter [   "?"   | CR | "point" | "list" | "i" | "." |
       | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
list
```

Domino

```
 Enter [  "?"  | CR | "point" | "list" | "i" | "." |
       | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
list

List of phase names (abbreviations)
-----------------------------------
  andalusite (and)        anorthite (an)          kyanite (ky)            quartz (q)
sillimanite (sill)


 to calculate                          enter
 ------------                          -----
 equilibrium phase diagram              "." (dot)
 isolines:
    special funtions:                          Key      min  max  step
    non-solution phases:                Name   Key      min  max  step
    solution phases:                    Name   Key  Nr  min  max  step
```

Domino

```
 Enter [  "?"  | CR | "point" | "list" | "i" | "." |
       | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
list

List of phase names (abbreviations)
-----------------------------------
  andalusite (and)        anorthite (an)          kyanite (ky)            quartz (q)
sillimanite (sill)


 to calculate                          enter
 ------------                          -----
 equilibrium phase diagram              "." (dot)
 isolines:
    special funtions:                          Key      min  max  step
    non-solution phases:                Name   Key      min  max  step
    solution phases:                    Name   Key  Nr  min  max  step

 For help with isoline definition type "i".


 Enter [  "?"  | CR | "point" | "list" | "i" | "." |
       | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
andalusite   rho   3.0   3.2   0.005
```

Domino

```
 Enter [  "?"  | CR | "point" | "list" | "i" | "." |
       | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
list

List of phase names (abbreviations)
-----------------------------------
  andalusite (and)        anorthite (an)          kyanite (ky)            quartz (q)
sillimanite (sill)


 to calculate                          enter
 ------------                          -----
 equilibrium phase diagram              "." (dot)
 isolines:
    special funtions:                          Key      min  max  step
    non-solution phases:                Name   Key      min  max  step
    solution phases:                    Name   Key  Nr  min  max  step

 For help with isoline definition type "i".


 Enter [  "?"  | CR | "point" | "list" | "i" | "." |
       | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
andalusite   rho   3.0   3.2   0.005

 --------------------
 labeling of reactions
 --------------------

 Labels: 1=assemblages, 2=new phases, 3=reactions, -1=special

 Enter [ "?" | CR | Label (prec  smooth) ] <1>?
```

accept this

Domino

```
...

...

...


 NUMBER OF LINES:  14    NUMBER OF POINTS: 104    max.ph.    9
 LEVEL:  5   SQUARE: (203 , 57 ) LINE     5   REACTION    5: OPEN END
      9  1145  Y =  3412.5000 ,      2 REACTIONS:    5   14
      7  1152  X =   616.4062 ,      2 REACTIONS:    5   11
 NUMBER OF LINES:  14    NUMBER OF POINTS: 108    max.ph.    9
 LEVEL:  5   SQUARE: (230 , 33 ) LINE     6   REACTION    6: OPEN END
      9  1161  Y =  2812.5000 ,      2 REACTIONS:    6   10
      5  1166  X =   658.5938 ,      1 REACTIONS:   10
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (257 , 10 ) LINE     7   REACTION    7: OPEN END
      3  1169  Y =  2237.5000 ,      0 REACTIONS:
      2  1171  X =   700.7812 ,      0 REACTIONS:
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (160 , 98 ) LINE    12   REACTION   12: OPEN END
      6  1177  Y =  4437.5000 ,      0 REACTIONS:
      5  1182  X =   549.2188 ,      1 REACTIONS:   12
 NUMBER OF LINES:  14    NUMBER OF POINTS: 112    max.ph.    9

exit DOMINO
CPU time:    0h 00m 00.08s
```

Creates file “**coplot**” in working directory

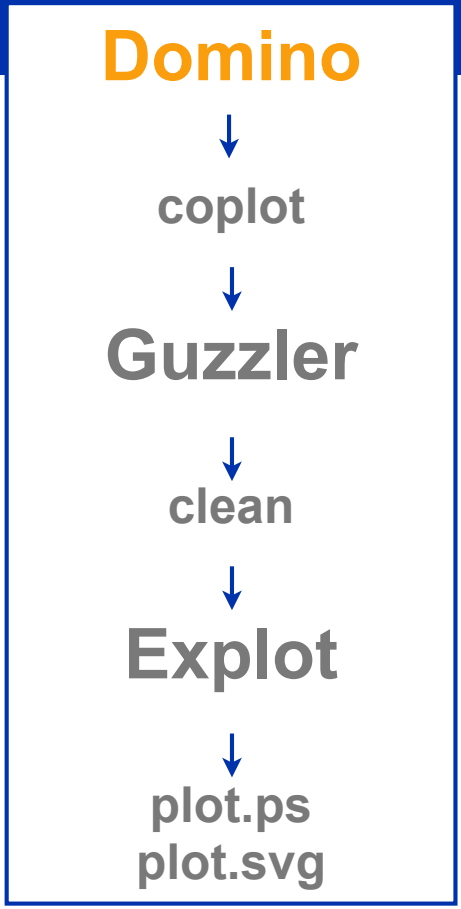
Domino

...

...

...

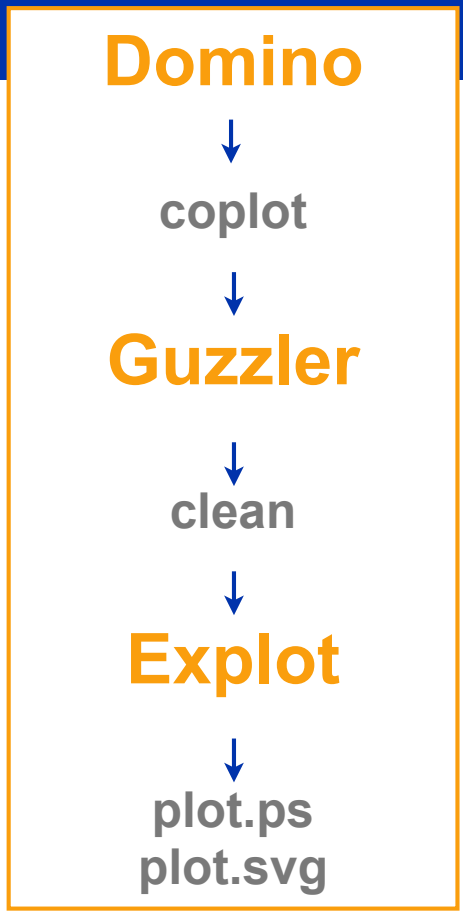
```
 NUMBER OF LINES:  14    NUMBER OF POINTS: 104    max.ph.    9
 LEVEL:  5   SQUARE: (203 , 57 ) LINE     5   REACTION    5: OPEN END
      9  1145  Y =  3412.5000 ,      2 REACTIONS:    5   14
      7  1152  X =   616.4062 ,      2 REACTIONS:    5   11
 NUMBER OF LINES:  14    NUMBER OF POINTS: 108    max.ph.    9
 LEVEL:  5   SQUARE: (230 , 33 ) LINE     6   REACTION    6: OPEN END
      9  1161  Y =  2812.5000 ,      2 REACTIONS:    6   10
      5  1166  X =   658.5938 ,      1 REACTIONS:   10
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (257 , 10 ) LINE     7   REACTION    7: OPEN END
      3  1169  Y =  2237.5000 ,      0 REACTIONS:
      2  1171  X =   700.7812 ,      0 REACTIONS:
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (160 , 98 ) LINE    12   REACTION   12: OPEN END
      6  1177  Y =  4437.5000 ,      0 REACTIONS:
      5  1182  X =   549.2188 ,      1 REACTIONS:   12
 NUMBER OF LINES:  14    NUMBER OF POINTS: 112    max.ph.    9

exit DOMINO
CPU time:    0h 00m 00.08s
```



Creates file “**coplot**” in working directory

Domino

```
...
...
...

 NUMBER OF LINES:  14    NUMBER OF POINTS: 104    max.ph.    9
 LEVEL:  5   SQUARE: (203 , 57 ) LINE     5   REACTION    5: OPEN END
      9  1145  Y =  3412.5000 ,      2 REACTIONS:    5   14
      7  1152  X =   616.4062 ,      2 REACTIONS:    5   11
 NUMBER OF LINES:  14    NUMBER OF POINTS: 108    max.ph.    9
 LEVEL:  5   SQUARE: (230 , 33 ) LINE     6   REACTION    6: OPEN END
      9  1161  Y =  2812.5000 ,      2 REACTIONS:    6   10
      5  1166  X =   658.5938 ,      1 REACTIONS:   10
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (257 , 10 ) LINE     7   REACTION    7: OPEN END
      3  1169  Y =  2237.5000 ,      0 REACTIONS:
      2  1171  X =   700.7812 ,      0 REACTIONS:
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (160 , 98 ) LINE    12   REACTION   12: OPEN END
      6  1177  Y =  4437.5000 ,      0 REACTIONS:
      5  1182  X =   549.2188 ,      1 REACTIONS:   12
 NUMBER OF LINES:  14    NUMBER OF POINTS: 112    max.ph.    9

exit DOMINO
CPU time:    0h 00m 00.08s
```



Creates file “**coplot**” in working directory

Make sure to rename old plot.ps/plot.svg files before using Explot again as it would overwrite them!

Domino

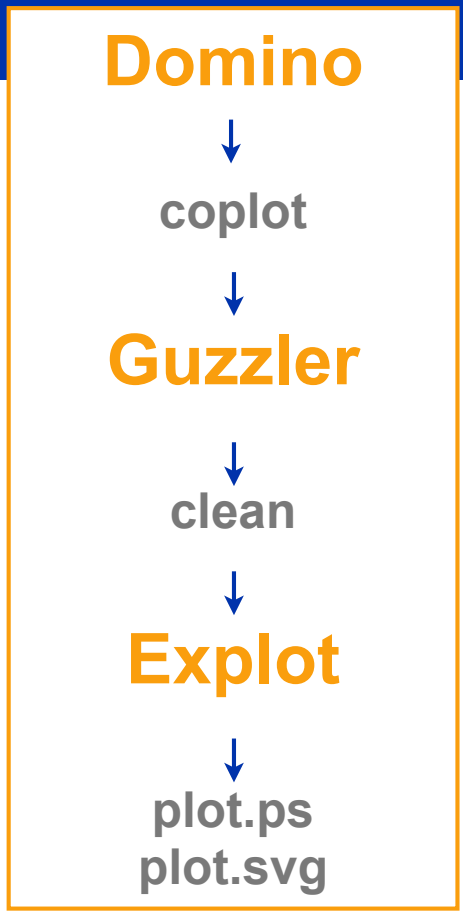
```
andalusite    rho    3.0    3.2    0.005
```

Repeat for kyanite and sillimanite (see below)!

```
kyanite    rho    3.5    3.7    0.005
```

```
sillimanite    rho    3.1    3.3    0.005
```

Rename files between steps and put all plots into one phase diagram!



Domino

Mac, Linux:

(1) Enter:
`domino`

Windows:

(1) Enter:
`domino`

Domino

```
--------------------
database definition
--------------------
Enter [ "?" | CR | "files" | "script" | database filename ] <ds5_5.txt>?


---------------------
definition of X-axis
---------------------

X-variable may be: TC, TK, P, A(abc), LNA(abc), LOGA(abc), BIN, TER

Enter [ "?" | "list" | CR | X-variable  X-min  X-max  (X-Grid)  (width)  (ptdist)] <TC   300    800>?


---------------------
definition of Y-axis
---------------------

Y-variable may be: TC, TK, P, PT, THG, A(abc), LNA(abc), LOGA(abc), BIN

Enter [ "?" | CR | "list" | Y-variable  Y-min  Y-max  (Y-Grid)  (height)] <P    2000    10000>?
```

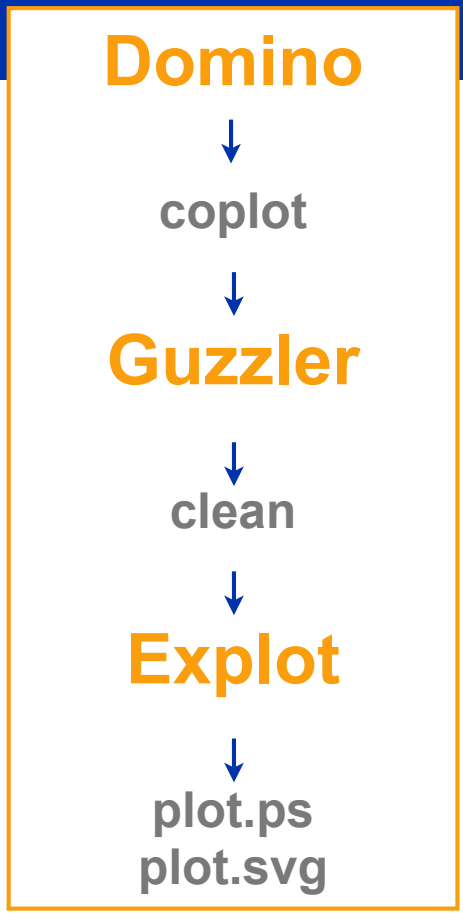
accept these
(previous input)

Domino

```
------------------------------
definition of calculation type
------------------------------

to calculate                          enter
------------                          -----
equilibrium phase diagram              "." (dot)
isolines:
   special funtions:                          Key       min  max  step
   non-solution phases:                Name   Key       min  max  step
   solution phases:                    Name   Key  Nr   min  max  step

For help with isoline definition type "i".


Enter [  "?"  | CR | "point" | "list" | "i" | "." |
      | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
kyanite   rho   3.5   3.7   0.005
```

Domino

```
...
...
...

 NUMBER OF LINES:  14    NUMBER OF POINTS: 104    max.ph.    9
 LEVEL:  5   SQUARE: (203 , 57 ) LINE     5   REACTION    5: OPEN END
      9  1145  Y =  3412.5000 ,      2 REACTIONS:    5   14
      7  1152  X =   616.4062 ,      2 REACTIONS:    5   11
 NUMBER OF LINES:  14    NUMBER OF POINTS: 108    max.ph.    9
 LEVEL:  5   SQUARE: (230 , 33 ) LINE     6   REACTION    6: OPEN END
      9  1161  Y =  2812.5000 ,      2 REACTIONS:    6   10
      5  1166  X =   658.5938 ,      1 REACTIONS:   10
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (257 , 10 ) LINE     7   REACTION    7: OPEN END
      3  1169  Y =  2237.5000 ,      0 REACTIONS:
      2  1171  X =   700.7812 ,      0 REACTIONS:
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (160 , 98 ) LINE    12   REACTION   12: OPEN END
      6  1177  Y =  4437.5000 ,      0 REACTIONS:
      5  1182  X =   549.2188 ,      1 REACTIONS:   12
 NUMBER OF LINES:  14    NUMBER OF POINTS: 112    max.ph.    9

exit DOMINO
CPU time:    0h 00m 00.08s
```



Creates file “**coplot**” in working directory

Make sure to rename old plot.ps/plot.svg files before using Explot again as it would overwrite them!

Domino

Mac, Linux:

(1) Enter:
`domino`

Windows:

(1) Enter:
`domino`

Domino

```
--------------------
database definition
--------------------
Enter [ "?" | CR | "files" | "script" | database filename ] <ds5_5.txt>?


---------------------
definition of X-axis
---------------------

X-variable may be: TC, TK, P, A(abc), LNA(abc), LOGA(abc), BIN, TER

Enter [ "?" | "list" | CR | X-variable  X-min  X-max  (X-Grid)  (width)  (ptdist)] <TC   300    800>?


---------------------
definition of Y-axis
---------------------

Y-variable may be: TC, TK, P, PT, THG, A(abc), LNA(abc), LOGA(abc), BIN

Enter [ "?" | CR | "list" | Y-variable  Y-min  Y-max  (Y-Grid)  (height)] <P    2000    10000>?
```

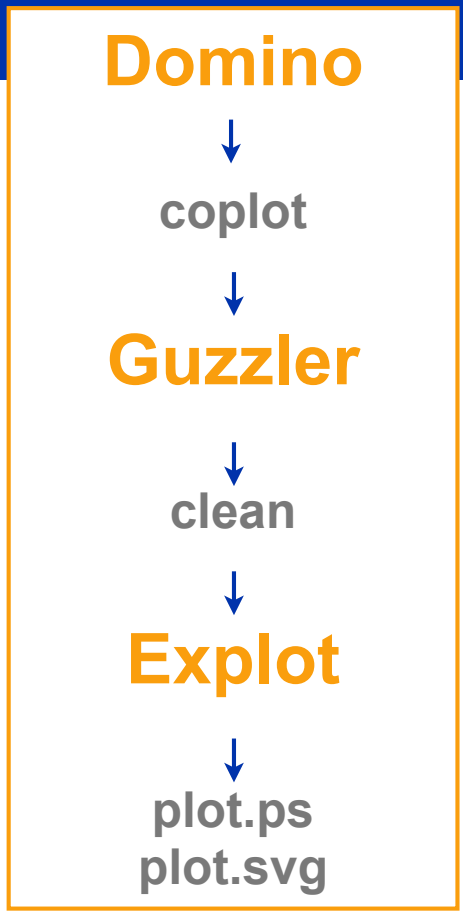
accept these
(previous input)

Domino

```
------------------------------
definition of calculation type
------------------------------

to calculate                          enter
------------                          -----
equilibrium phase diagram              "." (dot)
isolines:
   special funtions:                          Key       min  max  step
   non-solution phases:                Name   Key       min  max  step
   solution phases:                    Name   Key  Nr   min  max  step

For help with isoline definition type "i".


Enter [  "?"  | CR | "point" | "list" | "i" | "." |
      | "pix" ix iy | (Phase)  Key  (Nr)  min  max  step ] <.>?
sillimanite   rho    3.1    3.3   0.005
```

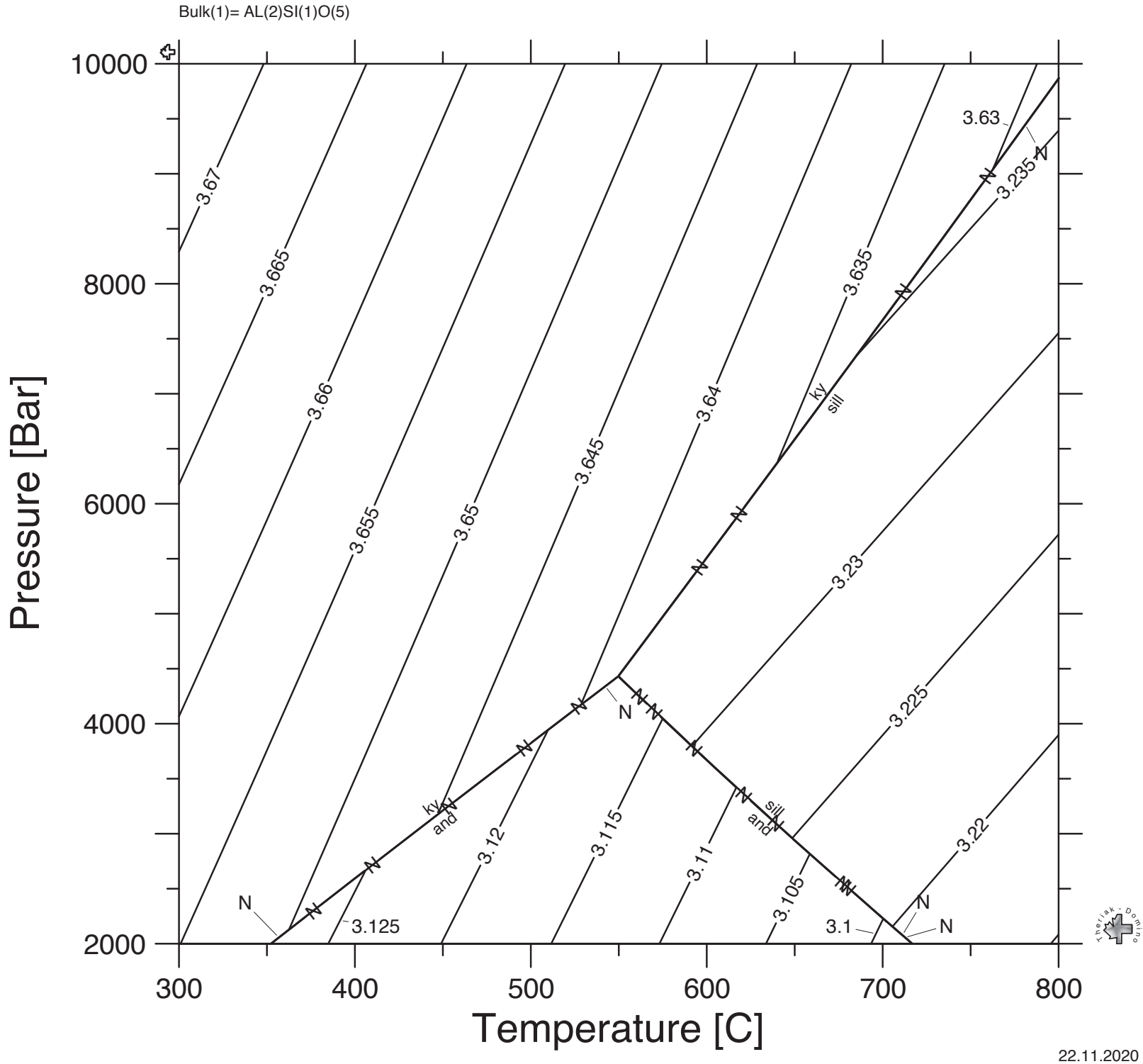
Domino

```
...
...
...

 NUMBER OF LINES:  14    NUMBER OF POINTS: 104    max.ph.    9
 LEVEL:  5   SQUARE: (203 , 57 ) LINE     5   REACTION    5: OPEN END
      9  1145  Y =  3412.5000 ,      2 REACTIONS:    5   14
      7  1152  X =   616.4062 ,      2 REACTIONS:    5   11
 NUMBER OF LINES:  14    NUMBER OF POINTS: 108    max.ph.    9
 LEVEL:  5   SQUARE: (230 , 33 ) LINE     6   REACTION    6: OPEN END
      9  1161  Y =  2812.5000 ,      2 REACTIONS:    6   10
      5  1166  X =   658.5938 ,      1 REACTIONS:   10
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (257 , 10 ) LINE     7   REACTION    7: OPEN END
      3  1169  Y =  2237.5000 ,      0 REACTIONS:
      2  1171  X =   700.7812 ,      0 REACTIONS:
 NUMBER OF LINES:  14    NUMBER OF POINTS: 111    max.ph.    9
 LEVEL:  5   SQUARE: (160 , 98 ) LINE    12   REACTION   12: OPEN END
      6  1177  Y =  4437.5000 ,      0 REACTIONS:
      5  1182  X =   549.2188 ,      1 REACTIONS:   12
 NUMBER OF LINES:  14    NUMBER OF POINTS: 112    max.ph.    9

exit DOMINO
CPU time:    0h 00m 00.08s
```



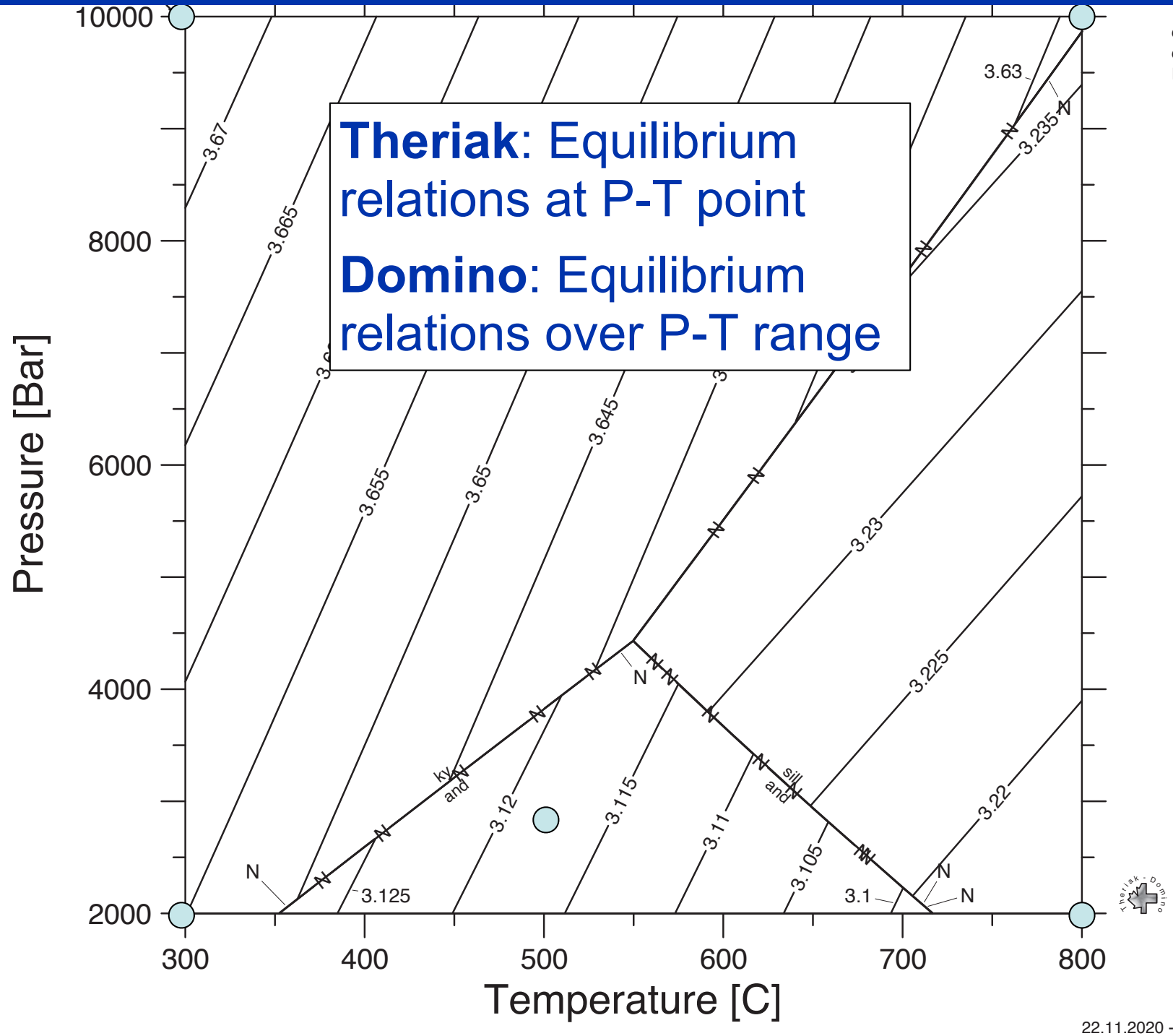
Creates file “**coplot**” in working directory

Make sure to rename old plot.ps/plot.svg files before using Explot again as it would overwrite them!



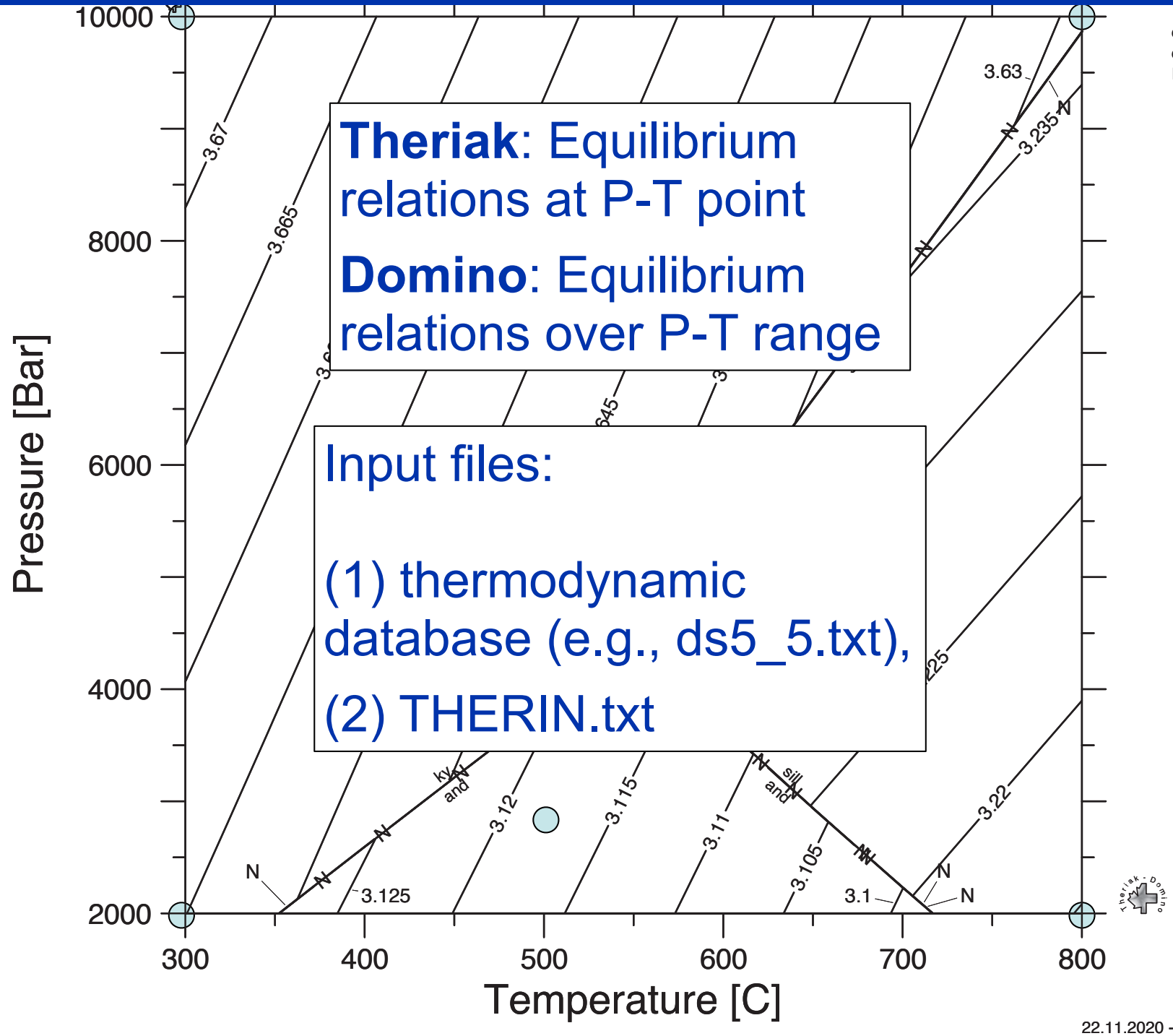
22.11.2020 - 21:47:00 CPU time: 0h 00m 00.08s

Summary



22.11.2020 - 21:47:00 CPU time: 0h 00m 00.08s

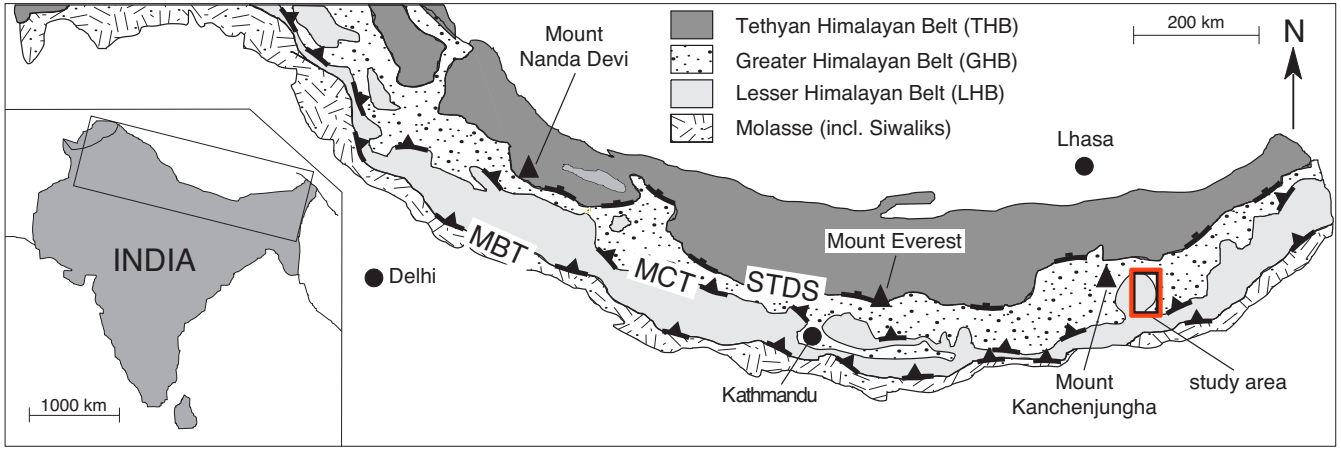
Summary

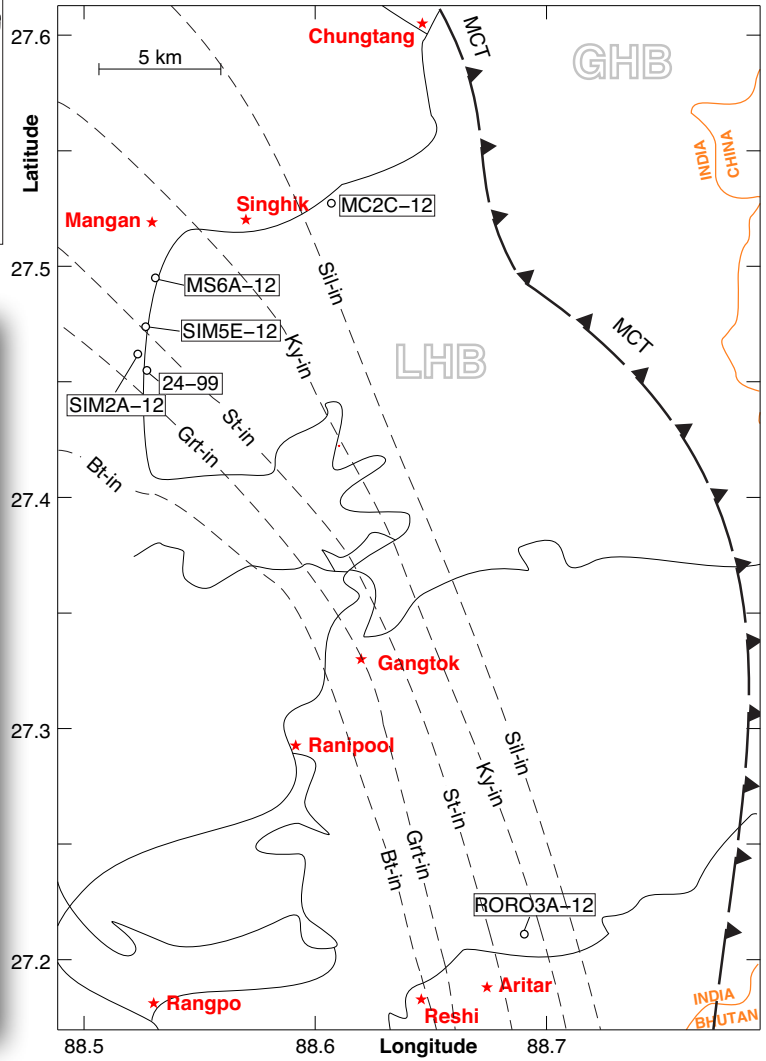


22.11.2020 - 21:47:00 CPU time: 0h 00m 00.08s

Theriak-Domino modelling of realistic systems

Lesser Himalayan Belt, Sikkim, India





Gaidies et al. (2015)

Theriak-Domino modelling of realistic systems

Given is the bulk chemical composition of a Barrovian garnet-zone mica schist from the Sikkim Himalaya (NE India).

Calculate a P-T equilibrium assemblage diagram using the database ds5_5.txt, assuming saturation with respect to H2O. Also assume that all iron is present as ferrous Fe.

T-range: 500 - 600 °C

P-range: 2500 - 6000 Bar

	wt%		Mol of element
SiO2	64.85		
TiO2	0.61		
Al2O3	18.73		
Fe2O3	6.44		
FeO	0		
MnO	0.05		
MgO	1.89		
CaO	0.55		
Na2O	0.87		
K2O	3.6		
LOI	2.36		

THERIN.txt:

```
0    ??????????????????????????     * A nice rock from Sikkim
```

Theriak-Domino modelling of realistic systems

Given is the bulk chemical composition of a Barrovian garnet-zone mica schist from the Sikkim Himalaya (NE India).

Calculate a P-T equilibrium assemblage diagram using the database ds5_5.txt, assuming saturation with respect to H2O. Also assume that all iron is present as ferrous Fe.

T-range: 500 - 600 °C

P-range: 2500 - 6000 Bar

	wt%	Mol.wt	Mol of element
SiO2	64.85	60.08	63.6
TiO2	0.61	79.88	0.45
Al2O3	18.73	101.96	21.65
Fe2O3	6.44	159.69	0
FeO	0	71.85	4.76
MnO	0.05	70.94	0.04
MgO	1.89	40.3	2.76
CaO	0.55	56.08	0.58
Na2O	0.87	61.98	1.66
K2O	3.6	94.2	4.5
LOI	2.36		
H2O			100.00

THERIN.txt:

```
0    SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)
```

Theriak-Domino modelling of realistic systems

THERIN.txt:

```
!-------------------------------------------------------------------------------------
    600    9500
0   SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)     * A nice rock from Sikkim
0   AL(2)SI(1)O(5)     * my first test run
0   SI(17)AL(8)K(1)NA(1)H(100)O(?)     *
0   SI(14)AL(5)K(1)H(100)O(?)     *
0   SI(17)AL(8)K(1)NA(0)H(100)O(?)     *
0   SI(17)AL(8)K(0)NA(1)H(100)O(?)     *
0   SI(17)AL(8)K(1)NA(1)H(100)O(?)     * my second test run
```

Mac, Linux:

(1) Enter:

```
domino
```

Windows:

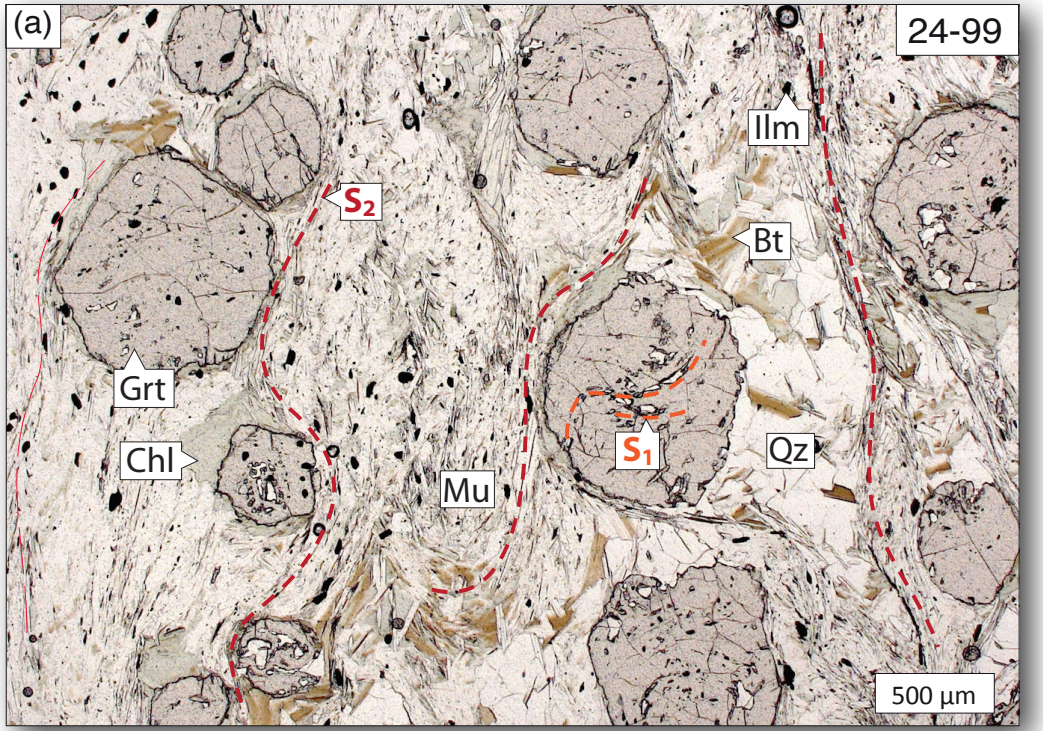
(1) Enter:

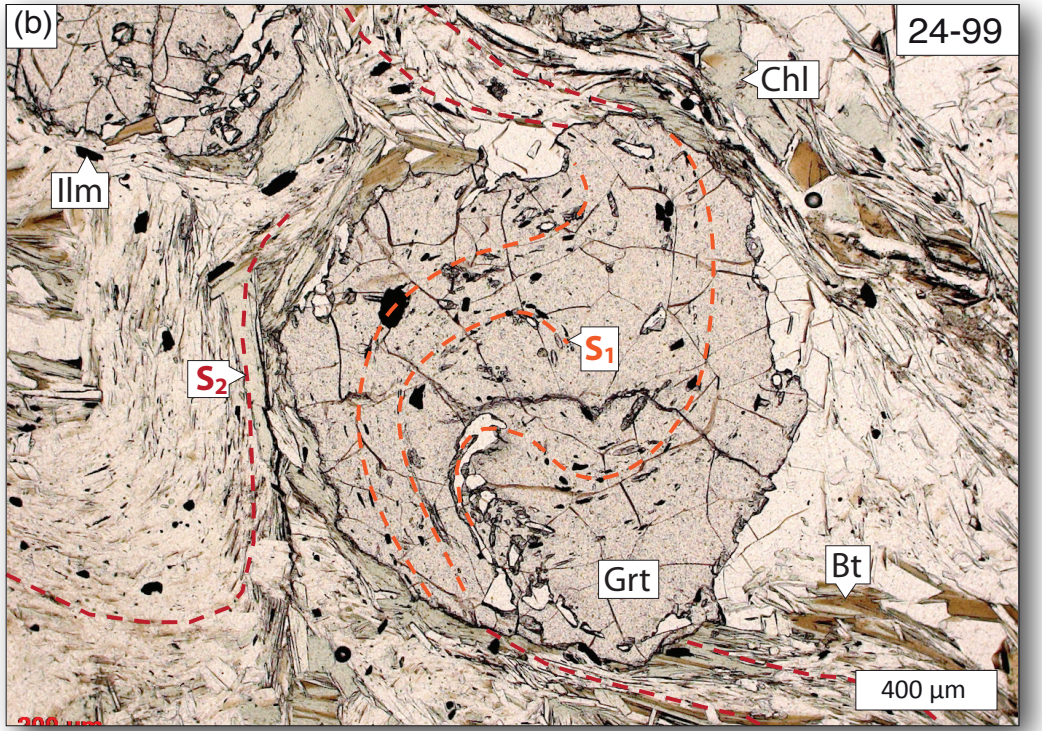
```
domino
```

```
X-axis
Y-axis
calculation type
labelling of reactions
```

```
TC    500     600
P    2500    6000
.
1
```

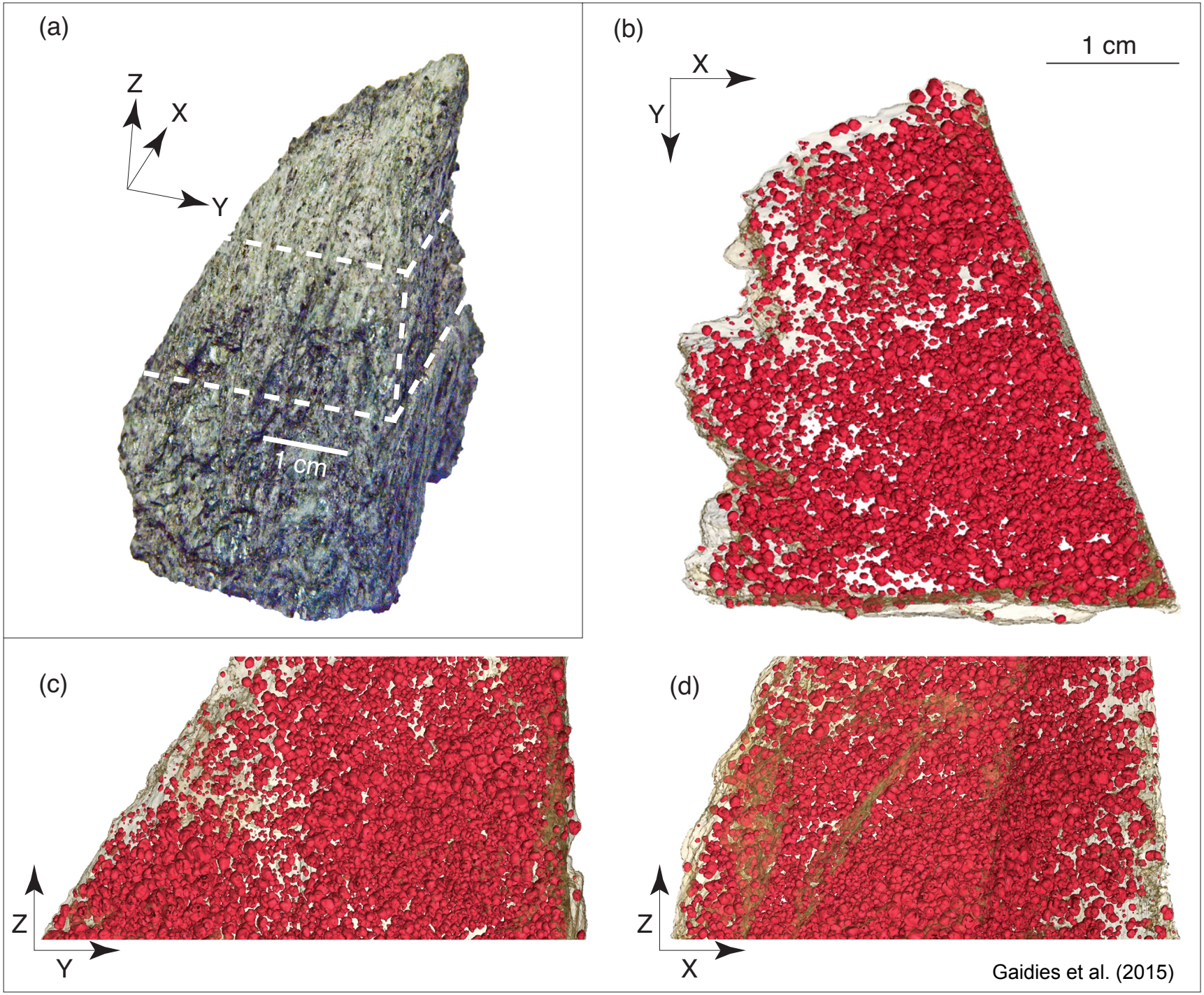
Theriak-Domino modelling of realistic systems

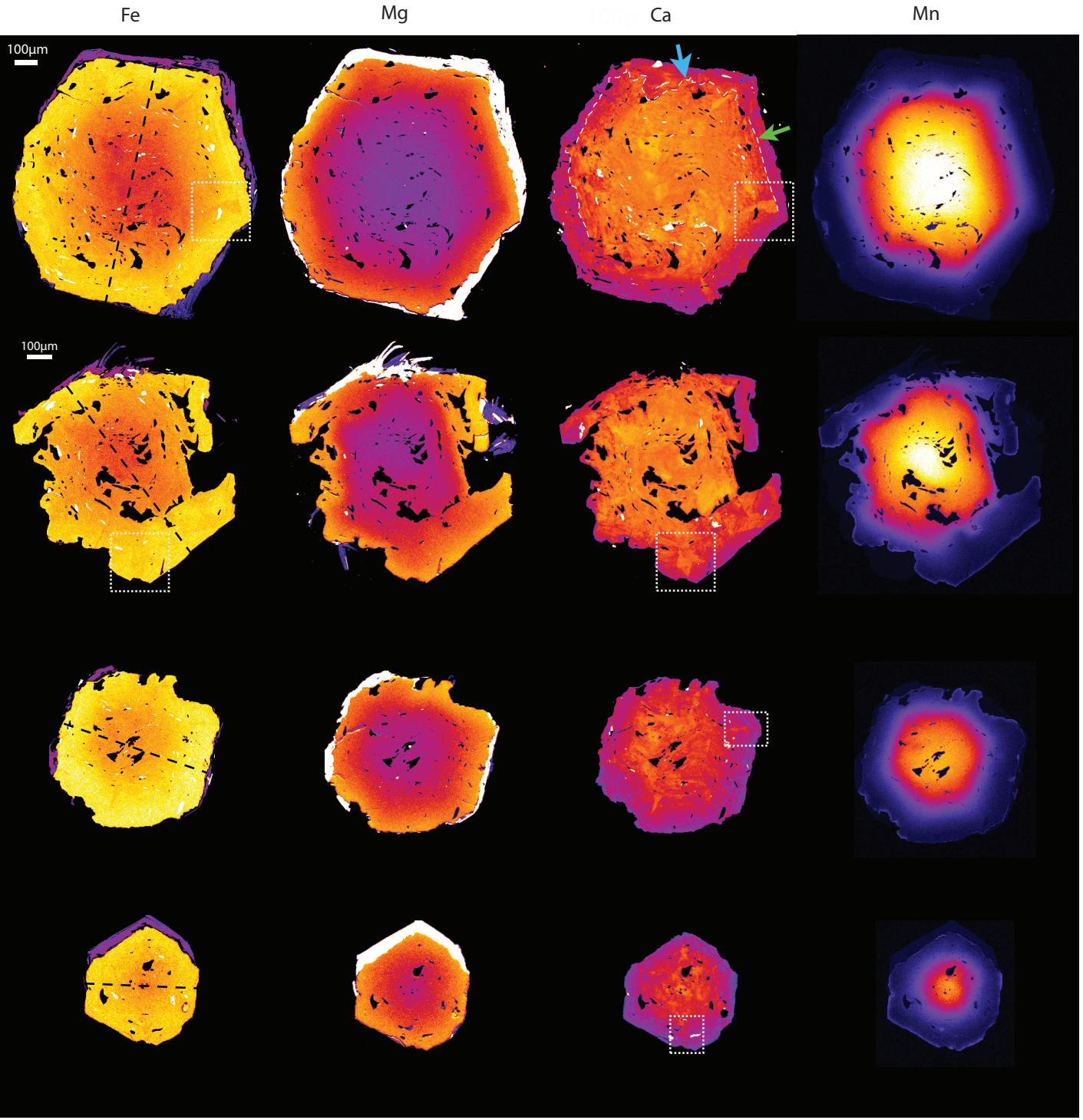


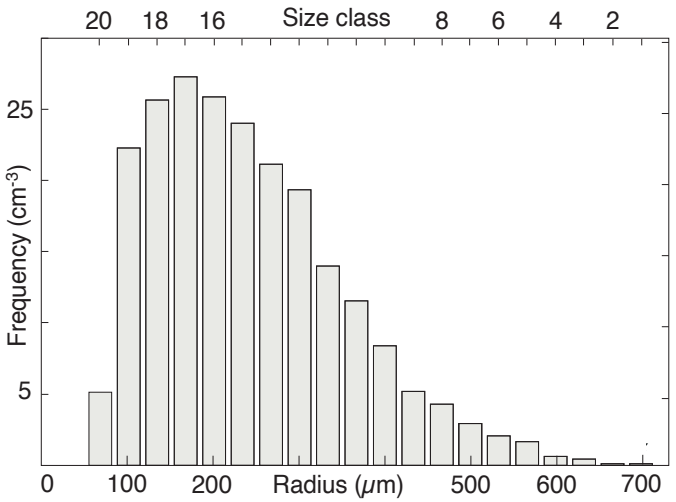


George & Gaidies (2017)

Theriak-Domino modelling of realistic systems







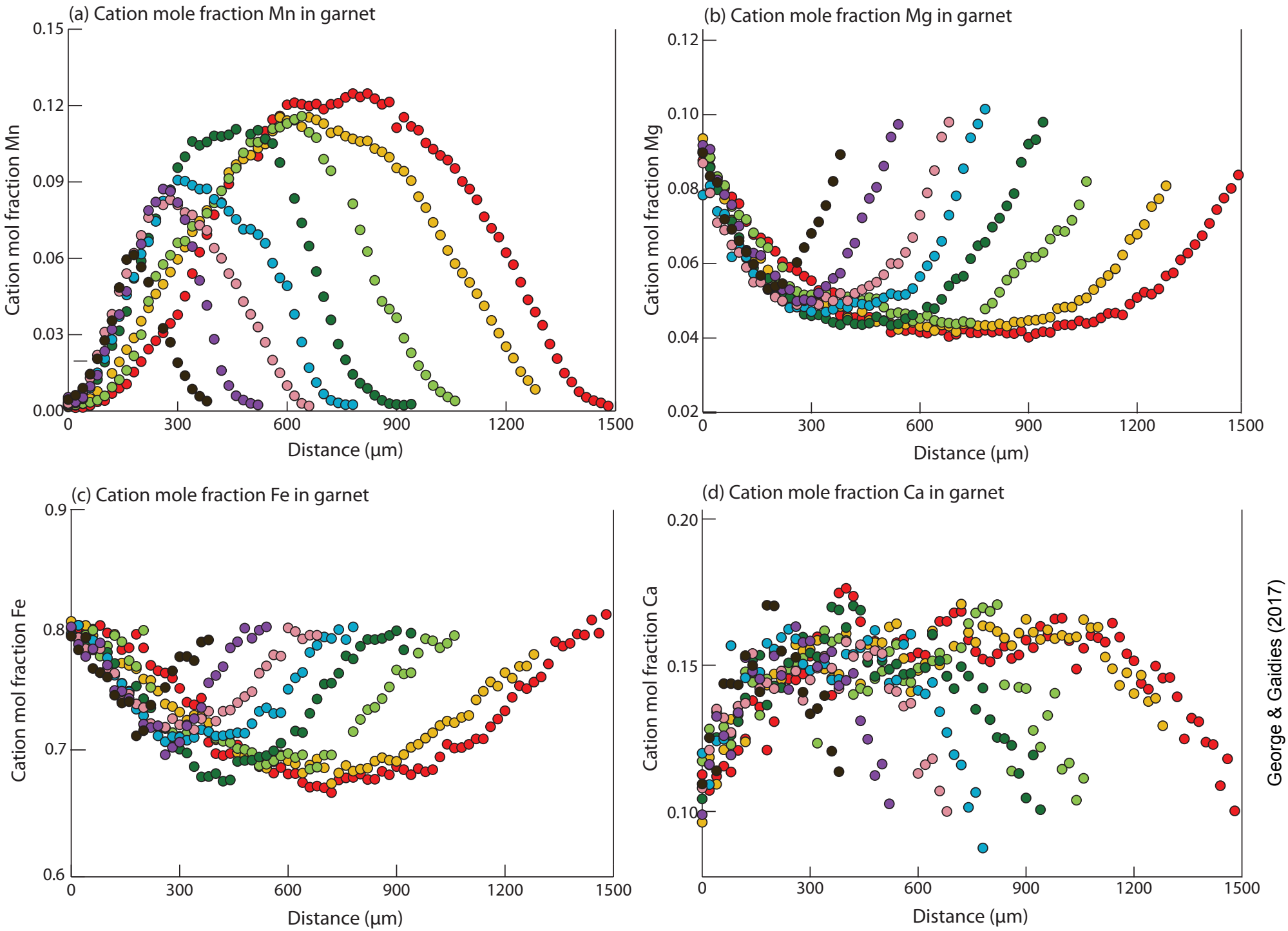
George & Gaidies (2017)

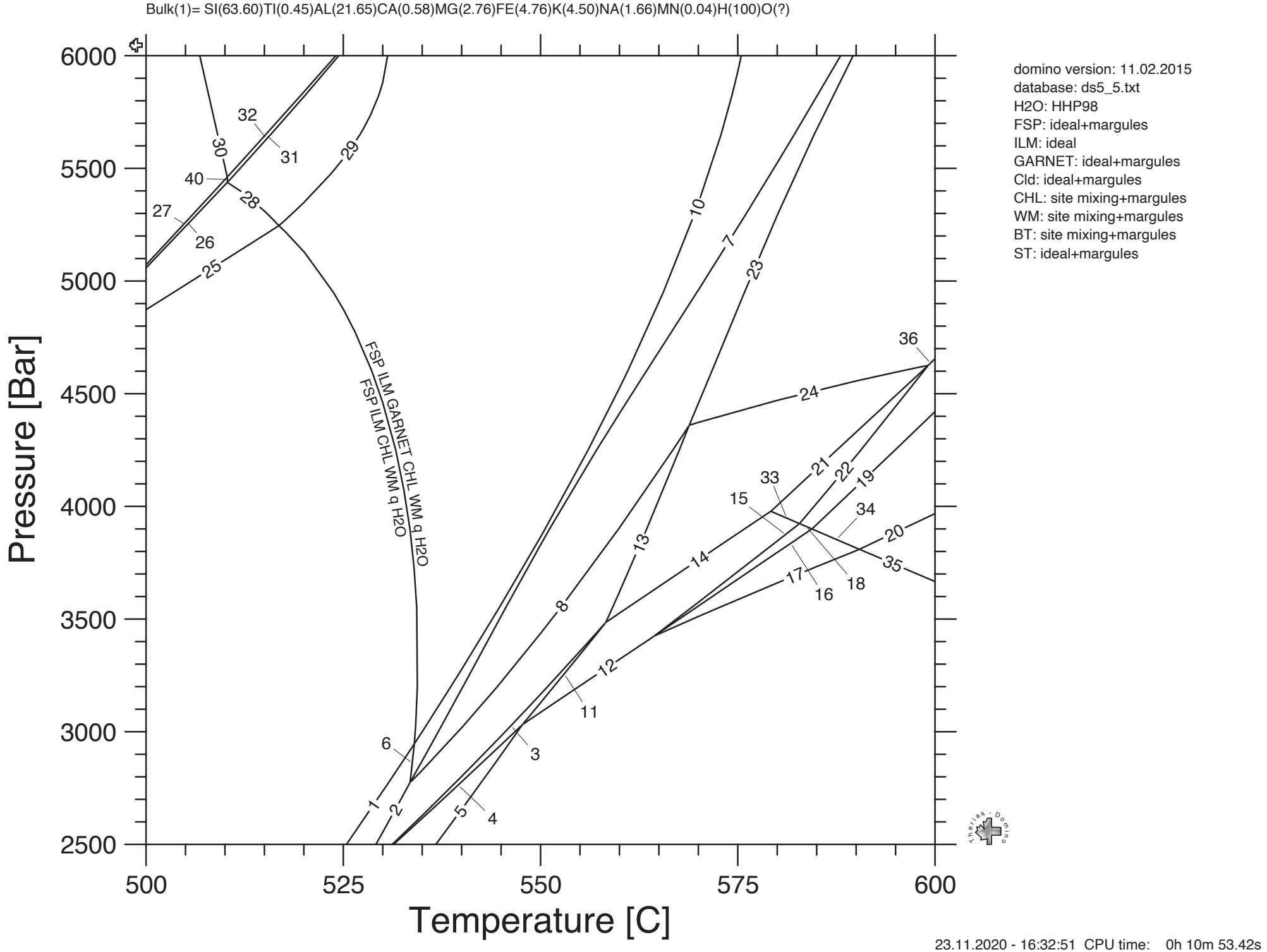
Relative count

low

high

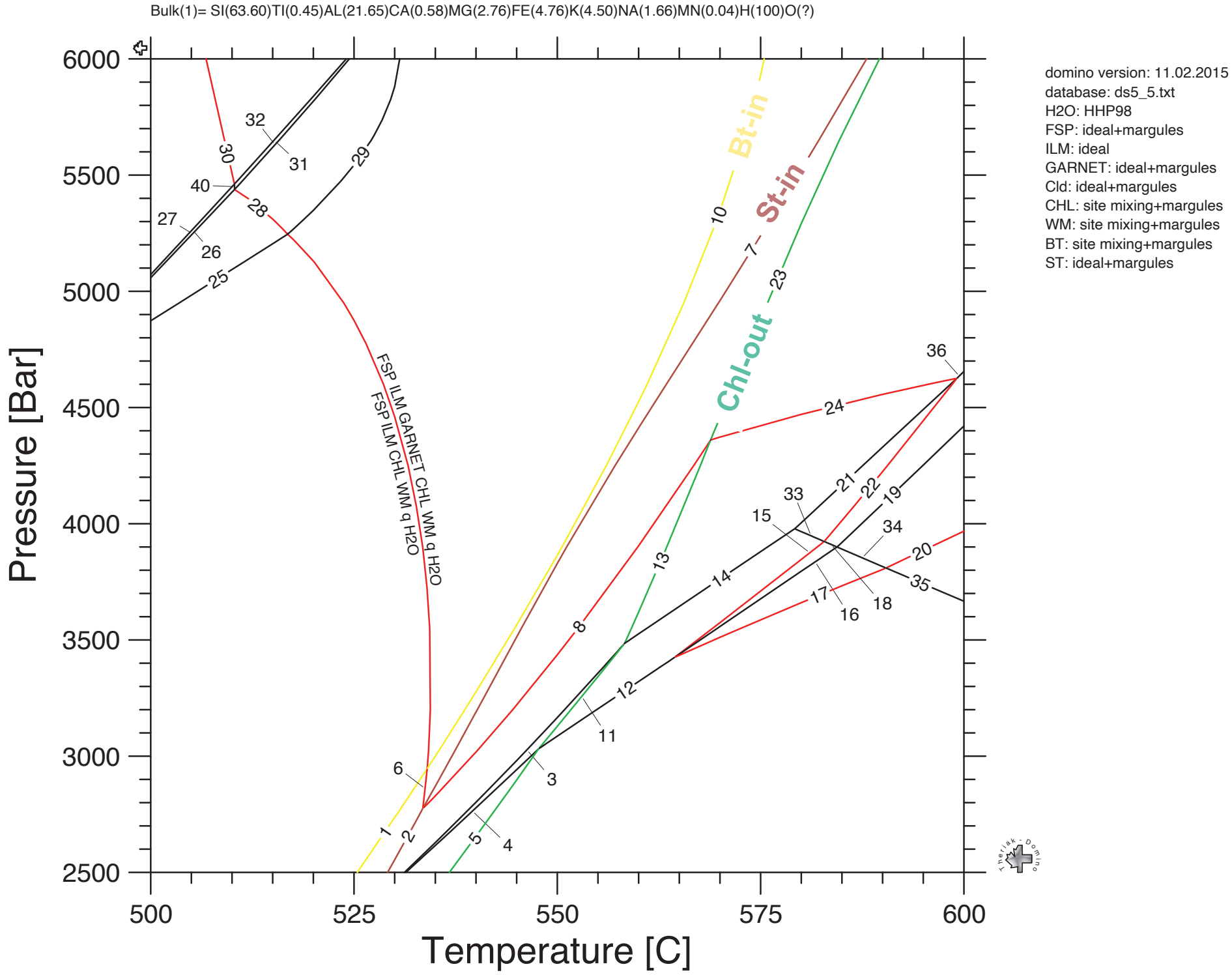
Theriak-Domino modelling of realistic systems

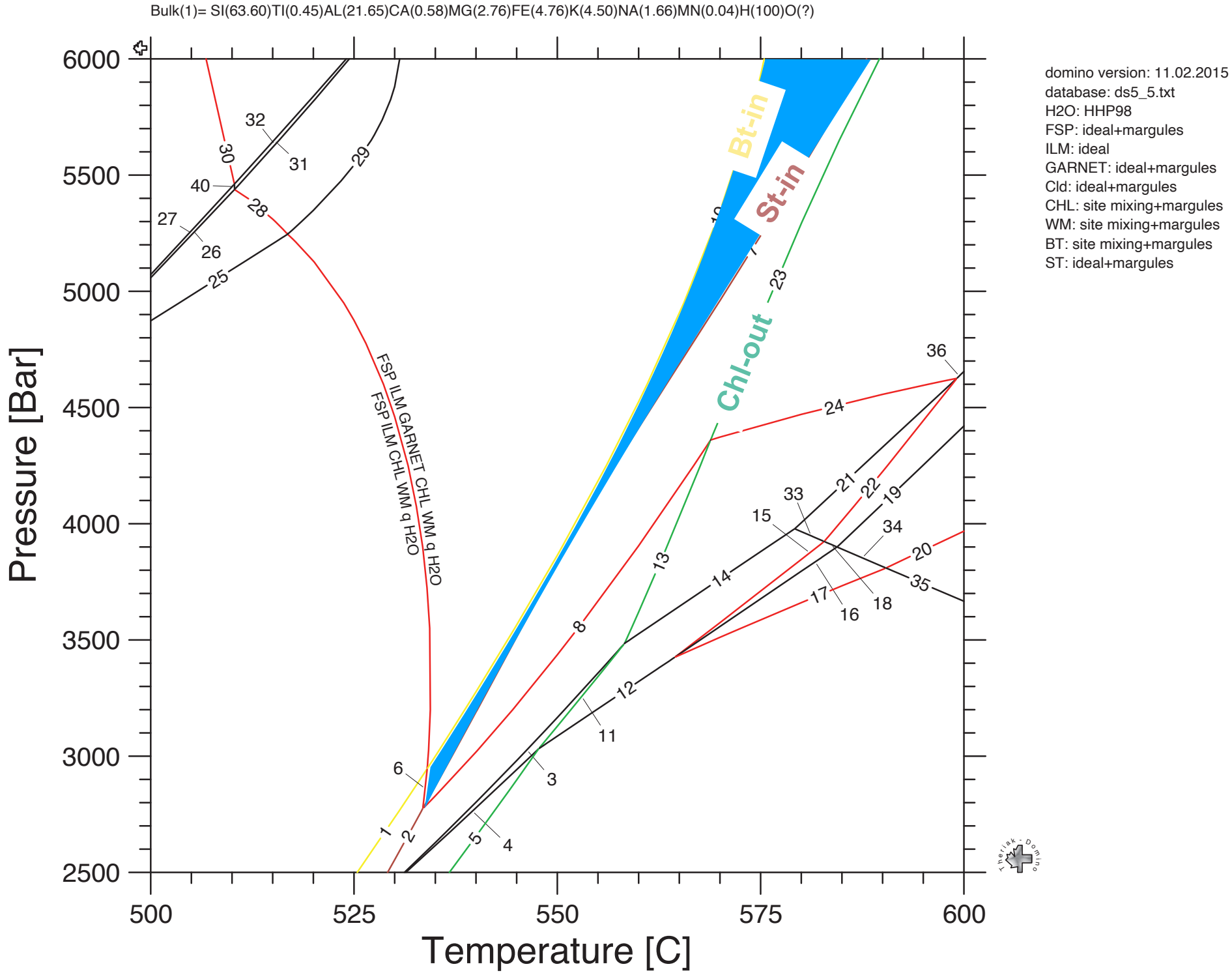



Bulk(1)= SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)
domino version: 11.02.2015
database: ds5_5.txt
H2O: HHP98
FSP: ideal+margules
ILM: ideal
GARNET: ideal+margules
Cld: ideal+margules
CHL: site mixing+margules
WM: site mixing+margules
BT: site mixing+margules
ST: ideal+margules
FSP ILM GARNET CHL WM q H2O
FSP ILM CHL WM q H2O
Pressure [Bar]
Temperature [C]
6000
5500
5000
4500
4000
3500
3000
2500
500
525
550
575
600
23.11.2020 - 16:32:51 CPU time: 0h 10m 53.42s

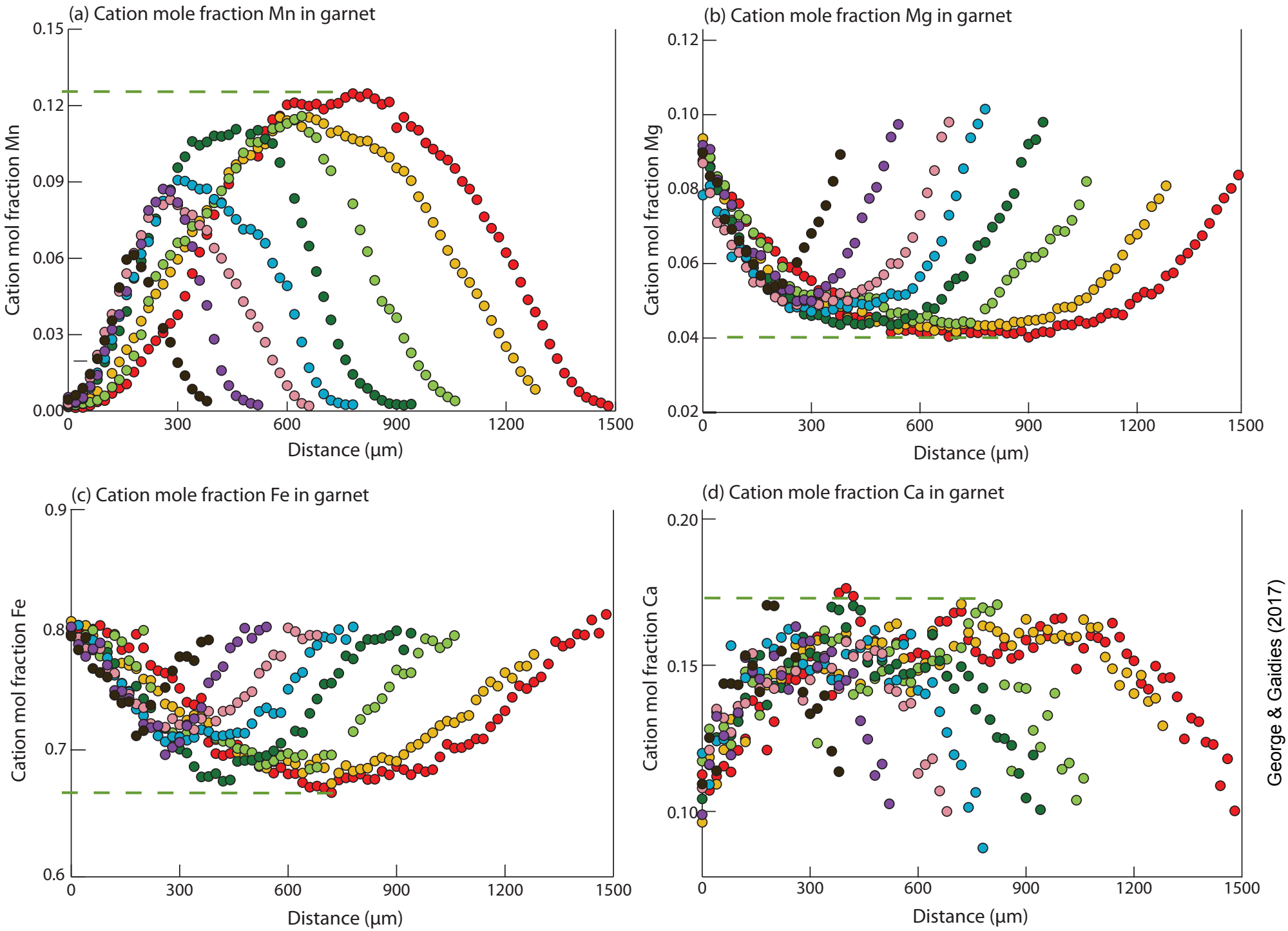
File "**table**" in working directory

```
 1):  FSP ILM CHL WM q H2O = FSP ILM CHL WM BT q H2O
 2):  FSP ILM CHL WM BT q H2O = FSP ILM CHL WM BT ST q H2O
 3):  FSP ILM CHL WM BT ST q H2O = FSP ILM CHL WM BT ST and q H2O
 4):  FSP ILM CHL WM BT ST and q H2O = FSP ILM CHL WM BT and q H2O
 5):  FSP ILM CHL WM BT and q H2O = FSP ILM WM BT and q H2O
 6):  FSP ILM CHL WM BT q H2O = FSP ILM GARNET CHL WM BT q H2O
 7):  FSP ILM GARNET CHL WM BT q H2O = FSP ILM GARNET CHL WM BT ST q H2O
 8):  FSP ILM GARNET CHL WM BT ST q H2O = FSP ILM CHL WM BT ST q H2O
 9):  FSP ILM CHL WM q H2O = FSP ILM GARNET CHL WM q H2O
10):  FSP ILM GARNET CHL WM q H2O = FSP ILM GARNET CHL WM BT q H2O
11):  FSP ILM CHL WM BT ST and q H2O = FSP ILM WM BT ST and q H2O
12):  FSP ILM WM BT ST and q H2O = FSP ILM WM BT and q H2O
13):  FSP ILM CHL WM BT ST q H2O = FSP ILM WM BT ST q H2O
14):  FSP ILM WM BT ST q H2O = FSP ILM WM BT ST and q H2O
15):  FSP ILM WM BT ST and q H2O = FSP ILM GARNET WM BT ST and q H2O
16):  FSP ILM GARNET WM BT ST and q H2O = FSP ILM GARNET WM BT and q H2O
17):  FSP ILM GARNET WM BT and q H2O = FSP ILM WM BT and q H2O
18):  FSP ILM GARNET WM BT ST and q H2O = FSP ILM GARNET WM BT ST sill q H2O
19):  FSP ILM GARNET WM BT ST sill q H2O = FSP ILM GARNET WM BT sill q H2O
20):  FSP ILM GARNET WM BT sill q H2O = FSP ILM WM BT sill q H2O
21):  FSP ILM WM BT ST q H2O = FSP ILM WM BT ST sill q H2O
22):  FSP ILM WM BT ST sill q H2O = FSP ILM GARNET WM BT ST sill q H2O
23):  FSP ILM GARNET CHL WM BT ST q H2O = FSP ILM GARNET WM BT ST q H2O
24):  FSP ILM GARNET WM BT ST q H2O = FSP ILM WM BT ST q H2O
25):  FSP ILM CHL WM mrg q H2O = FSP ILM CHL WM q H2O
26):  FSP ILM CHL WM czo q H2O = FSP ILM CHL WM czo mrg q H2O
27):  FSP ILM CHL WM czo mrg q H2O = FSP ILM CHL WM mrg q H2O
28):  FSP ILM GARNET CHL WM mrg q H2O = FSP ILM CHL WM mrg q H2O
29):  FSP ILM GARNET CHL WM mrg q H2O = FSP ILM GARNET CHL WM q H2O
30):  FSP ILM CHL WM czo q H2O = FSP ILM GARNET CHL WM czo q H2O
31):  FSP ILM GARNET CHL WM czo q H2O = FSP ILM GARNET CHL WM czo mrg q H2O
32):  FSP ILM GARNET CHL WM czo mrg q H2O = FSP ILM GARNET CHL WM mrg q H2O
33):  FSP ILM WM BT ST sill q H2O = FSP ILM WM BT ST and q H2O
34):  FSP ILM GARNET WM BT sill q H2O = FSP ILM GARNET WM BT and q H2O
35):  FSP ILM WM BT sill q H2O = FSP ILM WM BT and q H2O
36):  FSP ILM GARNET WM BT ST sill q H2O = FSP ILM GARNET WM BT ST q H2O
37):  FSP ILM CHL WM BT ST q H2O = FSP ILM WM BT ST and q H2O
38):  FSP ILM GARNET CHL WM BT ST q H2O = FSP ILM WM BT ST q H2O
39):  FSP ILM GARNET CHL WM mrg q mt H2O = FSP ILM GARNET CHL WM mrg q H2O
40):  FSP ILM CHL WM czo mrg q H2O = FSP ILM GARNET CHL WM czo mrg q H2O
41):  FSP ILM WM BT ST sill q H2O = FSP ILM GARNET WM BT ST and q H2O
```


Bulk(1)= SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)
Pressure [Bar]
Temperature [C]
6000
5500
5000
4500
4000
3500
3000
2500
500
525
550
575
600
Bt-in
St-in
Chl-out
FSP ILM GARNET CHL WM q H2O
FSP ILM CHL WM q H2O
domino version: 11.02.2015
database: ds5_5.txt
H2O: HHP98
FSP: ideal+margules
ILM: ideal
GARNET: ideal+margules
Cld: ideal+margules
CHL: site mixing+margules
WM: site mixing+margules
BT: site mixing+margules
ST: ideal+margules


Bulk(1)= SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)
Pressure [Bar]
Temperature [C]
6000
5500
5000
4500
4000
3500
3000
2500
500
525
550
575
600
Bt-in
St-in
Chl-out
FSP ILM GARNET CHL WM q H2O
FSP ILM CHL WM q H2O
domino version: 11.02.2015
database: ds5_5.txt
H2O: HHP98
FSP: ideal+margules
ILM: ideal
GARNET: ideal+margules
Cld: ideal+margules
CHL: site mixing+margules
WM: site mixing+margules
BT: site mixing+margules
ST: ideal+margules

Theriak-Domino modelling of realistic systems



Scripts in Domino

Given is the bulk chemical composition of a Barrovian garnet-zone mica schist from the Sikkim Himalaya (NE India).

Use the **script** option of Domino to calculate isopleths and isolines for grossular, spessartine, pyrope and almandine, and vol% of garnet, respectively.

T-range: 500 - 600 °C

P-range: 2500 - 6000 Bar

	wt%	Mol.wt	Mol of element
SiO2	64.85	60.08	63.6
TiO2	0.61	79.88	0.45
Al2O3	18.73	101.96	21.65
Fe2O3	6.44	159.69	0
FeO	0	71.85	4.76
MnO	0.05	70.94	0.04
MgO	1.89	40.3	2.76
CaO	0.55	56.08	0.58
Na2O	0.87	61.98	1.66
K2O	3.6	94.2	4.5
LOI	2.36		
H2O			100.00

THERIN:

```
0   SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)
```

Scripts in Domino

Mac, Linux:

(1) Enter:
`domino`

Windows:

(1) Enter:
`domino`

Scripts in Domino

```
-------------------
database definition
-------------------
Enter [ "?" | CR | "files" | "script" | database filename ] <ds5_5.txt>?
script
```

Scripts in Domino

```
-------------------
database definition
-------------------
Enter [ "?" | CR | "files" | "script" | database filename ] < >?
script
```

```
DOMINO SCRIPTING
----------------
JOB filename: domjob

Enter [ "?" | CR | new JOB filename ] <domjob>?
```

accept this

Scripts in Domino

```
SCRIPT filename: script_001.txt

Enter [ "?" | CR | "end" | new SCRIPT filename ] <script_001.txt>?

Enter [ CR | database filename ] <ds5_5.txt>:
```

accept these

```
X-axis
Y-axis
calculation type
labelling of reactions
```

```
TC    500     600
P    2500    6000
GARNET  spss  1  0   1   0.02
1
```

Scripts in Domino

```
SCRIPT filename: script_001.txt

Enter [ "?" | CR | "end" | new SCRIPT filename ] <script_001.txt>?

Enter [ CR | database filename ] <ds5_5.txt>:
```

accept these

```
X-axis
Y-axis
calculation type
labelling of reactions
```

```
TC    500     600
P    2500    6000
GARNET  spss  1  0    1    0.02
1
```

name of solution

abbrev. of end-member

min max

spacing (mol-fraction)

Scripts in Domino

```
SCRIPT filename: script_001.txt

Enter [ "?" | CR | "end" | new SCRIPT filename ] <script_001.txt>?

Enter [ CR | database filename ] <ds5_5.txt>:
```

accept these

for phases with solvus

```
X-axis                    TC    500     600
Y-axis                    P    2500    6000
calculation type          GARNET  spss  1   0    1    0.02
labelling of reactions    1
```

name of solution

abbrev. of end-member

min max spacing (mol-fraction)

Scripts in Domino

```
SCRIPT filename: script_002.txt

Enter [ "?" | CR | "end" | new SCRIPT filename ] <script_002.txt>?

Enter [ CR | database filename ] <ds5_5.txt>:
```

accept these

```
X-axis
Y-axis
calculation type
labelling of reactions
```

```
TC    500     600
P    2500    6000
GARNET  alm  1  0   1   0.02
1
```

Scripts in Domino

```
SCRIPT filename: script_003.txt

Enter [ "?" | CR | "end" | new SCRIPT filename ] <script_003.txt>?

Enter [ CR | database filename ] <ds5_5.txt>:
```

accept these

```
X-axis
Y-axis
calculation type
labelling of reactions
```

```
TC    500     600
P    2500    6000
GARNET  py   1   0    1    0.02
1
```

Scripts in Domino

```
SCRIPT filename: script_004.txt

Enter [ "?" | CR | "end" | new SCRIPT filename ] <script_004.txt>?

Enter [ CR | database filename ] <ds5_5.txt>:
```

accept these

```
X-axis
Y-axis
calculation type
labelling of reactions
```

```
TC    500     600
P    2500    6000
GARNET  gr   1   0    0.5    0.02
1
```

Scripts in Domino

```
SCRIPT filename: script_005.txt

Enter [ "?" | CR | "end" | new SCRIPT filename ] <script_005.txt>?

Enter [ CR | database filename ] <ds5_5.txt>:
```

accept these

```
X-axis
Y-axis
calculation type
labelling of reactions
```

```
TC    500     600
P    2500    6000
GARNET  vol%  1     0    10    1
1
```

Scripts in Domino

```
SCRIPT filename: script_006.txt

Enter [ "?" | CR | "end" | new SCRIPT filename ] <script_006.txt>?
end
```

Scripts in Domino

Mac, Linux:

(1) Enter:
`chmod a+x domjob`

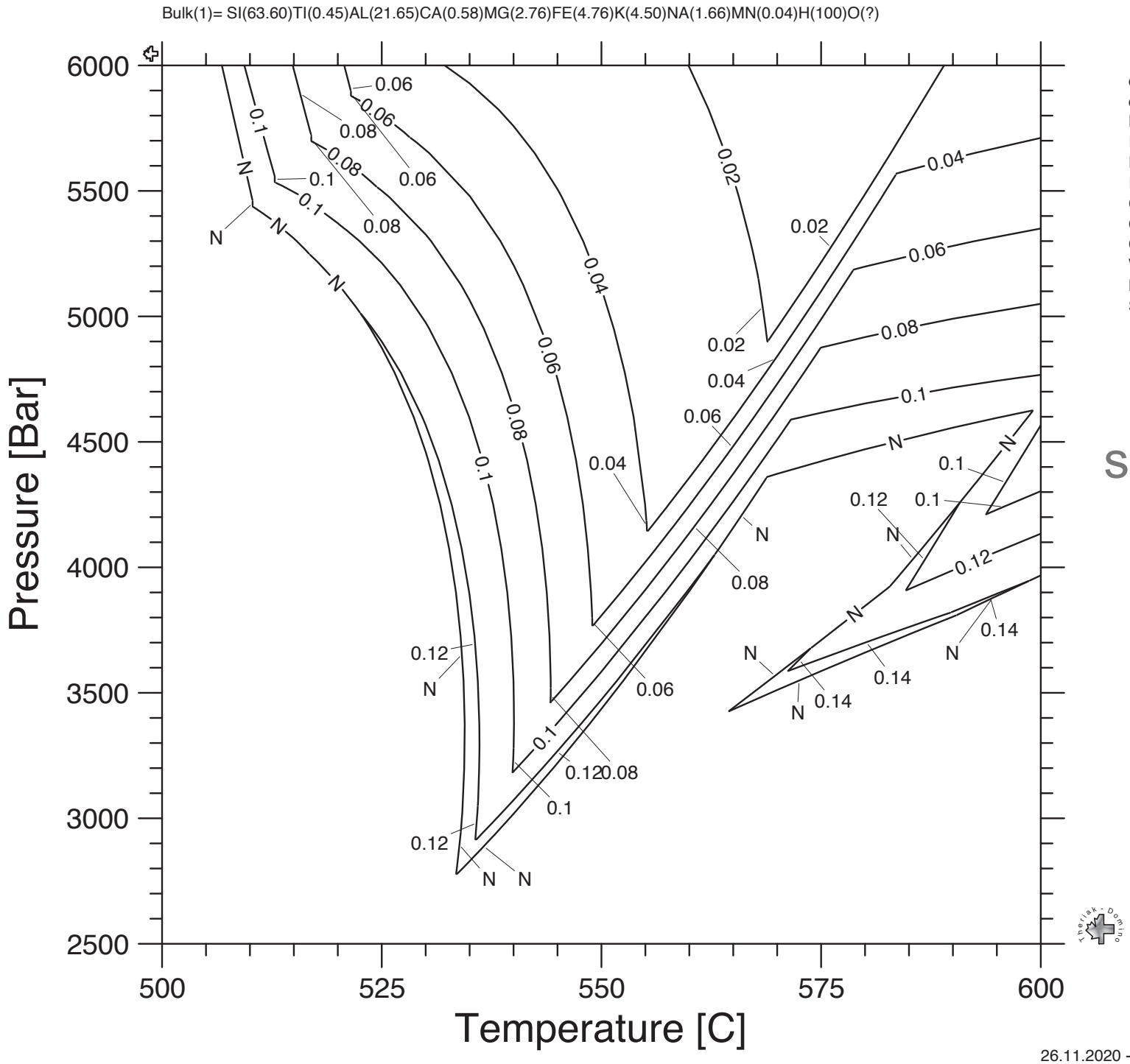
(2) Enter:
`domjob`

Windows:

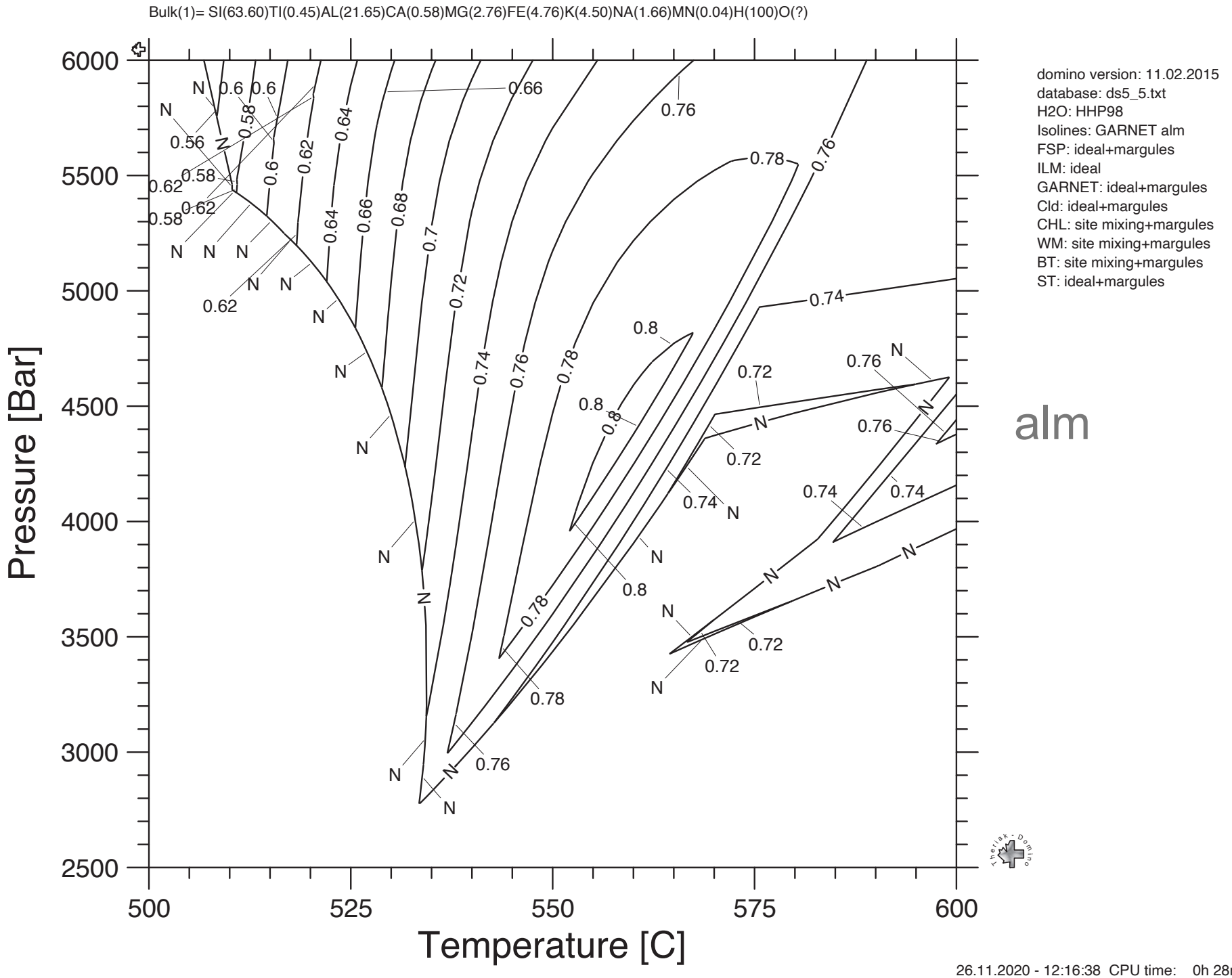
(1) In File Explorer:
Rename domjob to domjob.bat

(2) Enter (in console window):
`domjob.bat`

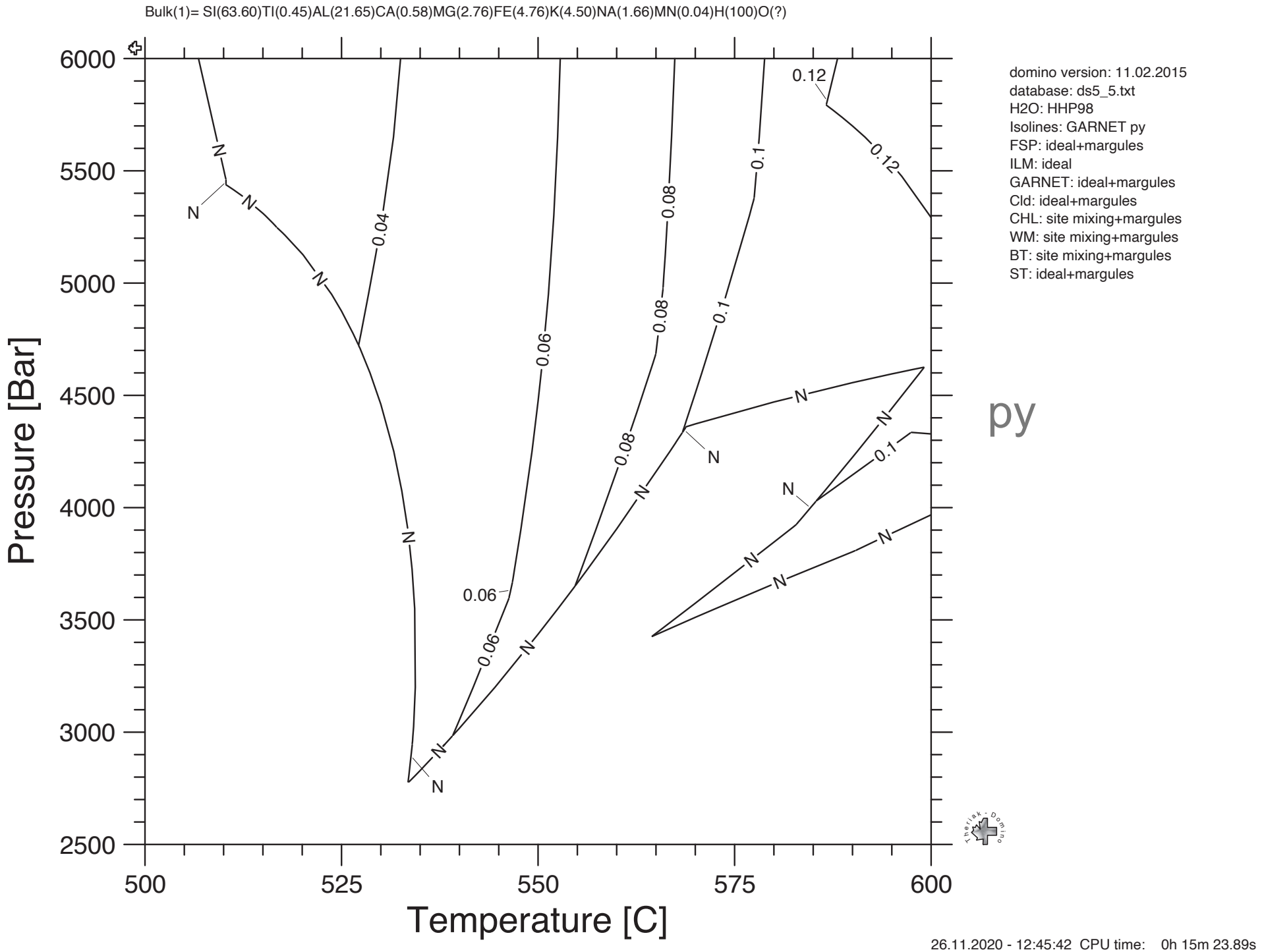
Scripts in Domino



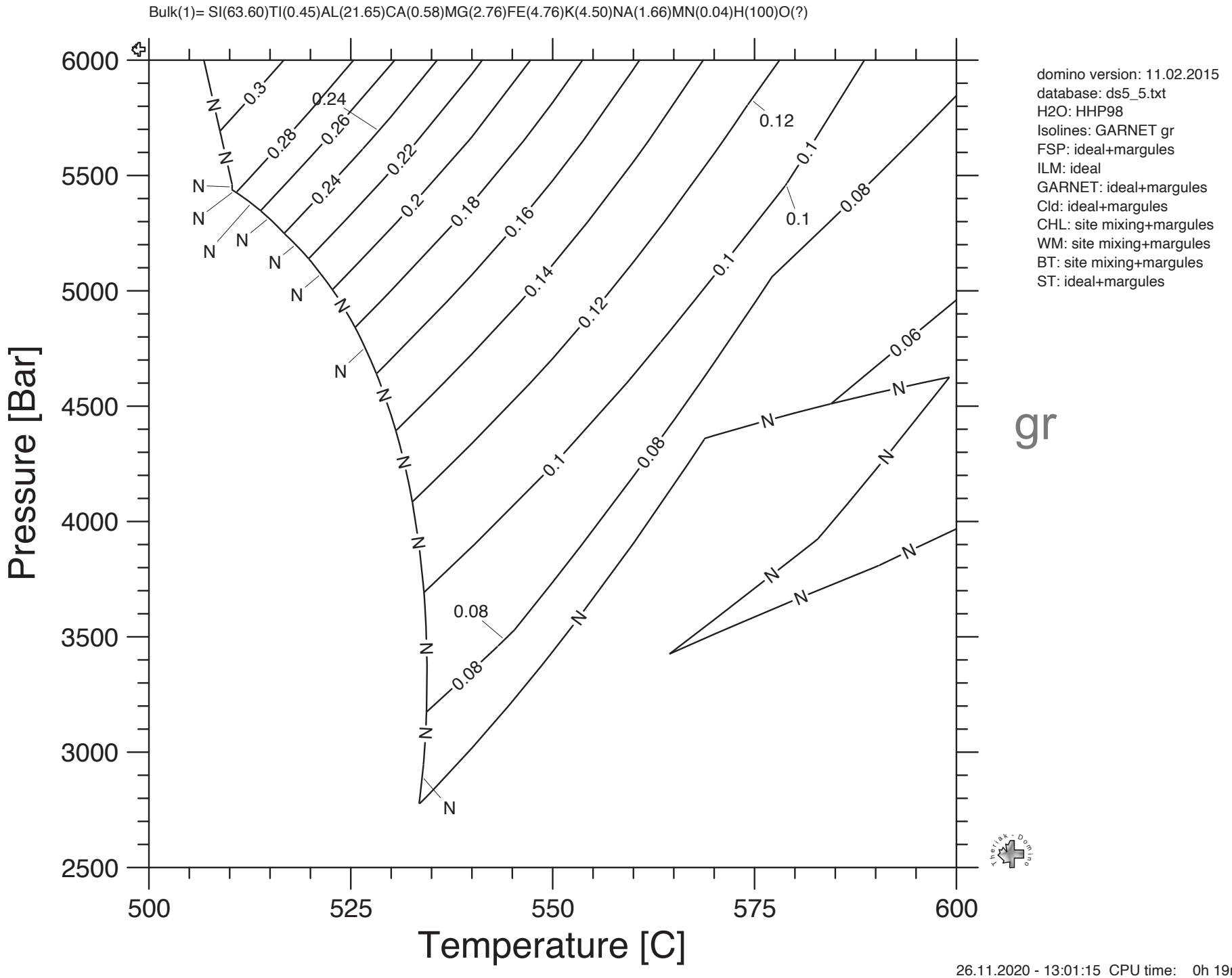
Scripts in Domino



Scripts in Domino

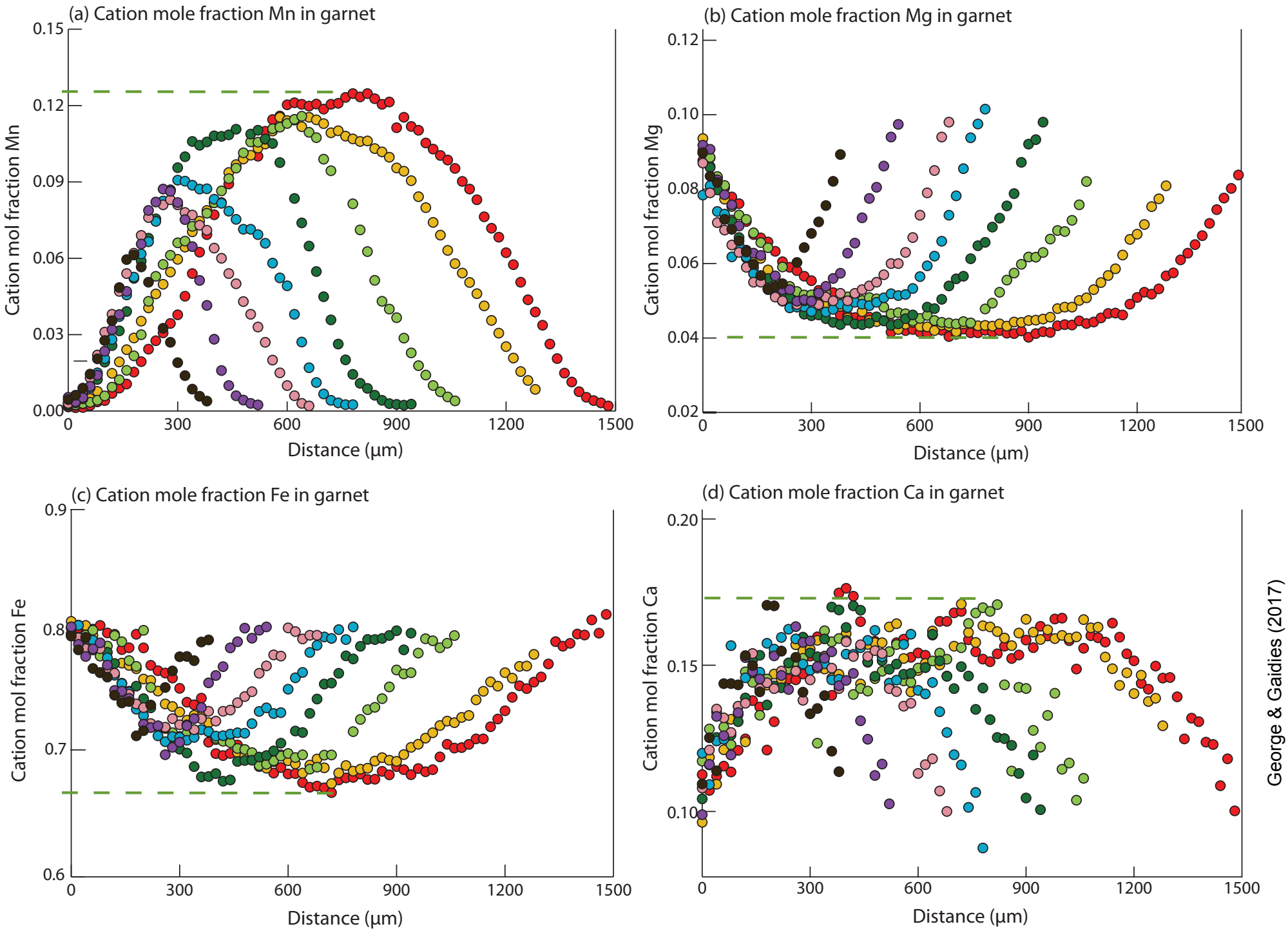


Scripts in Domino

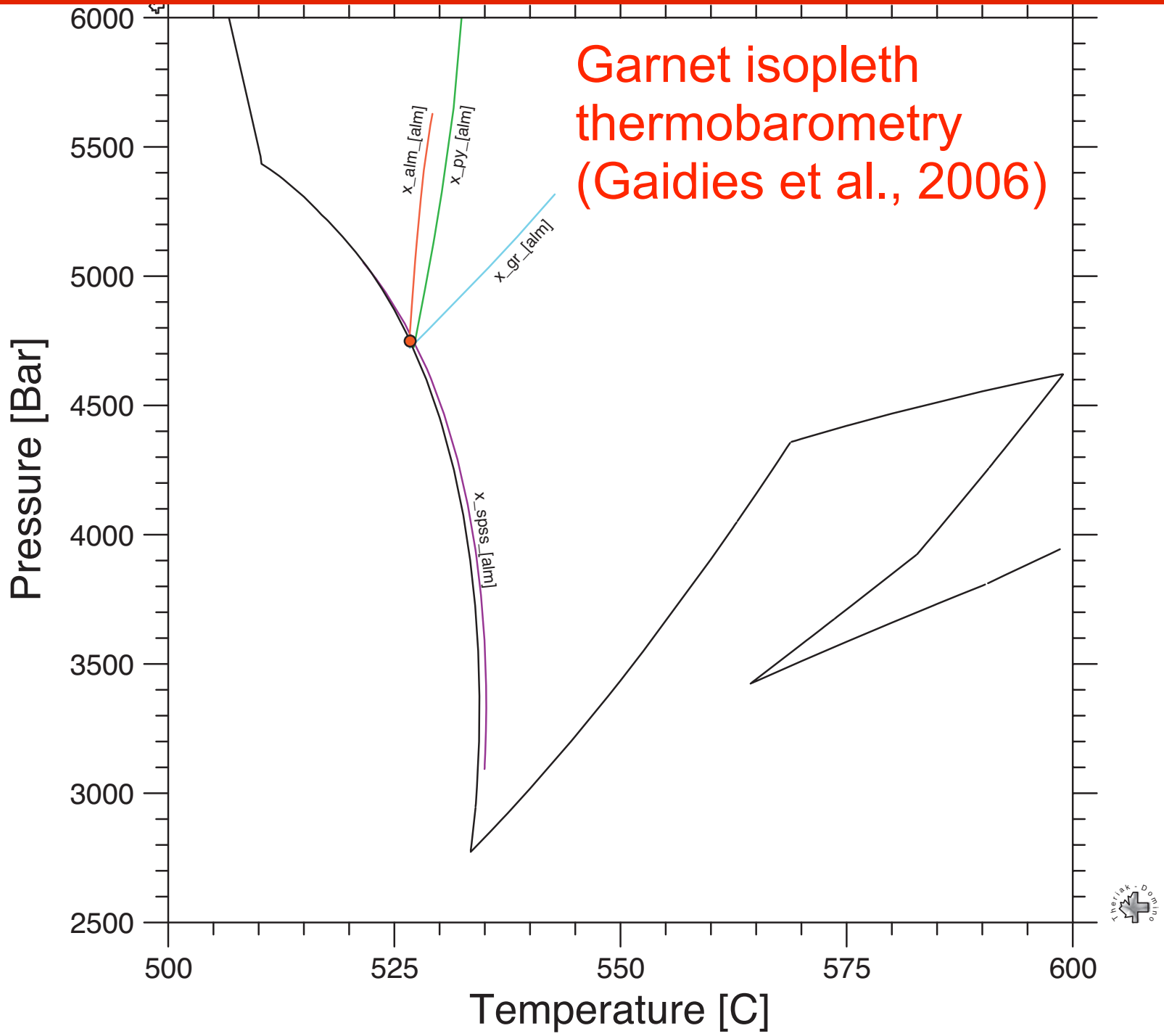


26.11.2020 - 13:01:15 CPU time: 0h 19m 19.53s

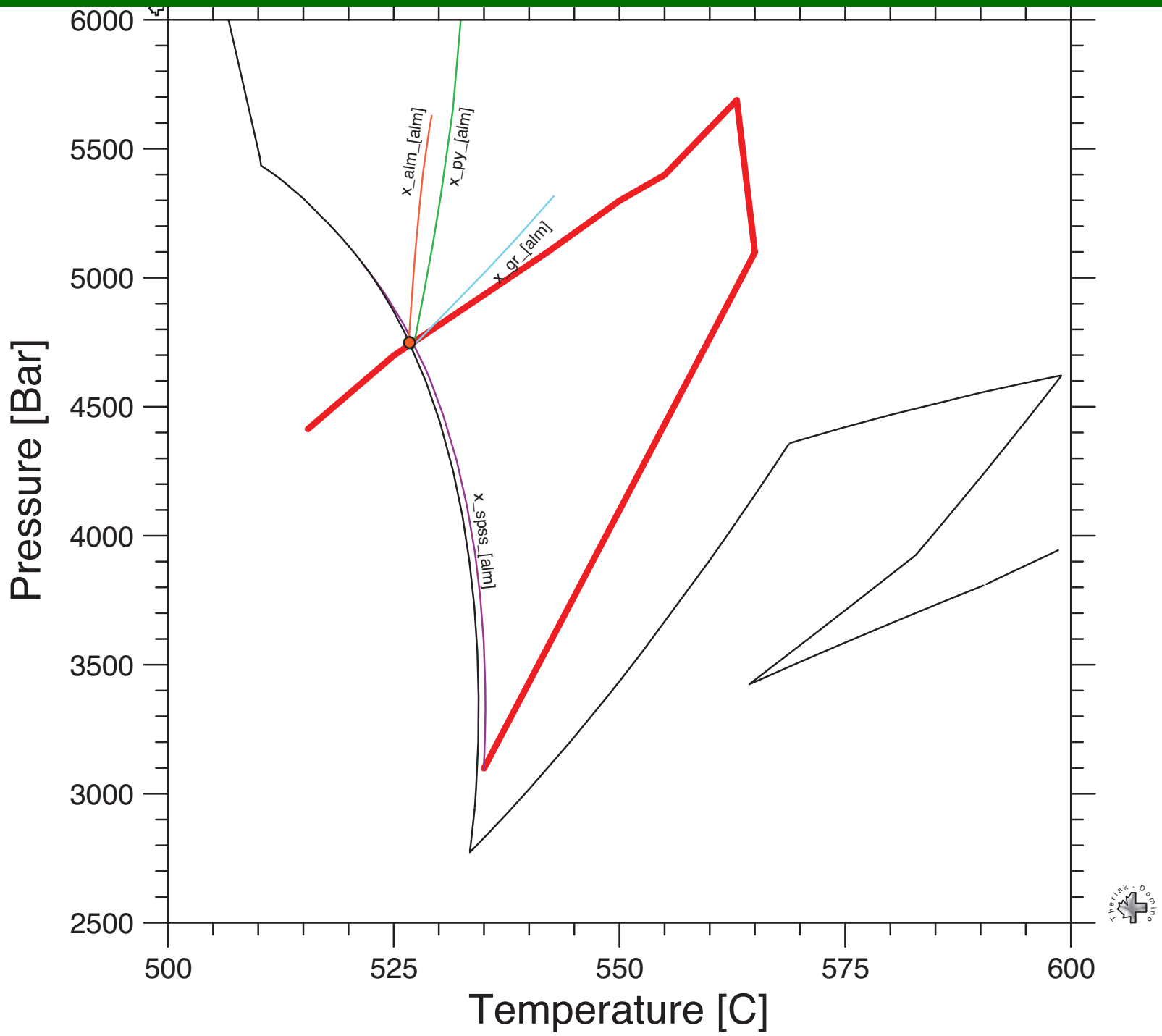
Theriak-Domino modelling of realistic systems



Theriak-Domino modelling of realistic systems



Theriak: Fractionation along a P-T path



Theriak: Fractionation along a P-T path

theriak command for fractionation

name of phase to be fractionated

degree of fractionation [%]

number of segments between TP points

path.txt:

```
REMOVE      GARNET     100
TP      525                4600              20
TP      542                5000              34
TP      550                5200              16
TP      555                5300              10
TP      563                5590              16
TP      565                5000              4
TP      535                3000              60
```

First T-P point of path

THERIN.txt:

```
     515     4300
0    SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)
```

Theriak: Fractionation along a P-T path

Mac, Linux:

replace with your Home Directory

(1) Open Terminal

(2) Enter:
`cd /Users/fredsmacbookpro/TheriakDominoMAC/GeochemSoc2020/Working`
or enter (if you followed the installation instructions):
`dom`

(3) Enter:
`theriak`

Windows:

(1) Use File Explorer and navigate to
C:\TheriakDominoWIN\GeochemSoc2020\Working

(2) Double-click start.bat (opens Command Prompt)

(3) Enter:
`theriak`

Theriak: Fractionation along a P-T path

```
 -------------------
 database definition
 -------------------
 Enter [ "?" | CR | "files" | database filename ] <ds5_5.txt>?


 database for this run: ds5_5.txt


 Input from file THERIN
 ----------------------
 T =  515.00 C     P =  4300.00 Bar
 0   SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)
* A nice rock from Sikkim

 ---------------------------
 define type of calculations
 ---------------------------
 Enter [ "?" | CR | "no" | "bin" | "loop" | filename ] < >?
path.txt
```

accept this
(hit return)

Theriak: Fractionation along a P-T path

```
 -------------------
 database definition
 -------------------
 Enter [ "?" | CR | "files" | database filename ] <ds5_5.txt>?


 database for this run: ds5_5.txt


 Input from file THERIN
 ----------------------
 T =  515.00 C     P =  4300.00 Bar
 0   SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)M
* A nice rock from Sikkim

 ---------------------------
 define type of calculations
 ---------------------------
 Enter [ "?" | CR | "no" | "bin" | "loop" | filename ] < >?
path.txt
```

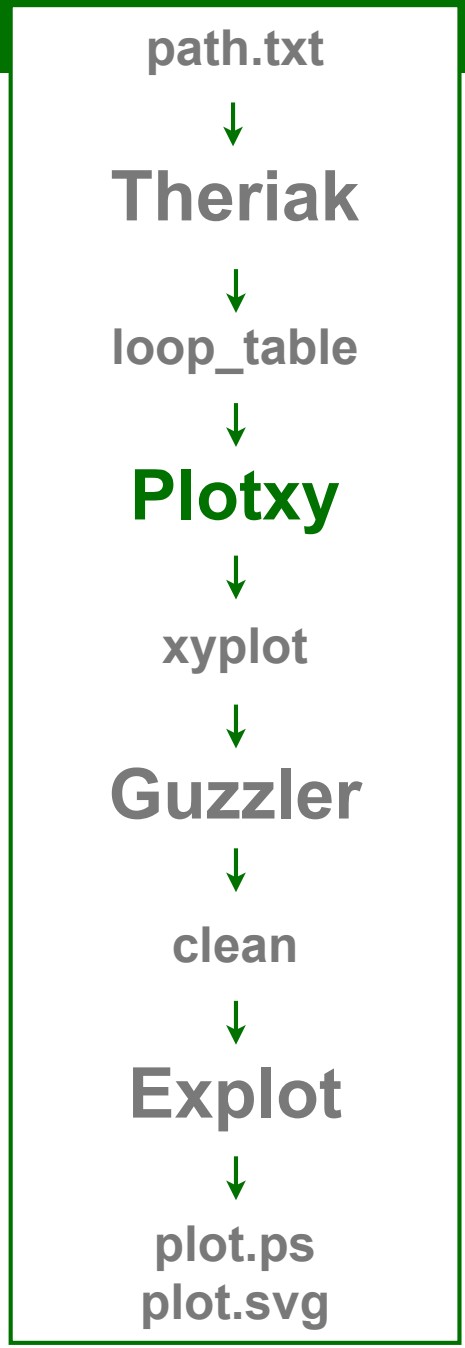
accept t
(hit retur

path.txt
↓
Theriak
↓
loop_table
↓
Plotxy
↓
xyplot
↓
Guzzler
↓
clean
↓
Explot
↓
plot.ps
plot.svg

Creates file "**loop_table**" in working directory

Theriak: Fractionation along a P-T path

Plot the chemical composition of garnet [mol-fractions of end-members] for each step along the P-T path.



Theriak: Fractionation along a P-T path

Plot the chemical composition of garnet [mol-fractions of end-members] for each step along the P-T path.

Mac, Linux:

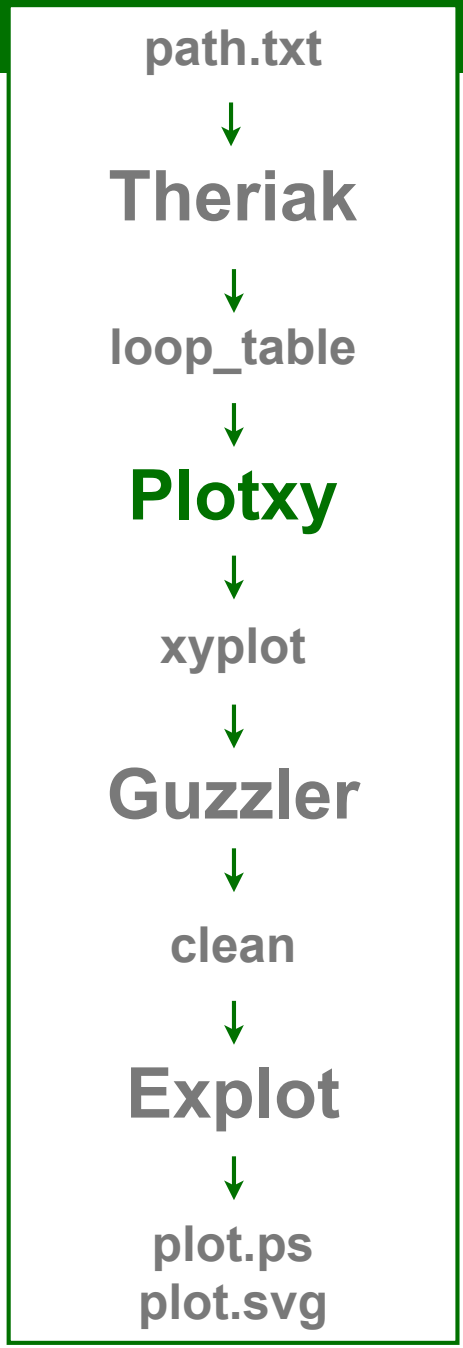
(1) Enter:

```
plotxy
```

Windows:

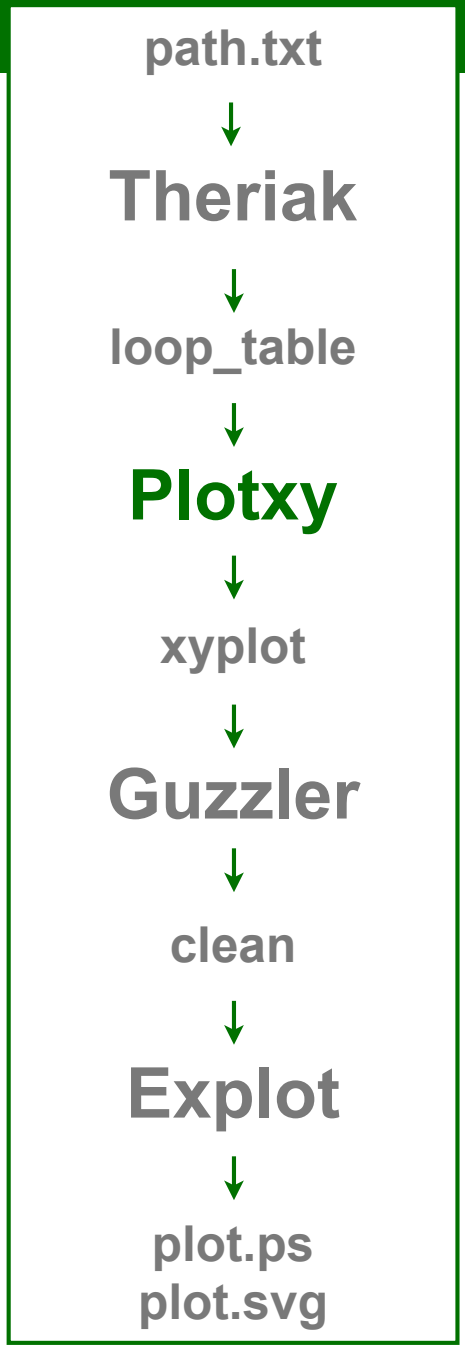
(1) Enter:

```
plotxy
```



Theriak: Fractionation along a P-T path

```
 ----------
 input file
 ----------
 Enter [ "?" | CR | "files" | filename ] < >?
loop_table
```



Theriak: Fractionation along a P-T path

```
Variables available:

[b]: b-rich solution  a : activity    blk: bulk     Mg# : Mg/(Mg+Fe)    mvol: molar volume
n  : mass [mol]       pc: percent     wt : weight   x   : mole fraction

  1: NR(step)           2: Pressure           3: Temperature        4: Al_pfu_[abh]       5: Al_pfu_[anc1]
  6: Al_pfu_[ann]       7: Al_pfu_[daph]      8: Al_pfu_[mu]        9: G_system          10: G_tot
 11: H_tot             12: Mg#_[alm]         13: Mg#_[ann]         14: Mg#_[daph]       15: Mg#_[ilm]
 16: Mg#_[mu]          17: PV-_tot           18: S_tot             19: Si_pfu_[abh]     20: Si_pfu_[anc1]
 31: V_[daph]          32: V_[ilm]           33: V_[mu]            34: V_q              35: V_solids
 61: a_san_[anc1]      62: a_spss_[alm]      63: blk_AL            64: blk_CA           65: blk_E
 66: blk_FE            67: blk_H             68: blk_K             69: blk_MG           70: blk_MN
 81: mvol_[daph]       82: mvol_[ilm]        83: mvol_[mu]         84: mvol_q           85: n_H2O
 86: n_H2O_H2O         87: n_H2O_[ann]       88: n_H2O_[daph]      89: n_H2O_[mu]       90: n_H2O_solids
 91: n_[abh]           92: n_[alm]           93: n_[anc1]          94: n_[ann]          95: n_[daph]
131: rho_[ann]        132: rho_[daph]       133: rho_[ilm]        134: rho_[mu]        135: rho_q
136: rho_solids       137: wt_H2O_H2O       138: wt_H2O_[ann]     139: wt_H2O_[daph]   140: wt_H2O_[mu]
141: wt_H2O_solids    142: x_Al(M1)_[ann]   143: x_Al(M1)_[daph]  144: x_Al(M2A)_[mu]  145:[daph]
181: x_anc1_[abh]     182: x_anc1_[anc1]    183: x_ann_[ann]      184: x_cel_[mu]      185: x_clin_[daph]
186: x_daph_[daph]    187: x_east_[ann]     188: x_fcel_[mu]      189: x_geik_[ilm]    190: x_gr_[alm]
191: x_ilm_[ilm]      192: x_mnbi_[ann]     193: x_mnchl_[daph]   194: x_mu_[mu]      195: x_obi_[ann]
196: x_pa_[mu]        197: x_phl_[ann]      198: x_pnt_[ilm]      199: x_py_[alm]      200: x_san_[abh]
201: x_san_[anc1]     202: x_spss_[alm]

definition example for axes: 3,5,6+7,8+9

Enter X-axis: [ "?" | CR | number(s) ] < >?
1

Enter Y-axis: [ "?" | CR | number(s) ] < >?
190,199,202
```

Theriak: Fractionation along a P-T path

accept this (hit return key)

```
Enter [ CR | X-min  X-max  width ]  <        1.00000000        160.00000000    15.000>?

 Enter [ CR | Y-min  Y-max  height ] <          0.00000000          0.16234446    15.000>?
0     0.2
```

Creates file "**xyplot**" in working directory

Theriak: Fractionation along a P-T path

accept this (hi

```
Enter [ CR | X-min   X-max   width ]  <          1.00000000          160.00000000

 Enter [ CR | Y-min   Y-max   height ] <            0.00000000            0.16234446
0      0.2
```

path.txt

↓

Theriak

↓

loop_table

↓

Plotxy

↓

xyplot

↓

Guzzler

↓

clean

↓

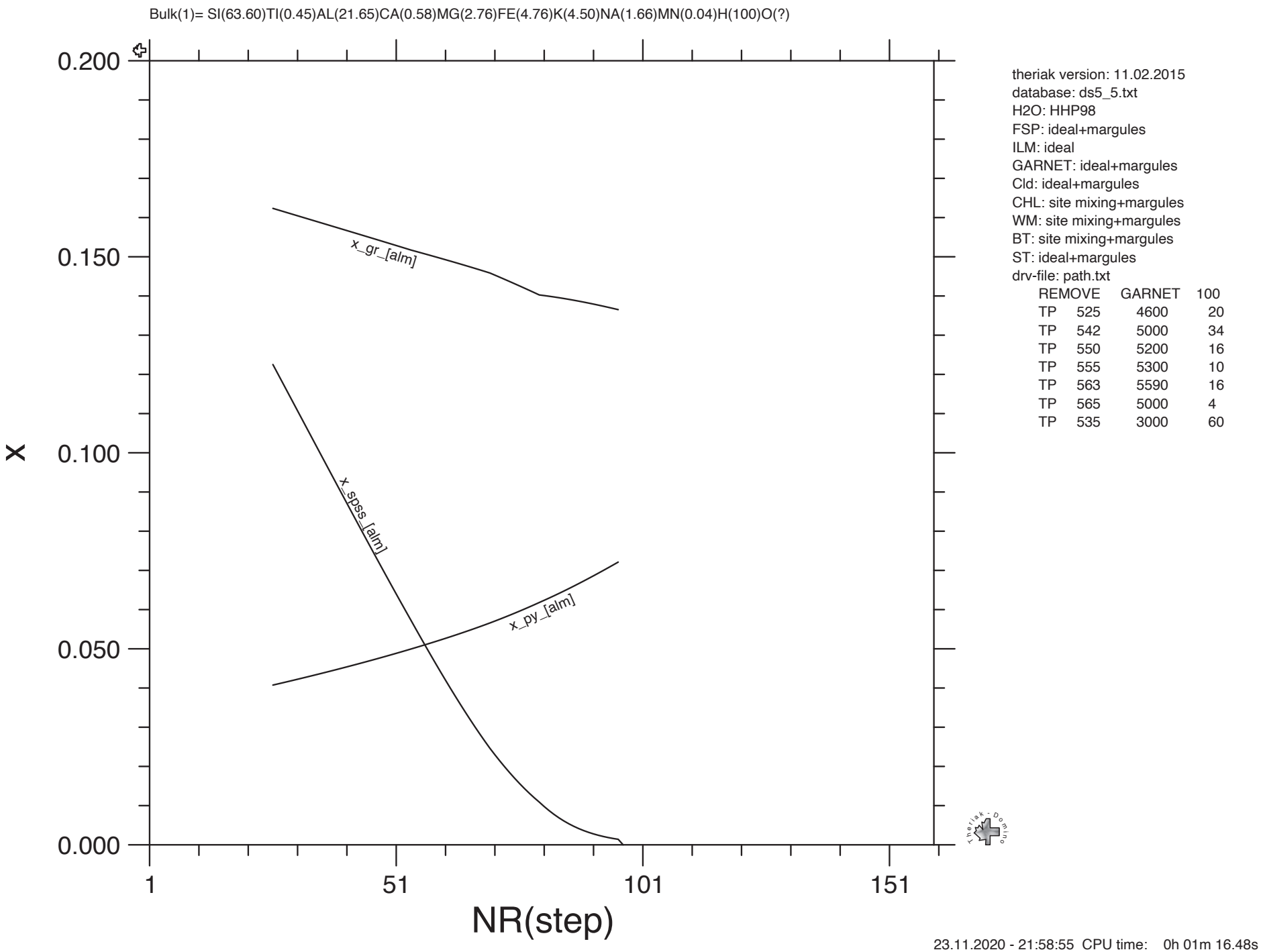
Explot

↓

plot.ps
plot.svg

Creates file "**xyplot**" in working directory

Theriak: Fractionation along a P-T path



Theriak: Fractionation along a P-T path

Plot the chemical composition of garnet [mol-fractions of end-members] for each step along the P-T path.

Mac, Linux:

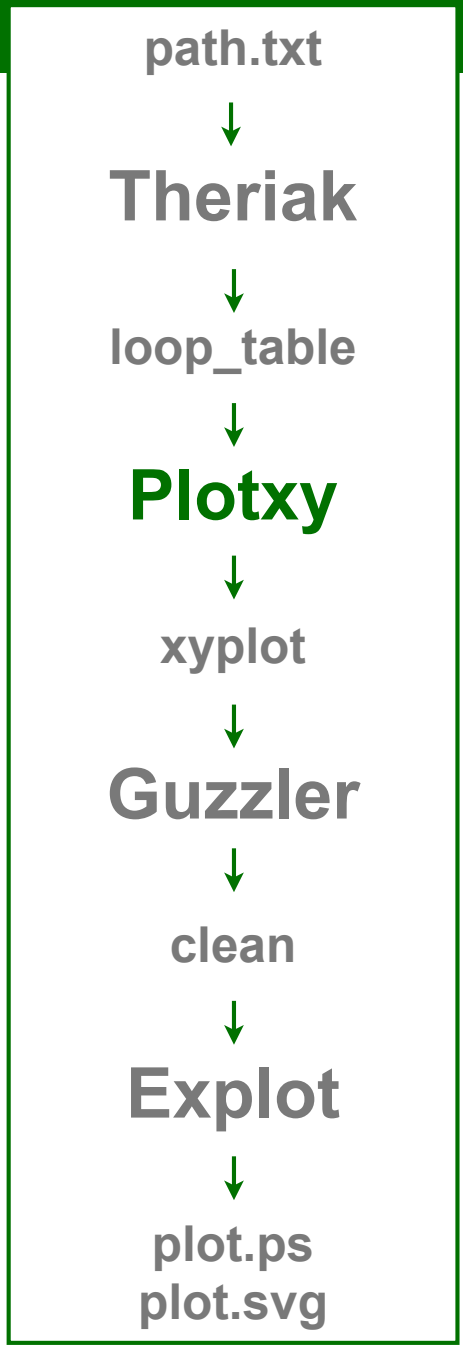
(1) Enter:

```
plotxy
```

Windows:

(1) Enter:

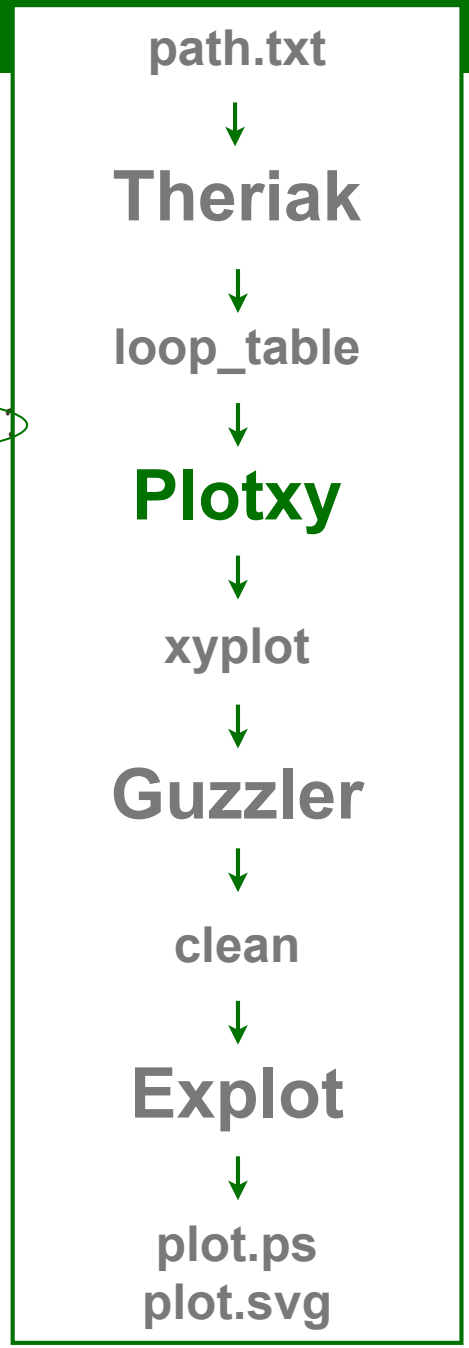
```
plotxy
```



Theriak: Fractionation along a P-T path

```
----------
input file
----------
Enter [ "?" | CR | "files" | filename ] <loop_table>
```

accept this (hit return key)



Theriak: Fractionation along a P-T path

```
Variables available:

[b]: b-rich solution  a : activity    blk: bulk     Mg# : Mg/(Mg+Fe)    mvol: molar volume
n  : mass [mol]       pc: percent     wt : weight   x   : mole fraction

  1: NR(step)           2: Pressure           3: Temperature        4: Al_pfu_[abh]       5: Al_pfu_[anc1]
  6: Al_pfu_[ann]       7: Al_pfu_[daph]      8: Al_pfu_[mu]        9: G_system          10: G_tot
 11: H_tot             12: Mg#_[alm]         13: Mg#_[ann]         14: Mg#_[daph]       15: Mg#_[ilm]
 16: Mg#_[mu]          17: PV-_tot           18: S_tot             19: Si_pfu_[abh]     20: Si_pfu_[anc1]
 31: V_[daph]          32: V_[ilm]           33: V_[mu]            34: V_q              35: V_solids
 61: a_san_[anc1]      62: a_spss_[alm]      63: blk_AL            64: blk_CA           65: blk_E
 66: blk_FE            67: blk_H             68: blk_K             69: blk_MG           70: blk_MN
176: x_Si(T1)_[mu]    177: x_abh_[abh]      178: x_abh_[anc1]     179: x_alm_[alm]     180: x_ames_[daph]
181: x_anc1_[abh]     182: x_anc1_[anc1]    183: x_ann_[ann]      184: x_cel_[mu]      185: x_clin_[daph]
186: x_daph_[daph]    187: x_east_[ann]     188: x_fcel_[mu]      189: x_geik_[ilm]    190: x_gr_[alm]
191: x_ilm_[ilm]      192: x_mnbi_[ann]     193: x_mnchl_[daph]   194: x_mu_[mu]      195: x_obi_[ann]
196: x_pa_[mu]        197: x_phl_[ann]      198: x_pnt_[ilm]      199: x_py_[alm]      200: x_san_[abh]
201: x_san_[anc1]     202: x_spss_[alm]

definition example for axes: 3,5,6+7,8+9

Enter X-axis: [ "?" | CR | number(s) ] <1>?


Enter Y-axis: [ "?" | CR | number(s) ] <190,199,202>?
179
```

accept this

Theriak: Fractionation along a P-T path

accept this (hit return key)

```
Enter [ CR | X-min  X-max  width ]  <        1.00000000        160.00000000    15.000>?

 Enter [ CR | Y-min  Y-max  height ] <          0.00000000          0.79068261    15.000>?
0.6     0.8
```

Creates file "**xyplot**" in working directory

Theriak: Fractionation along a P-T path

accept this (hi

```
Enter [ CR | X-min   X-max   width ]  <          1.00000000          160.00000000

 Enter [ CR | Y-min   Y-max   height ] <           0.00000000           0.79068261
0.6      0.8
```

path.txt

↓

Theriak

↓

loop_table

↓

Plotxy

↓

xyplot

↓

Guzzler

↓

clean

↓

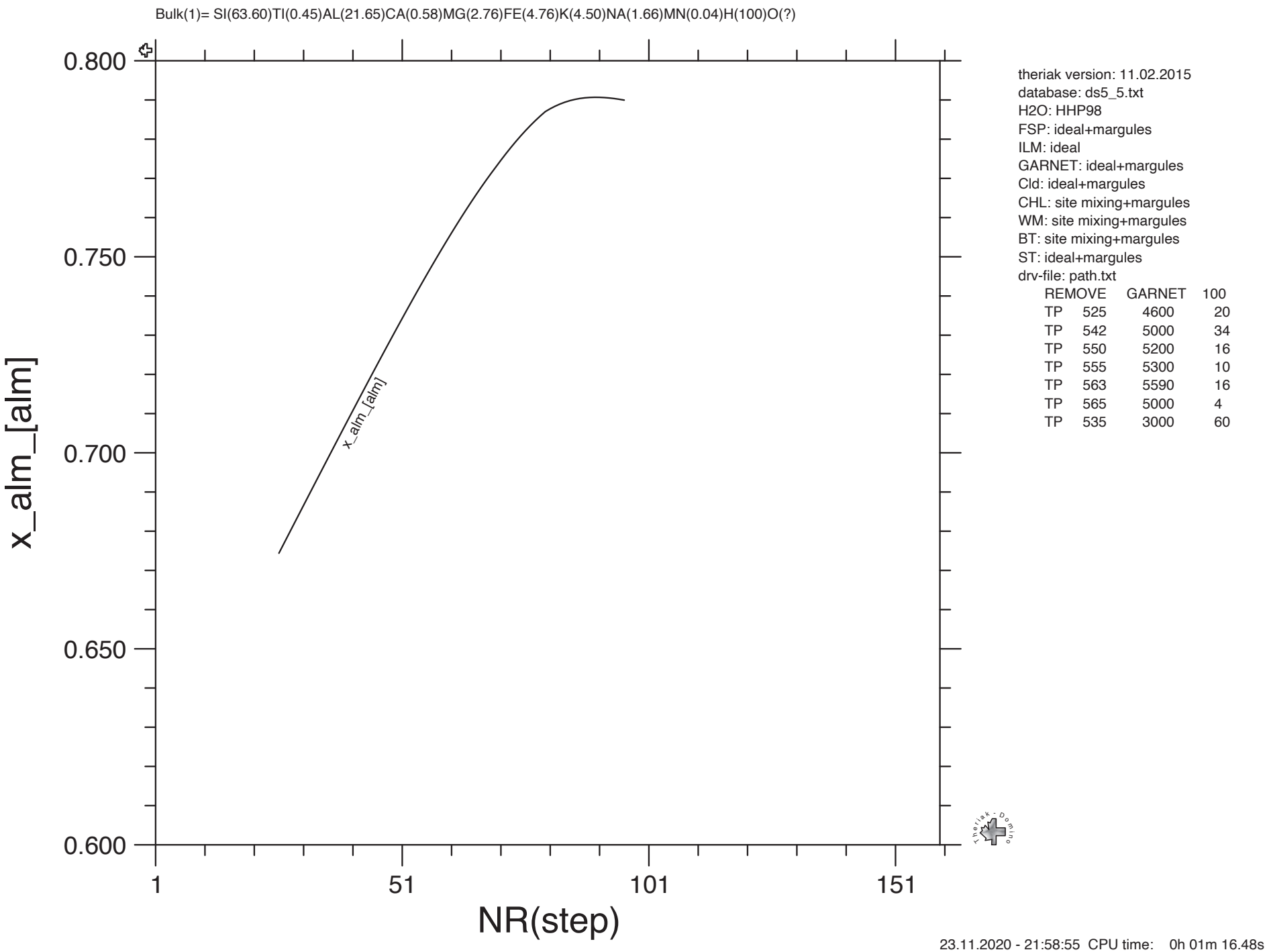
Explot

↓

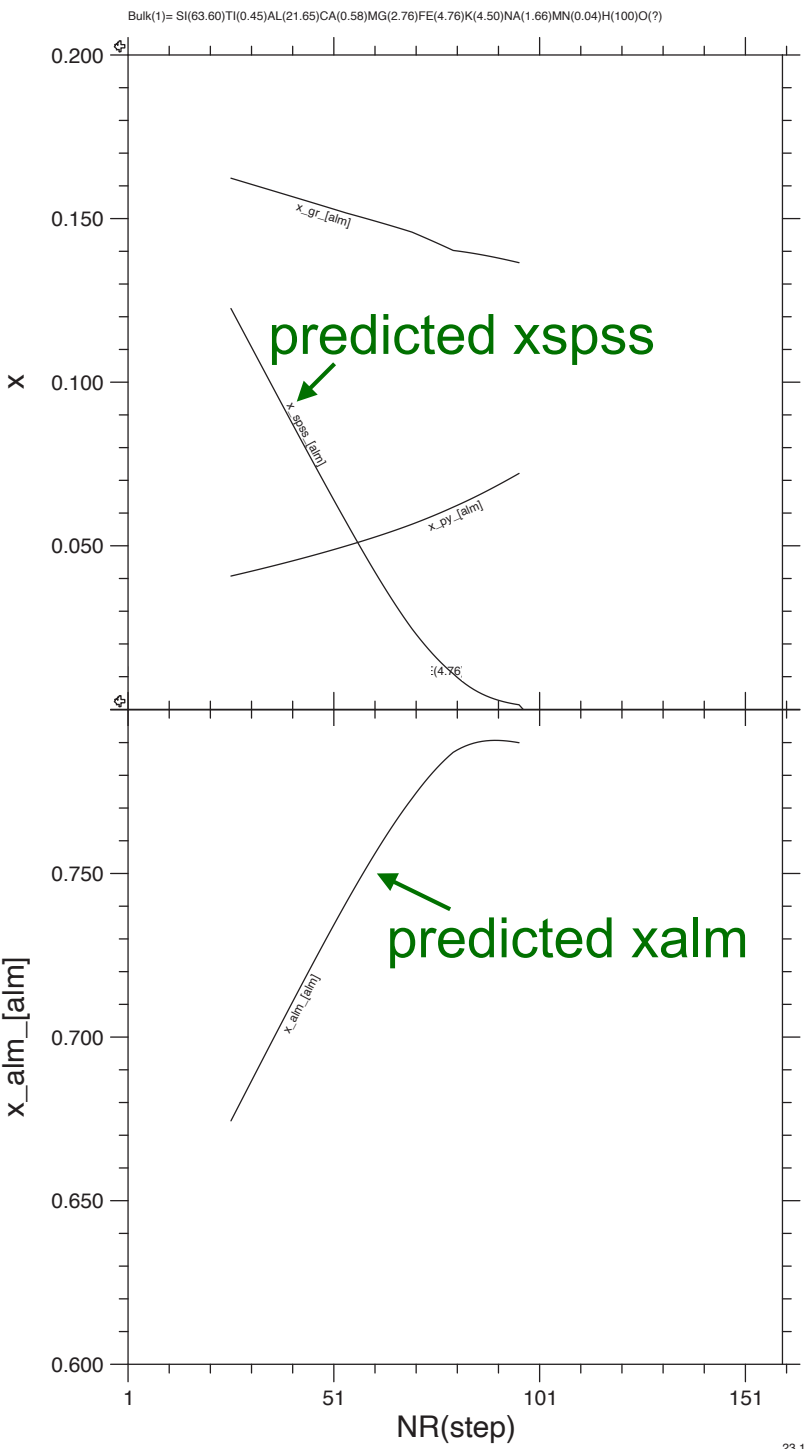
plot.ps
plot.svg

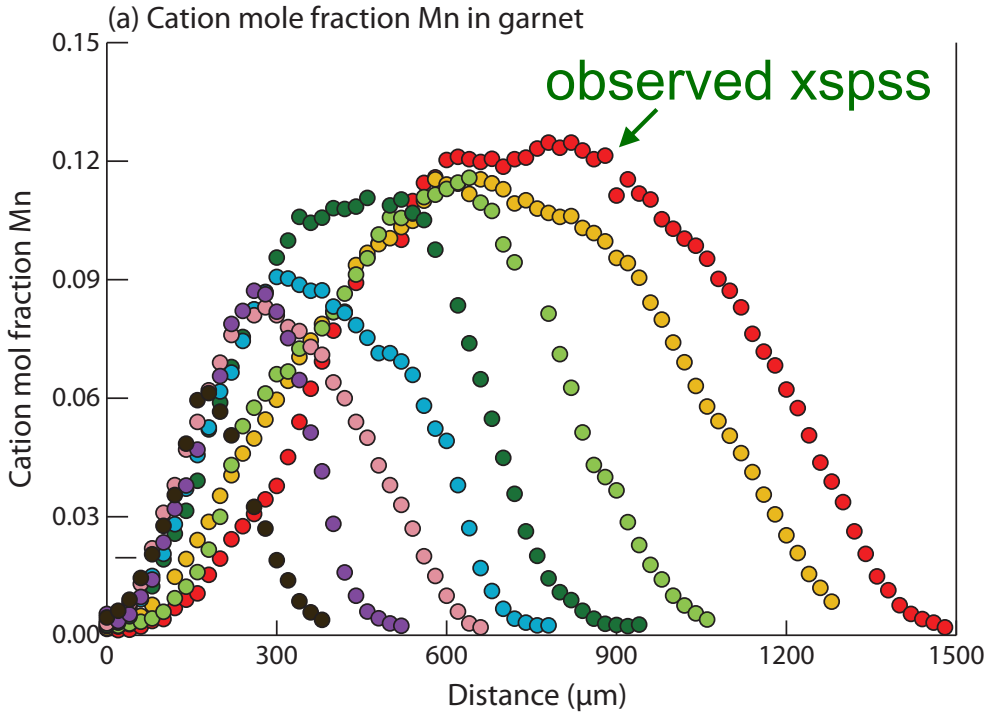
Creates file "**xyplot**" in working directory

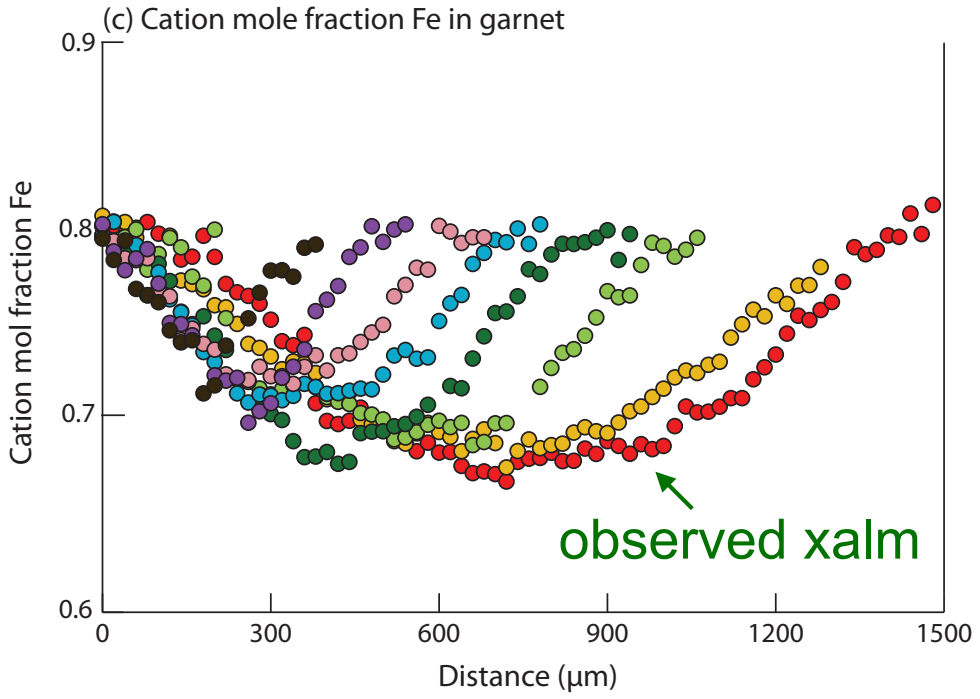
Theriak: Fractionation along a P-T path



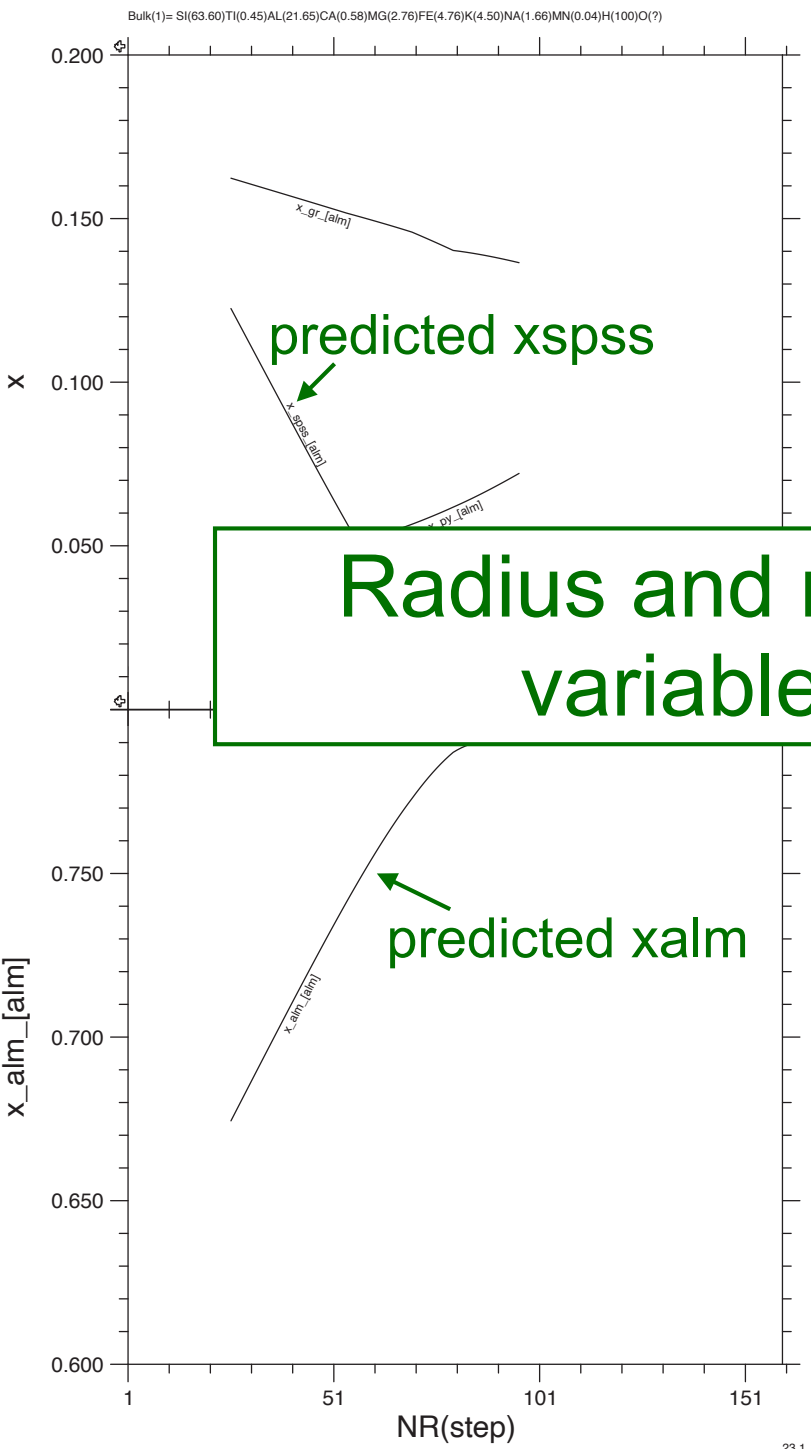
Theriak: Fractionation along a P-T path

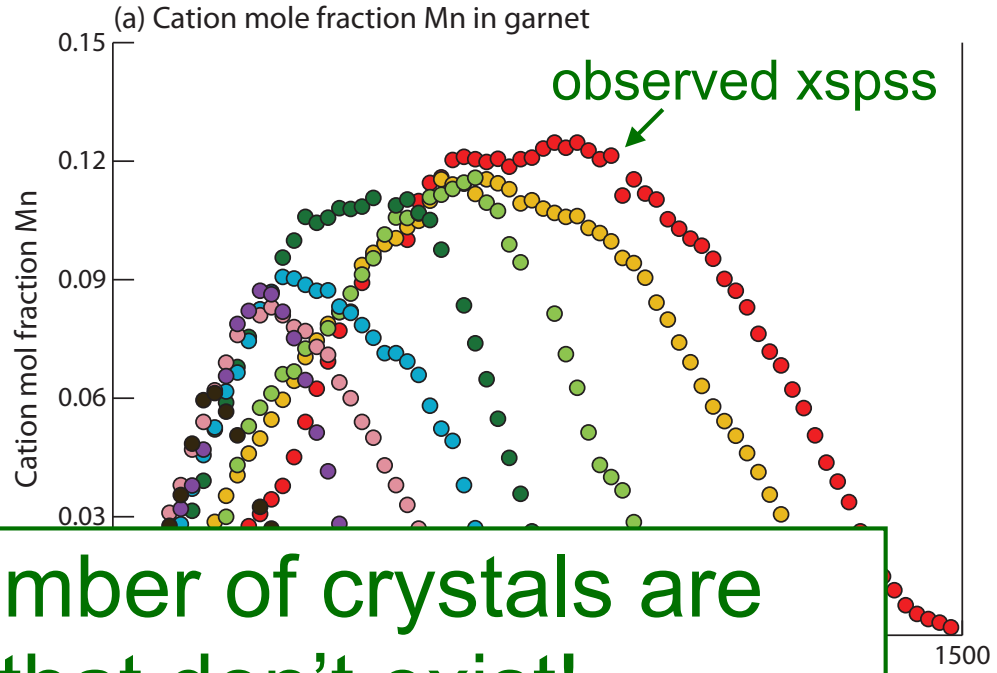




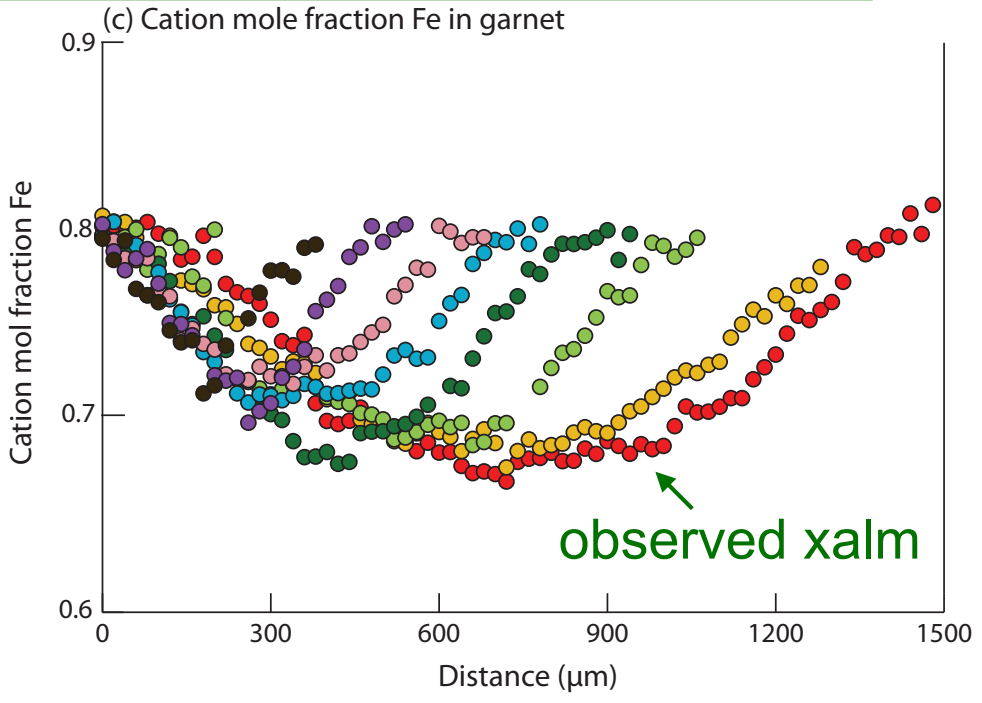


Theriak: Fractionation along a P-T path

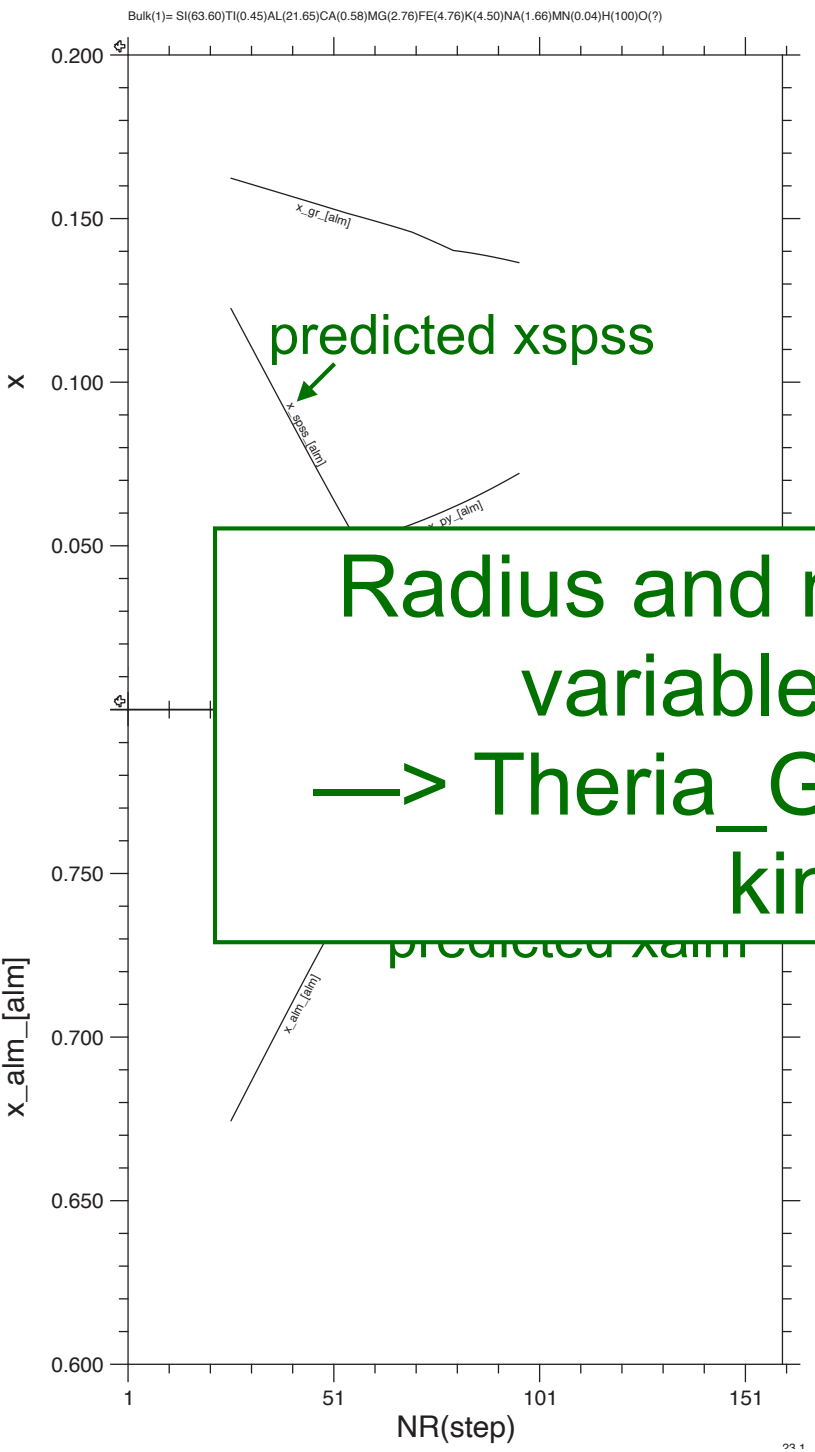


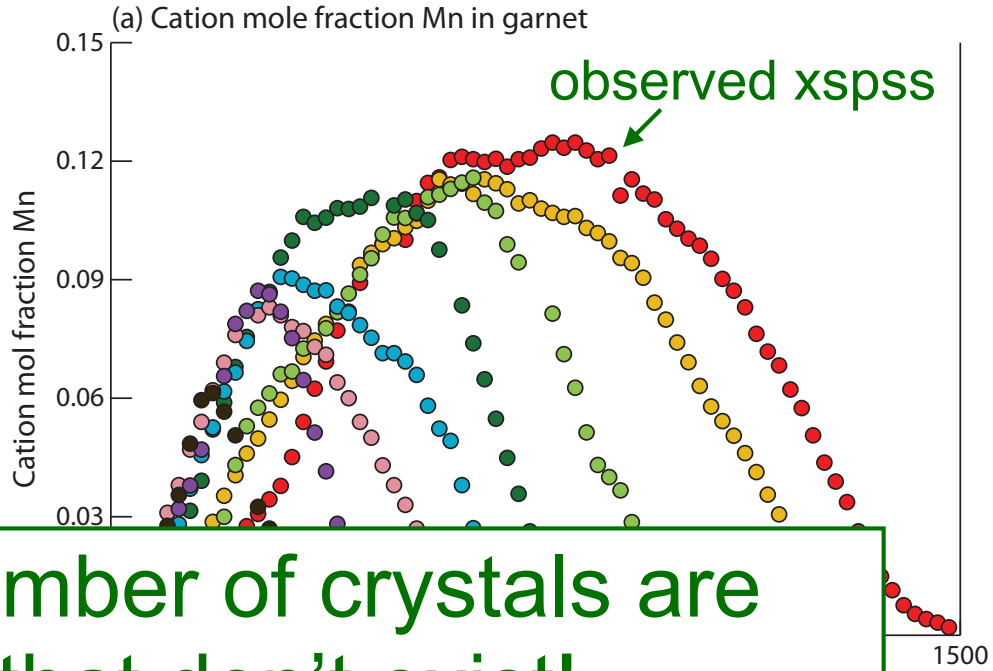


Radius and number of crystals are variables that don't exist!

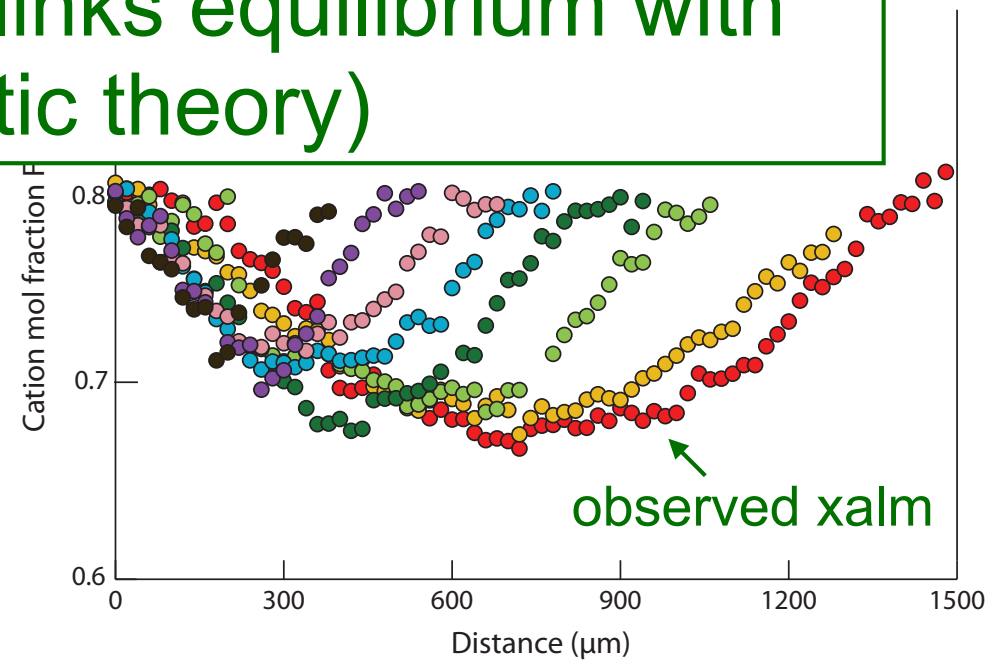


Theriak: Fractionation along a P-T path

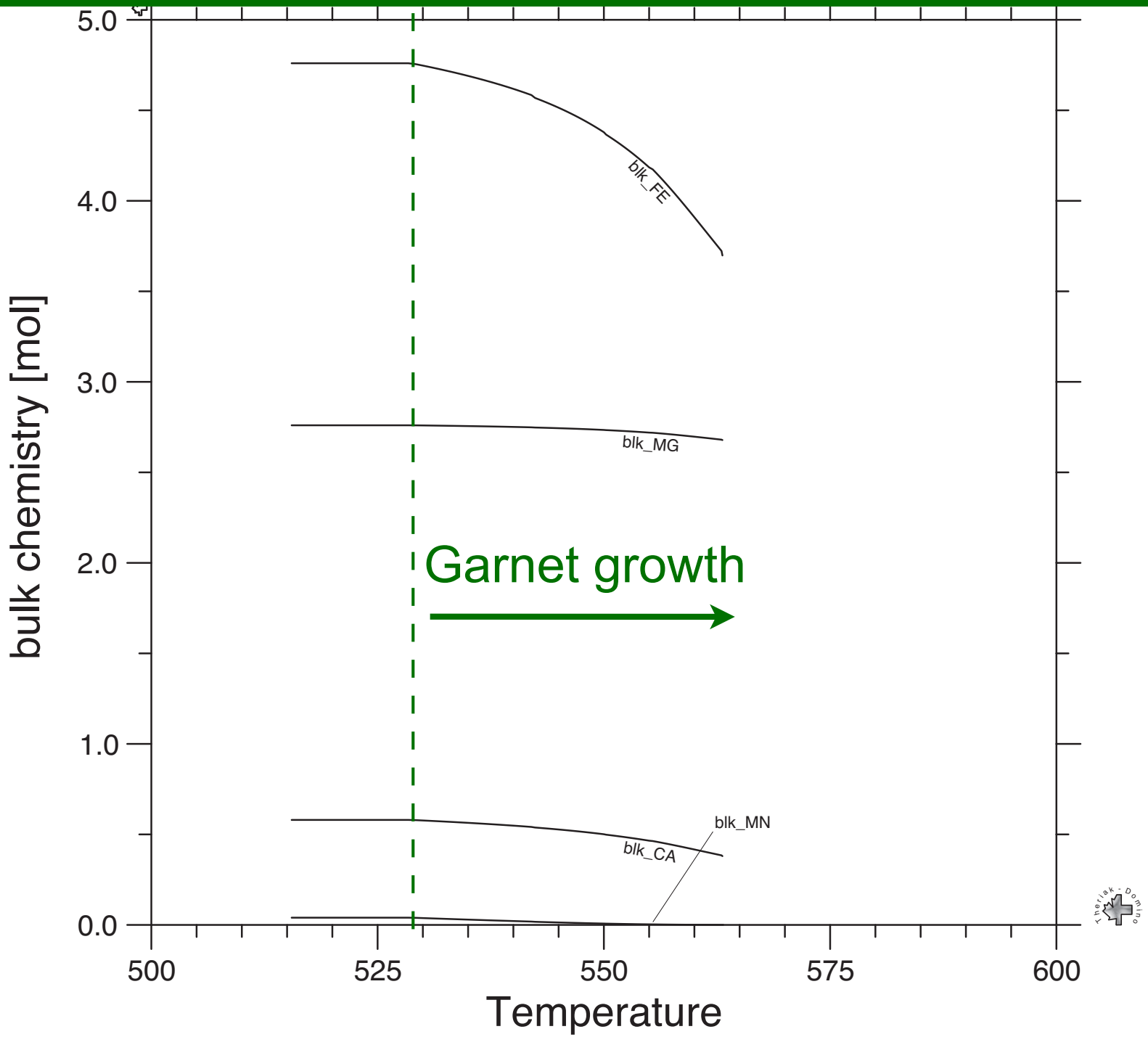




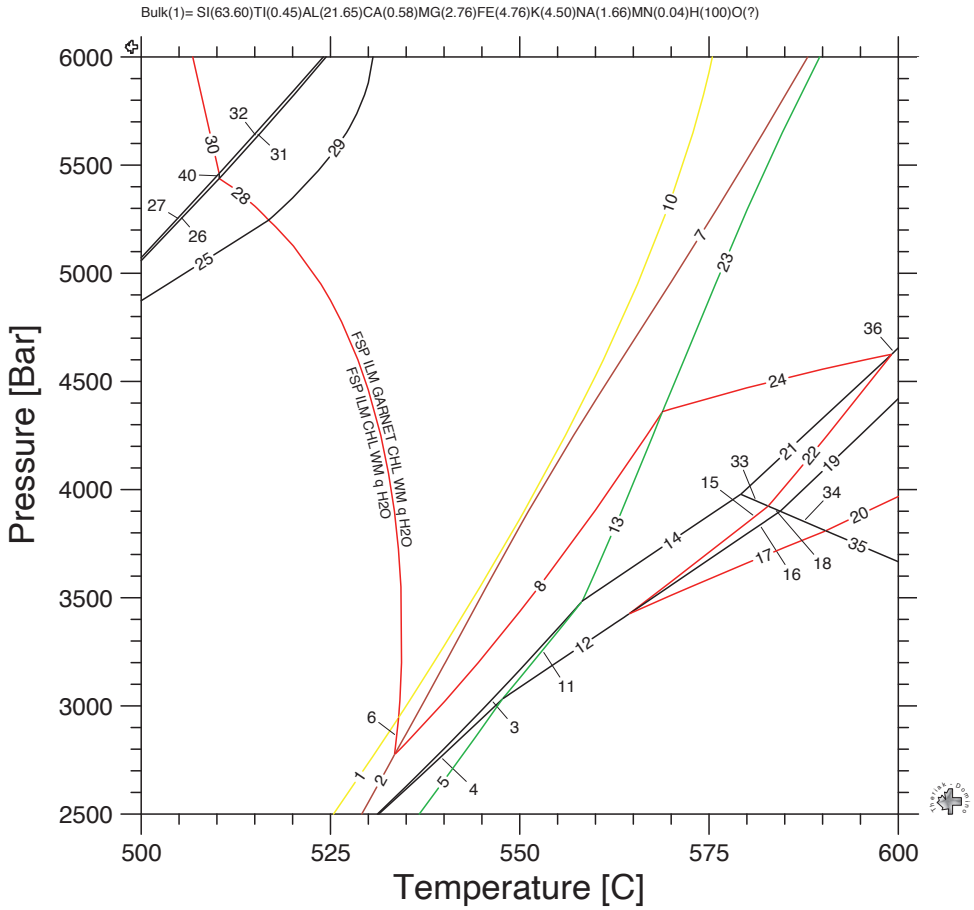
Radius and number of crystals are variables that don't exist!
—> Theria_G (links equilibrium with kinetic theory)

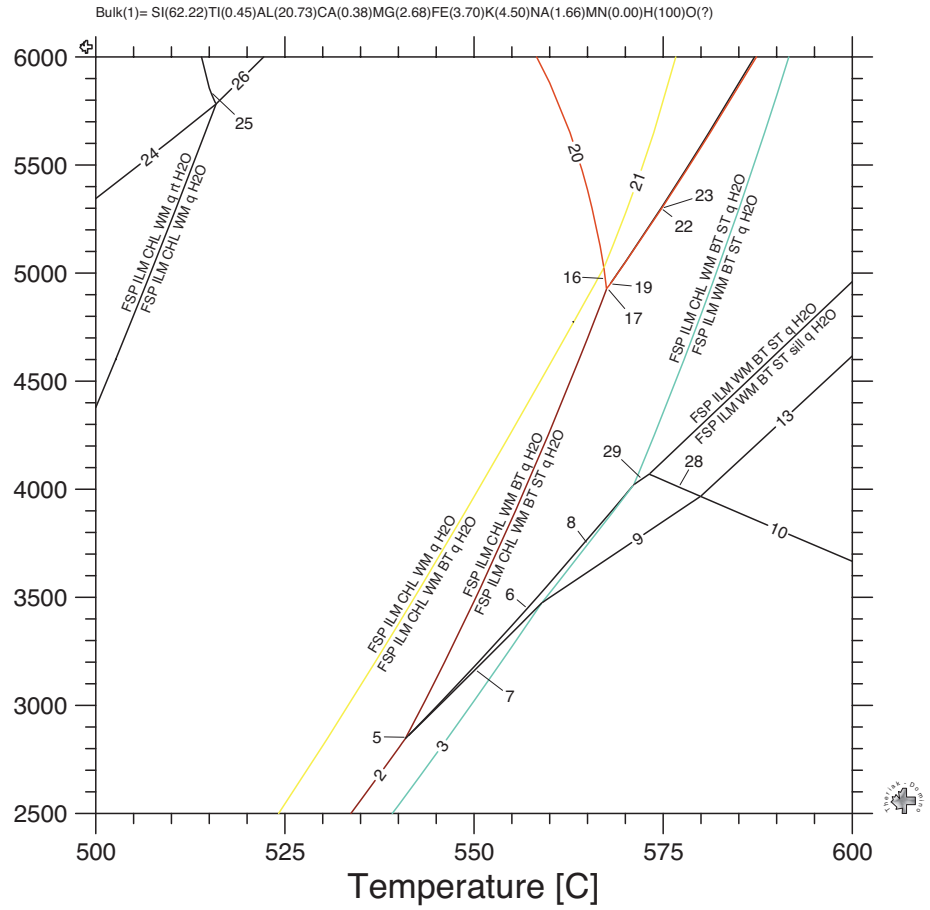


Theriak: Fractionation along a P-T path



Theriak: Fractionation along a P-T path



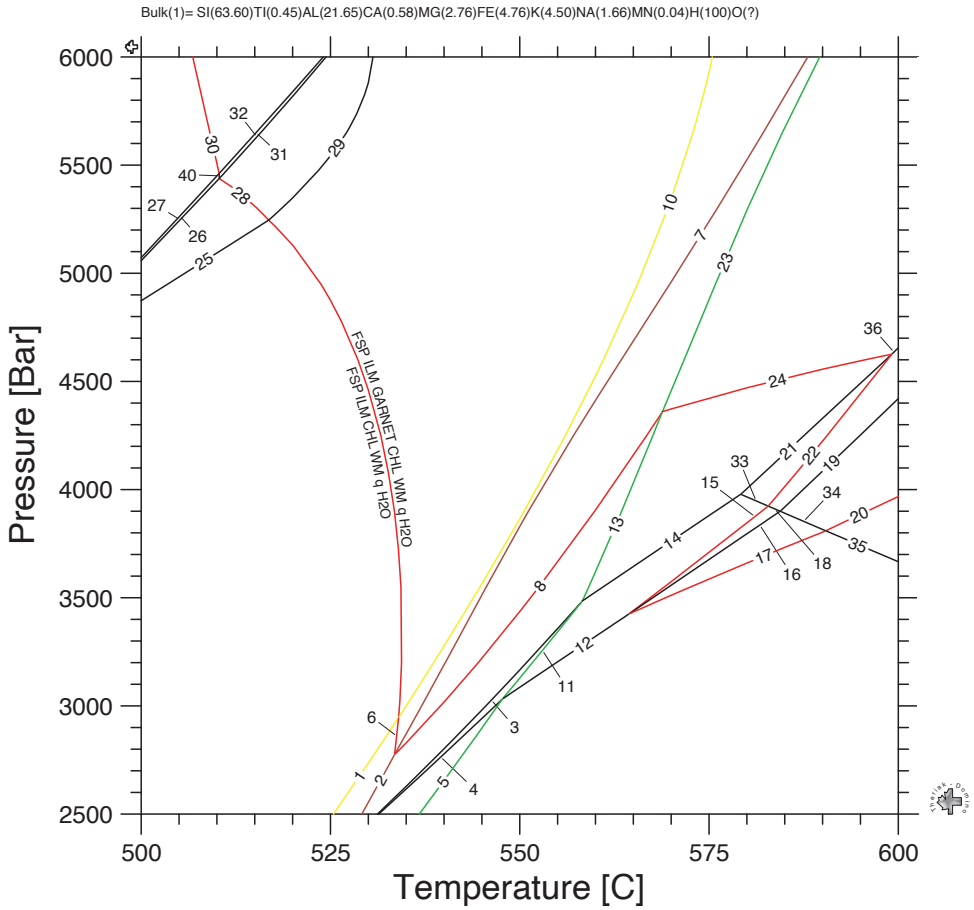


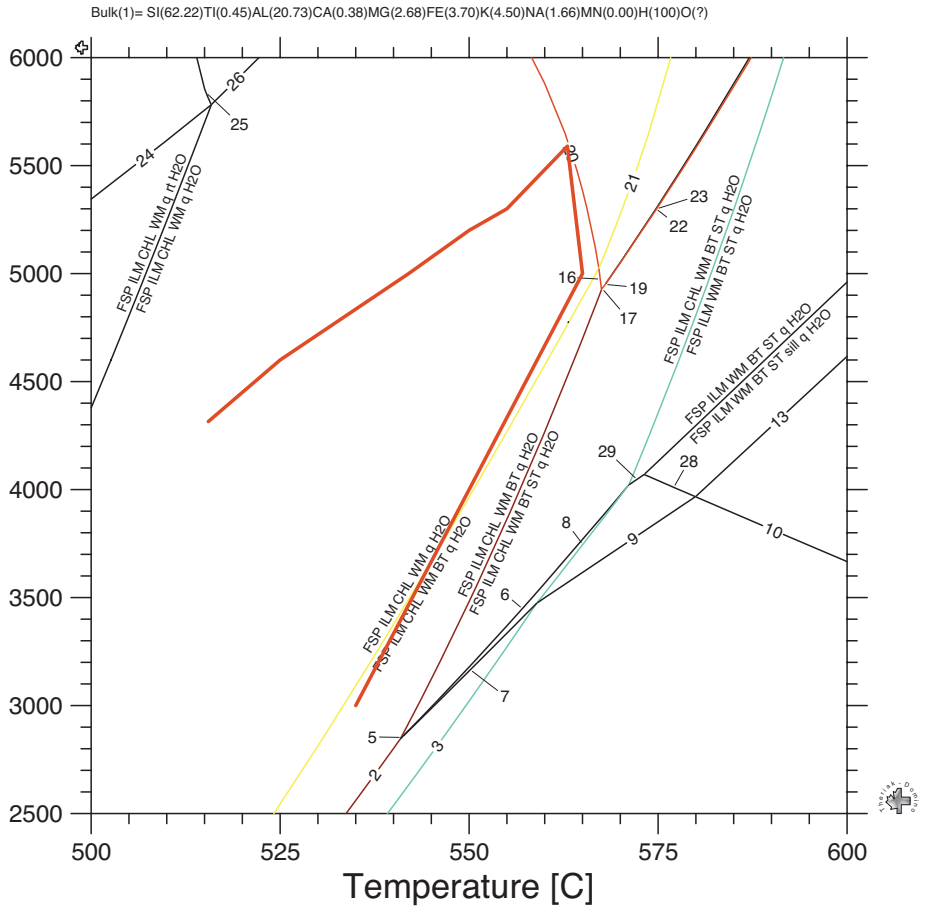
before

after

Garnet growth

Theriak: Fractionation along a P-T path



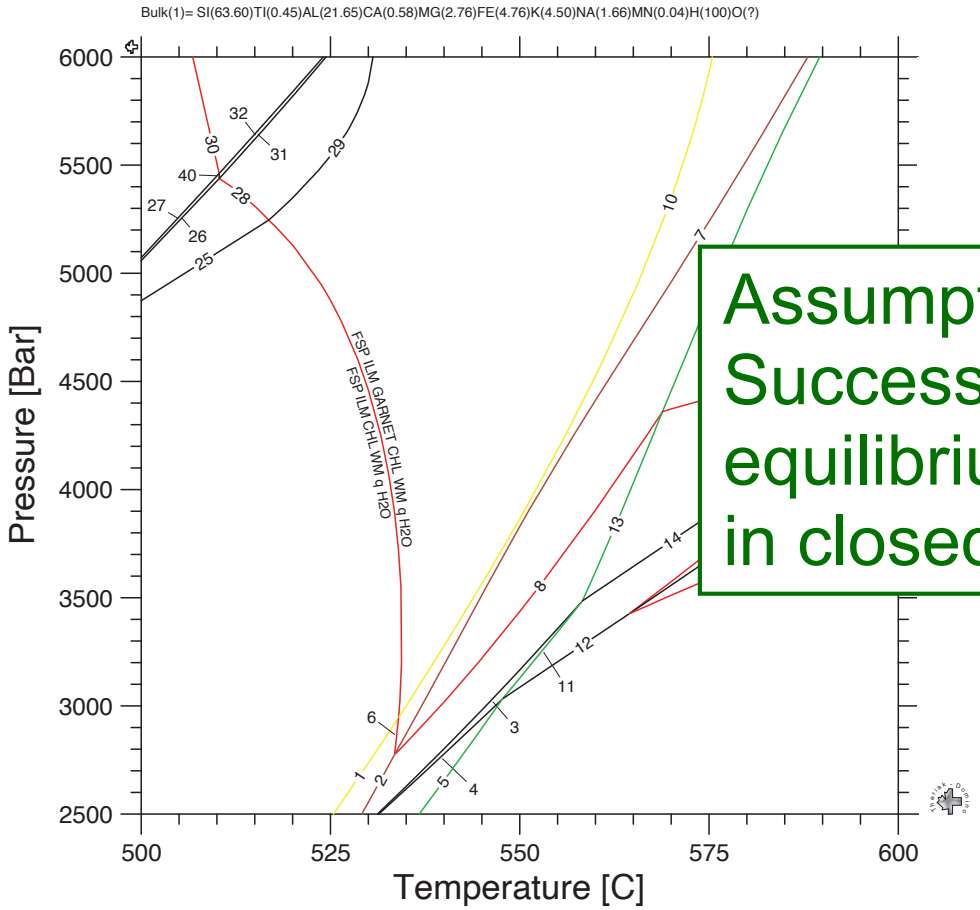


before

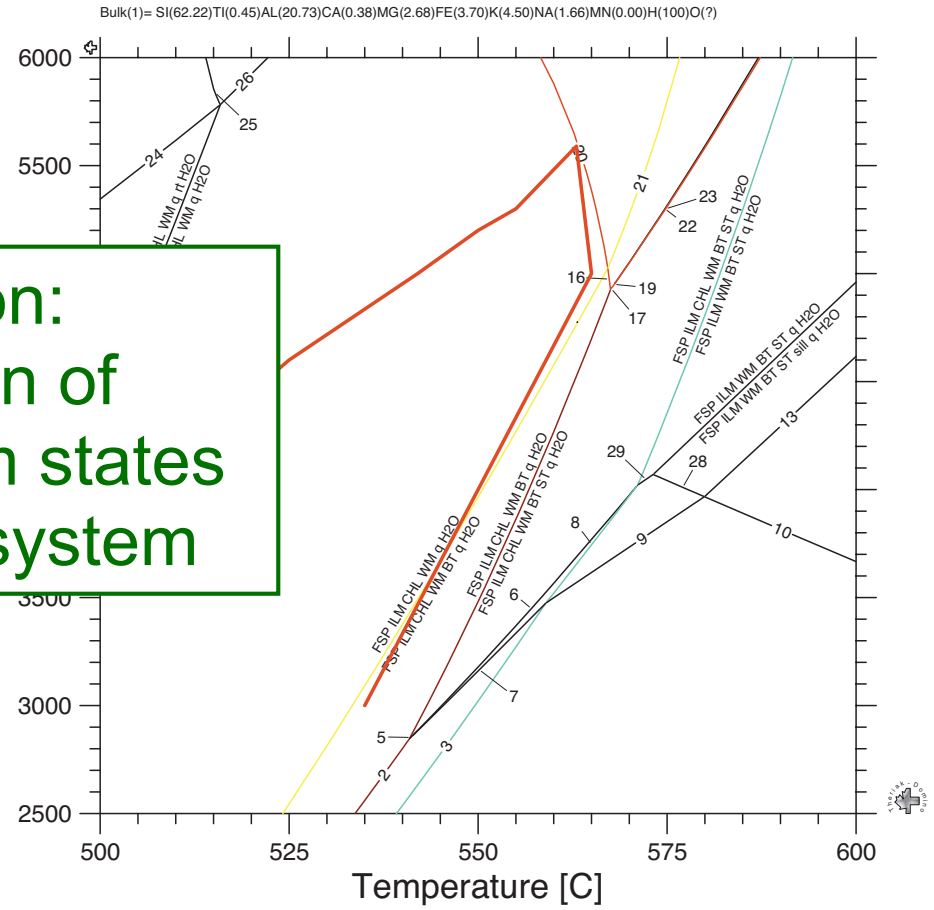
after

Garnet growth

Theriak: Fractionation along a P-T path



Assumption: Succession of equilibrium states in closed system



before

after

Garnet growth

geochemical society

The P-T-t Trajectory of Metamorphic Processes

Garnet crystallization simulations with Theria_G to estimate P-T-t trajectories of metamorphism

Fred Gaidies, Carleton U. (fred.gaidies@carleton.ca)

geochemical society

The P-T-t Trajectory of Metamorphic Processes

Garnet crystallization simulations with Theria_G to estimate P-T-t trajectories of metamorphism

Fred Gaidies, Carleton U. (fred.gaidies@carleton.ca)

Gaidies F, de Capitani C, Abart R (2008) THERIA_G: a software program to numerically model prograde garnet growth. Contributions to Mineralogy and Petrology 155:657-671

Gaidies F, Petley-Ragan A, Chakraborty S, Dasgupta S, Jones P (2015) Constraining the conditions of Barrovian metamorphism in Sikkim, India: P-T-t paths of garnet crystallization in the Lesser Himalayan Belt. Journal of Metamorphic Geology 33:23-44

George F, Gaidies F (2017) Characterisation of a garnet population from the Sikkim Himalaya: insights into the rates and mechanisms of porphyroblast crystallisation. Contributions to Mineralogy and Petrology 172:57

Garnet crystallization modelling with THERIA_G

THERIA_G

Considers:
1) Equilibrium thermodynamics
2) Multi-component diffusion
3) Chemical fractionation
4) Formation of a garnet population

Garnet crystallization modelling with THERIA_G

THERIA_G

Considers: 1) Equilibrium thermodynamics
2) Multi-component diffusion
3) Chemical fractionation
4) Formation of a garnet population

to calculate: phase content of rock
chemical compositions of all stable phases
volumes, number of moles, ..., of all stable phases

by Gibbs energy minimization for changing P-T-X
[theriak algorithm, de Capitani & Brown, 1987)

Garnet crystallization modelling with THERIA_G

THERIA_G

Considers: 1) Equilibrium thermodynamics
2) Multi-component diffusion
3) Chemical fractionation
4) Formation of a garnet population

to calculate: intracrystalline diffusion of Mn, Fe, Ca, Mg in garnet

concentration — diffusion coefficients

$$\frac{\partial C_i}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\sum_{j}^{n-1} D_{ij} r^2 \left(\frac{\partial C_j}{\partial r}\right)$$

time — radius

Garnet crystallization modelling with THERIA_G

THERIA_G

concentration

diffusion coefficients

$$\frac{\partial C_i}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\sum_{j}^{n-1} D_{ij} r^2 \left(\frac{\partial C_j}{\partial r}\right)$$

time

radius

charge

mole fraction

$$D_{ij} = D_i^\star \delta_{ij} - \left(\frac{D_i^\star z_i z_j X_i}{\sum_{k=1}^{n} z_k^2 X_k D_k^\star}\right)(D_j^\star - D_n^\star)$$

tracer diffusion coefficient

Garnet crystallization modelling with THERIA_G

THERIA_G

concentration

diffusion coefficients

$$\frac{\partial C_i}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\sum_{j}^{n-1} D_{ij} r^2 \left(\frac{\partial C_j}{\partial r}\right)$$

time

radius

charge

mole fraction

$$D_{ij} = D_i^{\star}\delta_{ij} - \left(\frac{D_i^{\star} z_i z_j X_i}{\sum_{k=1}^{n} z_k^2 X_k D_k^{\star}}\right)(D_j^{\star} - D_n^{\star})$$

tracer diffusion coefficient

activation energy

activation volume

$$D_i^{\star} = D_0 \exp\left(\frac{-E_a - (P-1)\Delta V^{+}}{RT}\right)$$

pre-exponential constant

Garnet crystallization modelling with THERIA_G

THERIA_G

Considers:
1) Equilibrium thermodynamics
2) Multi-component diffusion
3) Chemical fractionation
4) Formation of a garnet population

to calculate: the thermodynamically effective chemical composition of the model system

Garnet crystallization modelling with THERIA_G

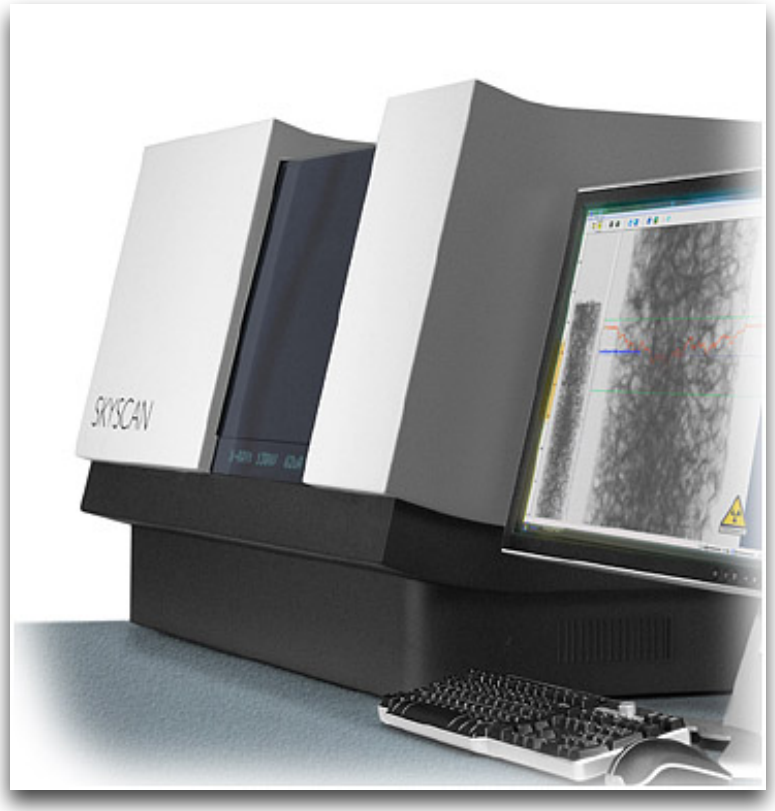
THERIA_G

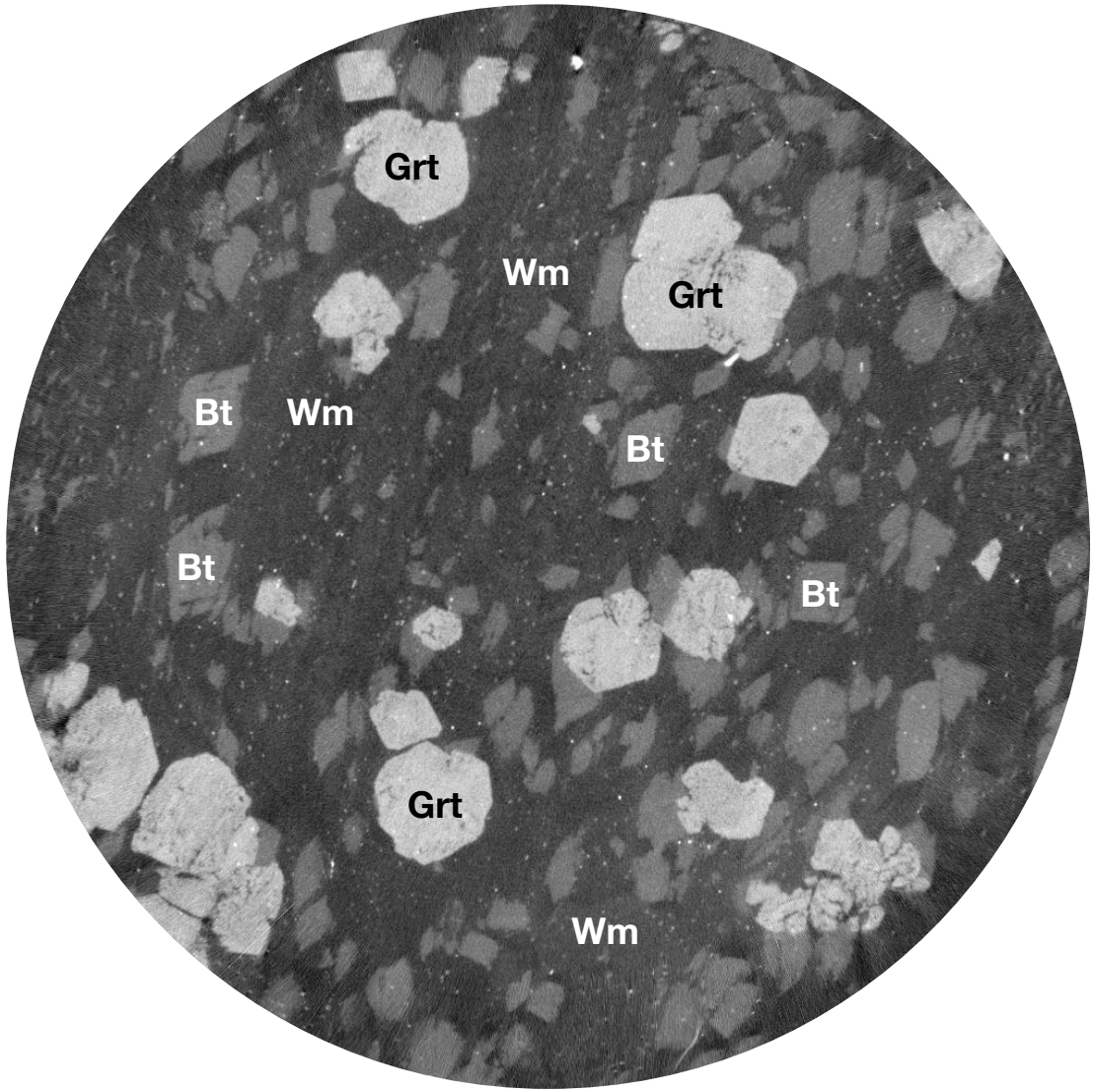
Considers:
1) Equilibrium thermodynamics
2) Multi-component diffusion
3) Chemical fractionation
4) Formation of a garnet population

to calculate: the chemical compositions and sizes of all garnet crystals in a rock accounting for their specific crystal growth histories

Garnet crystallization modelling with THERIA_G

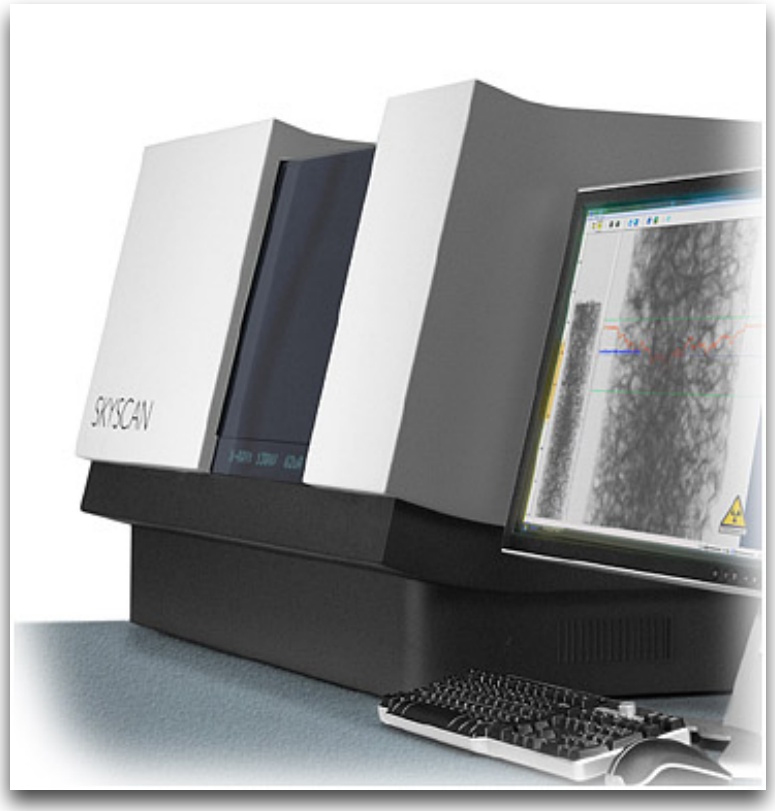
X-ray micro-computed tomography

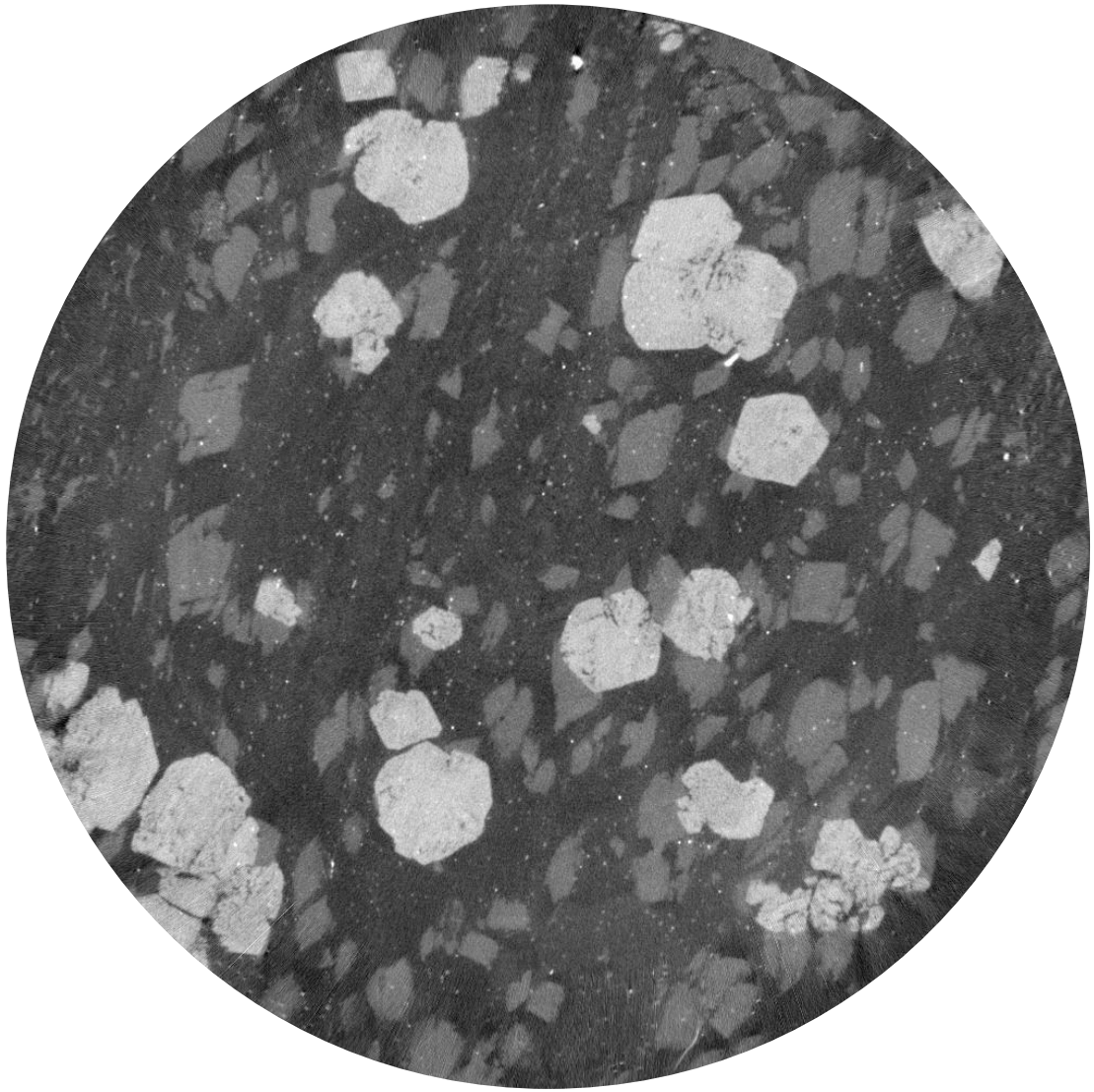




Garnet crystallization modelling with THERIA_G

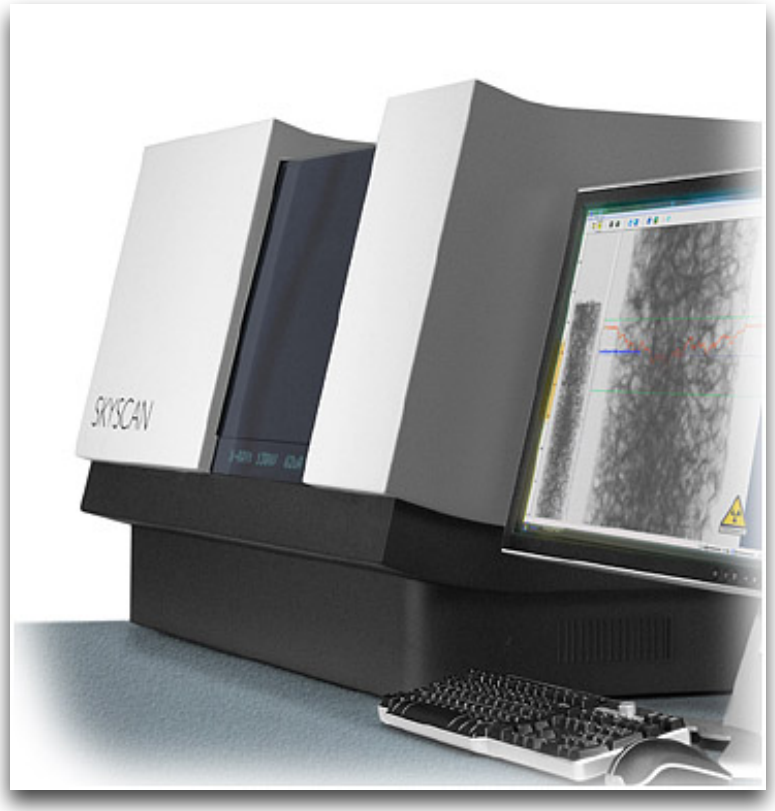
X-ray micro-computed tomography

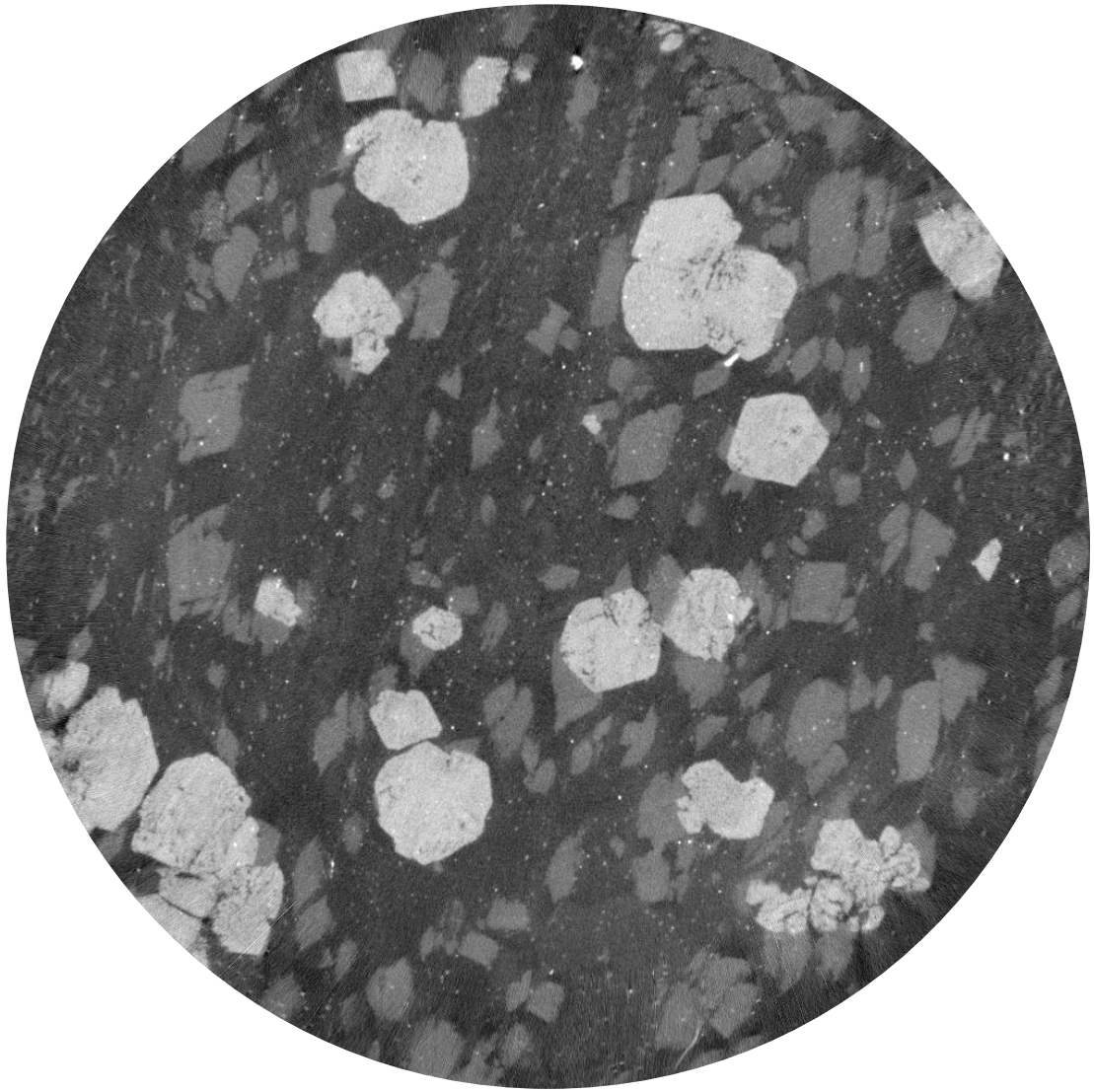




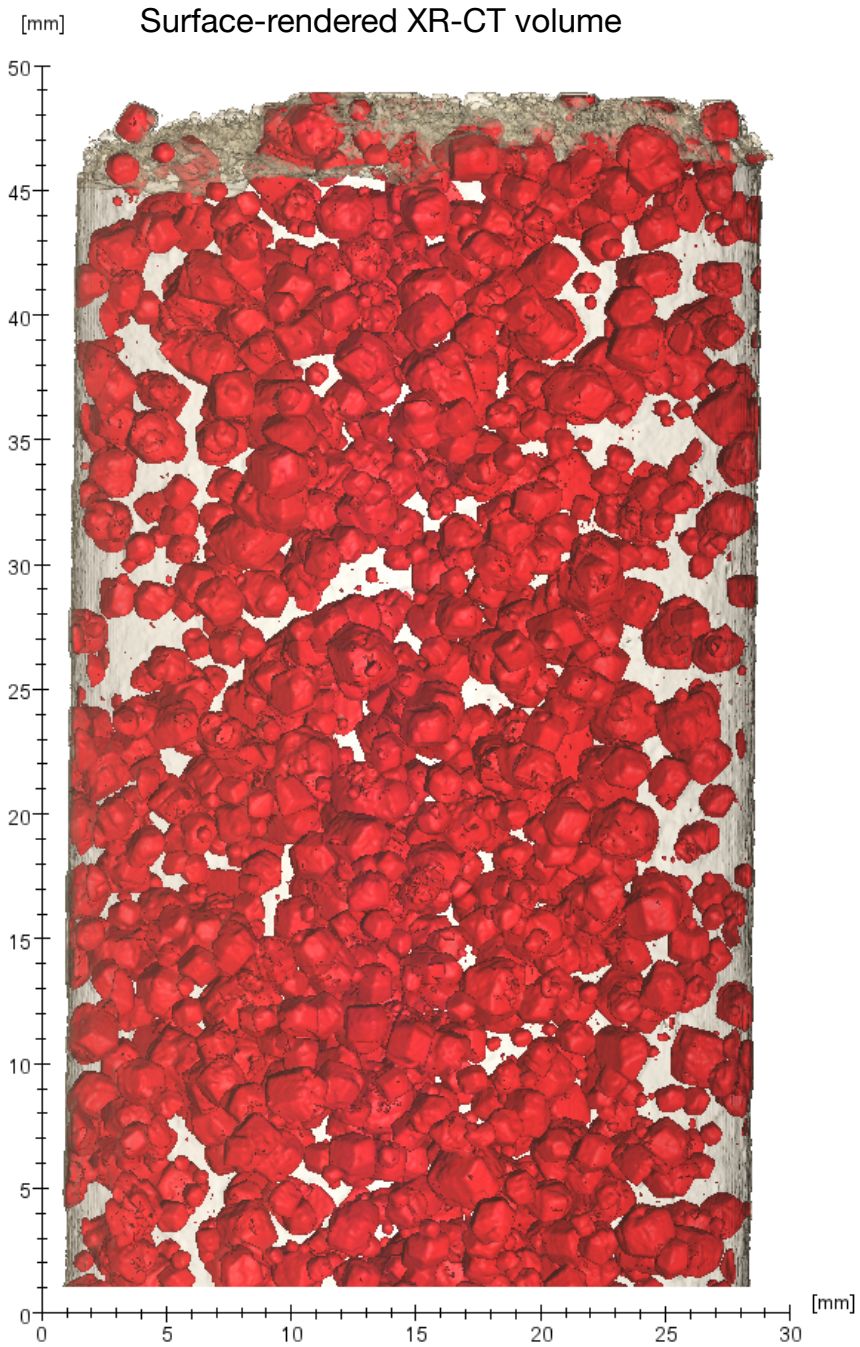
Garnet crystallization modelling with THERIA_G

X-ray micro-computed tomography

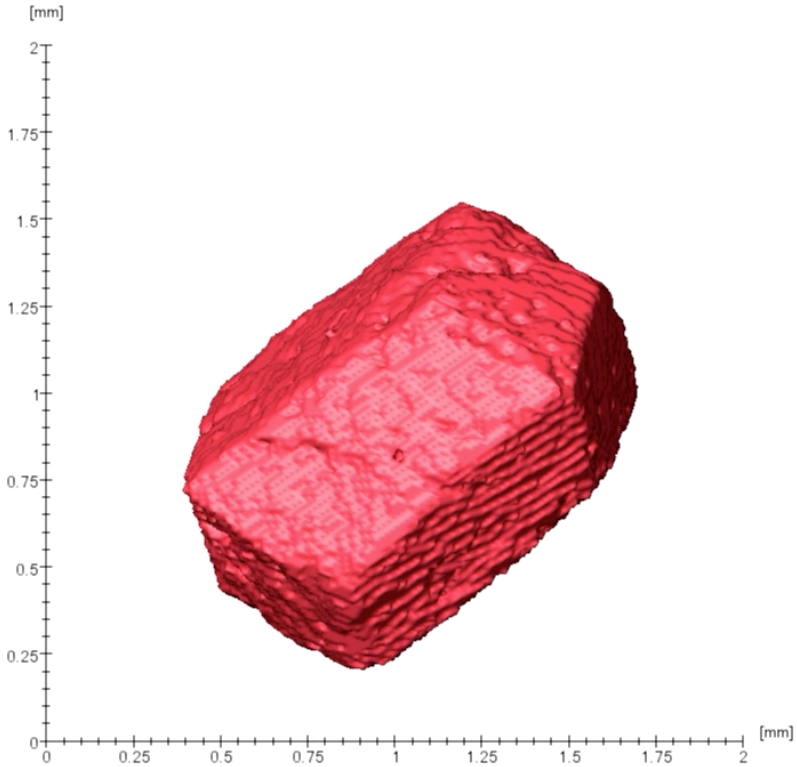




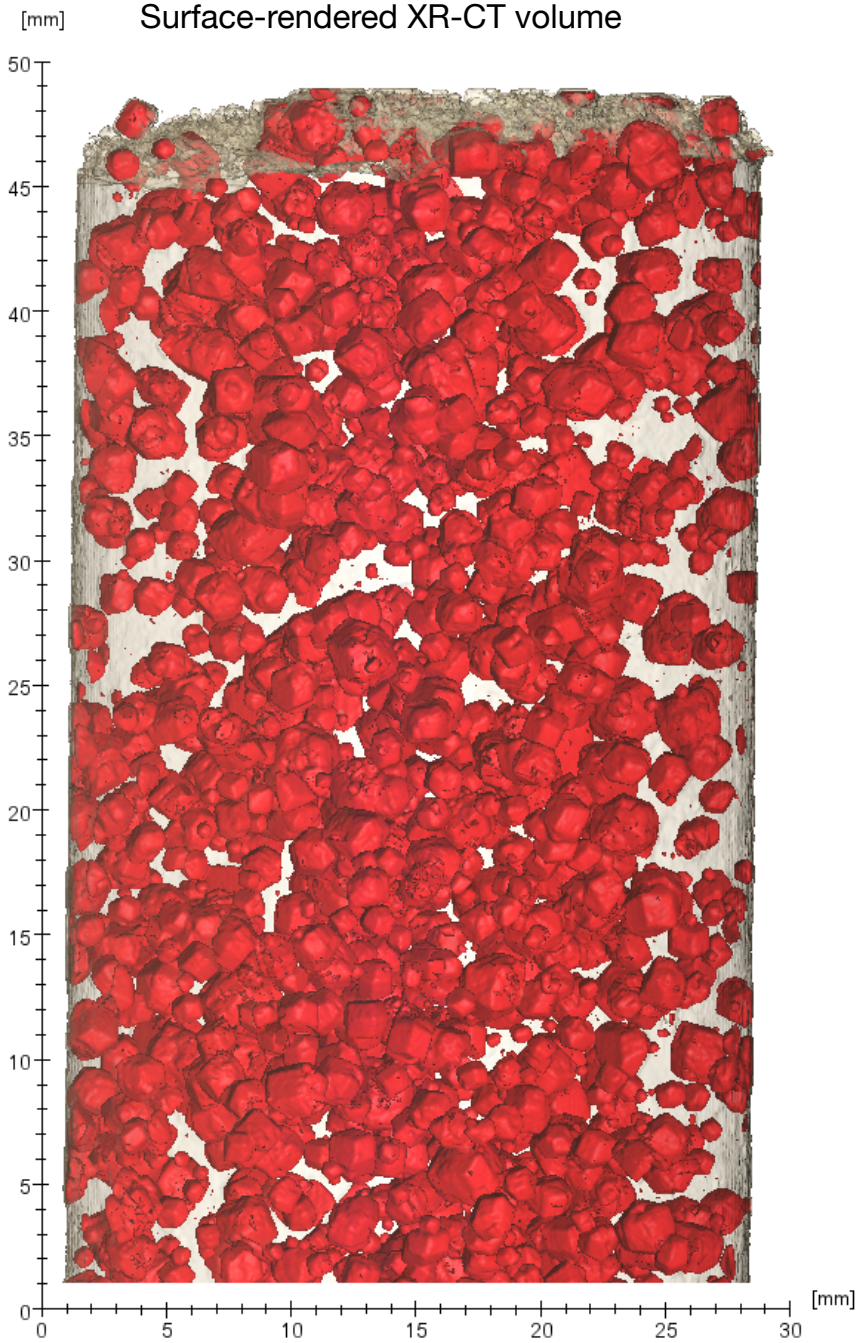
Garnet crystallization modelling with THERIA_G



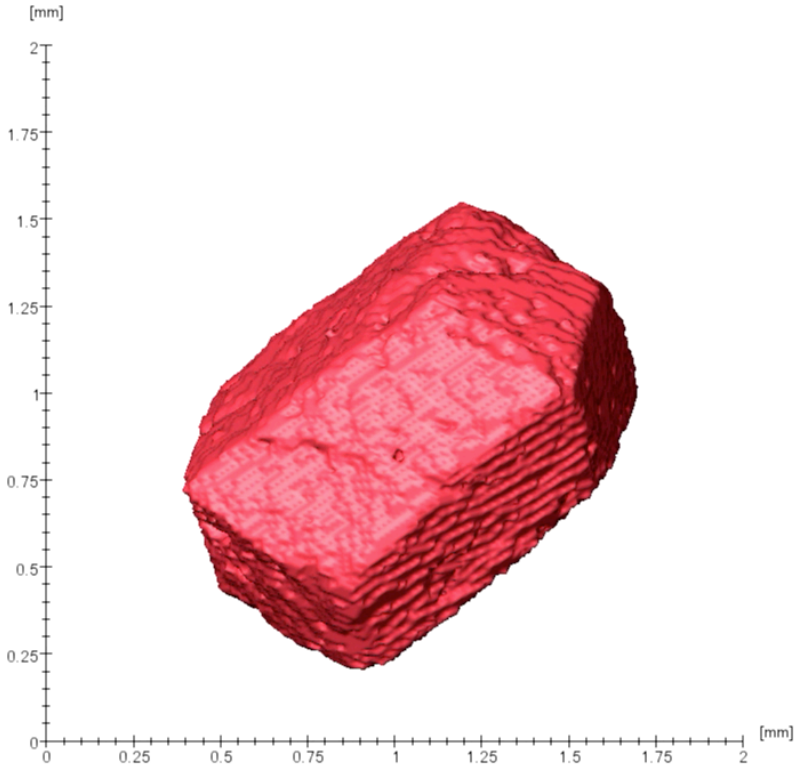
Garnet crystallization modelling with THERIA_G



Surface-rendered XR-CT volume



Garnet crystallization modelling with THERIA_G



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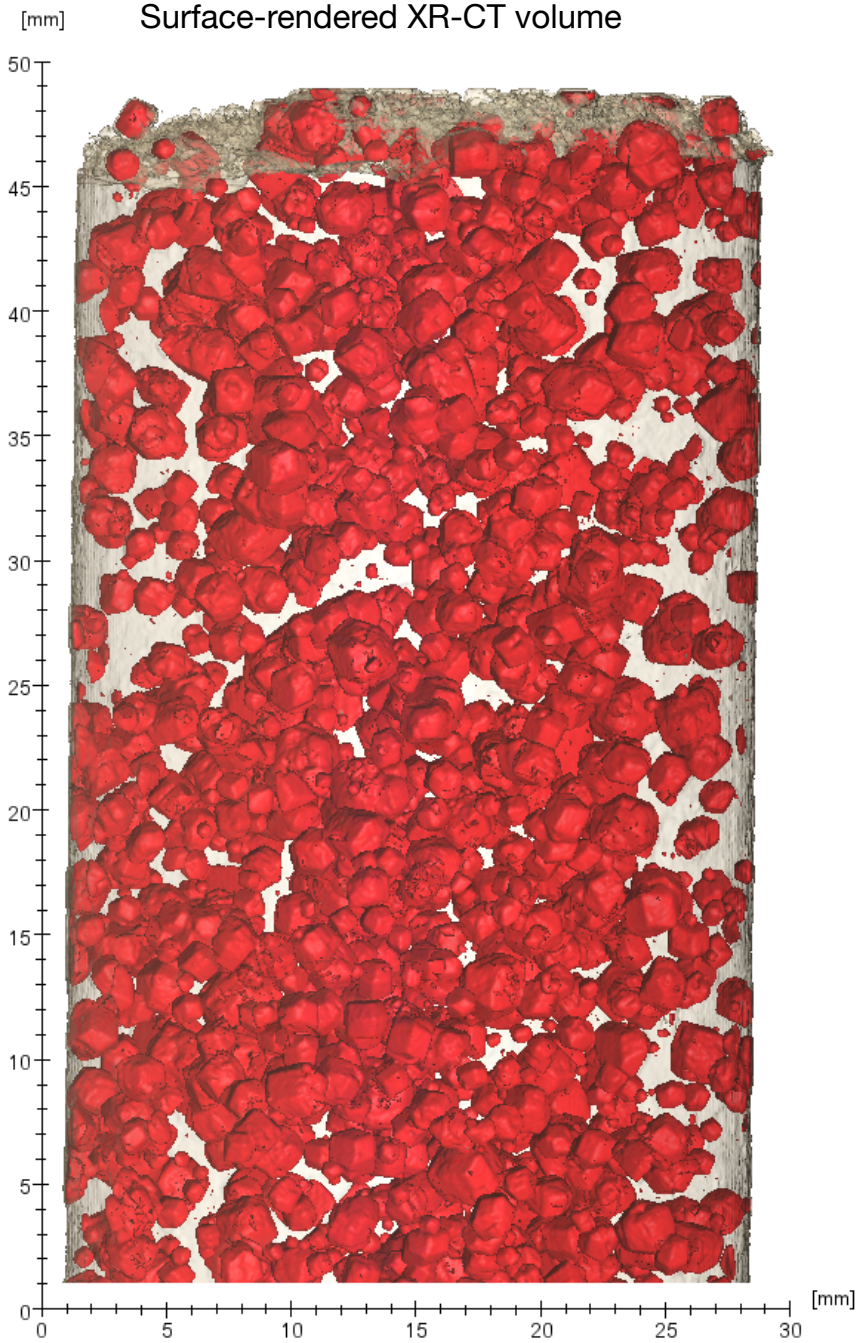
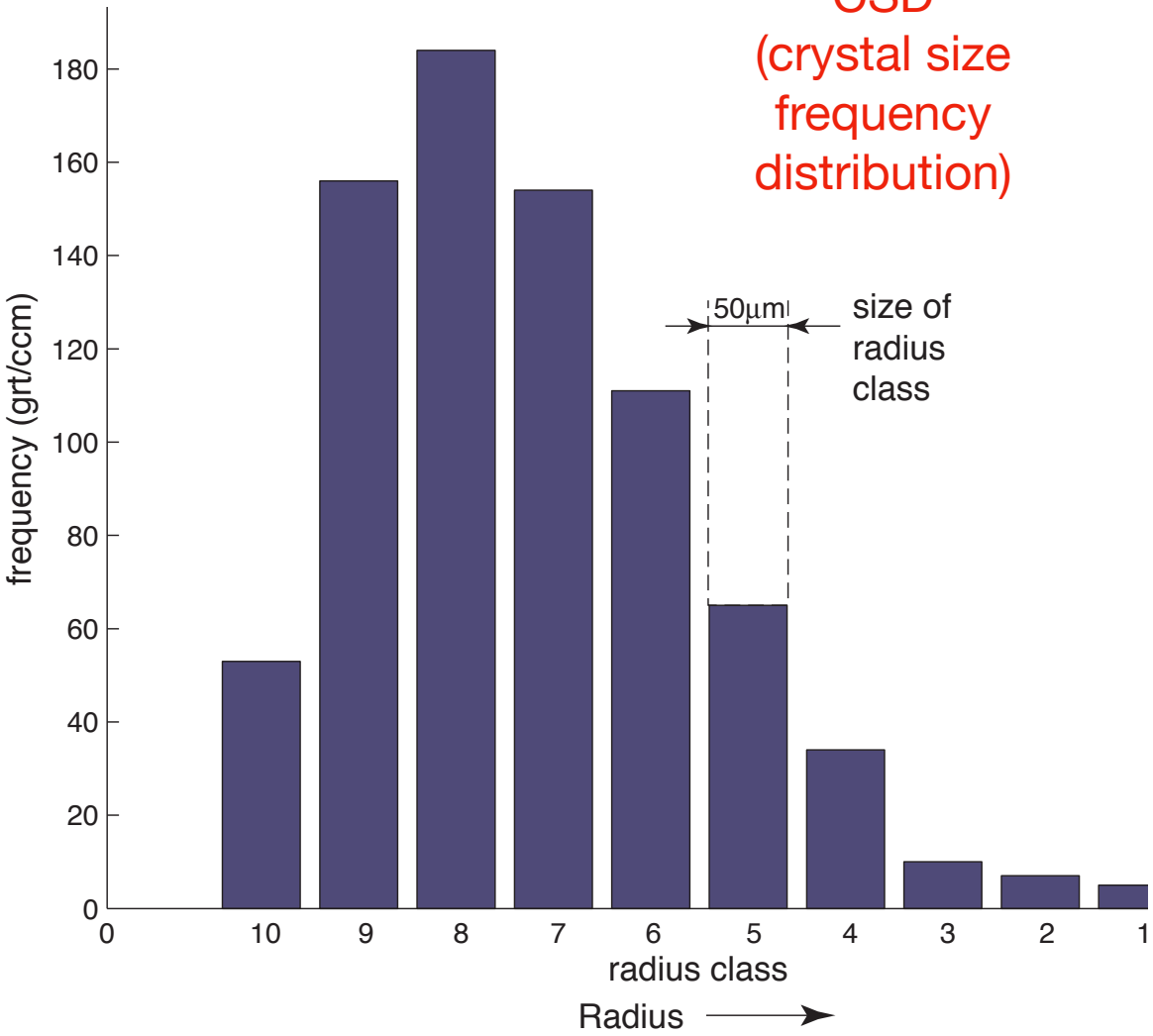


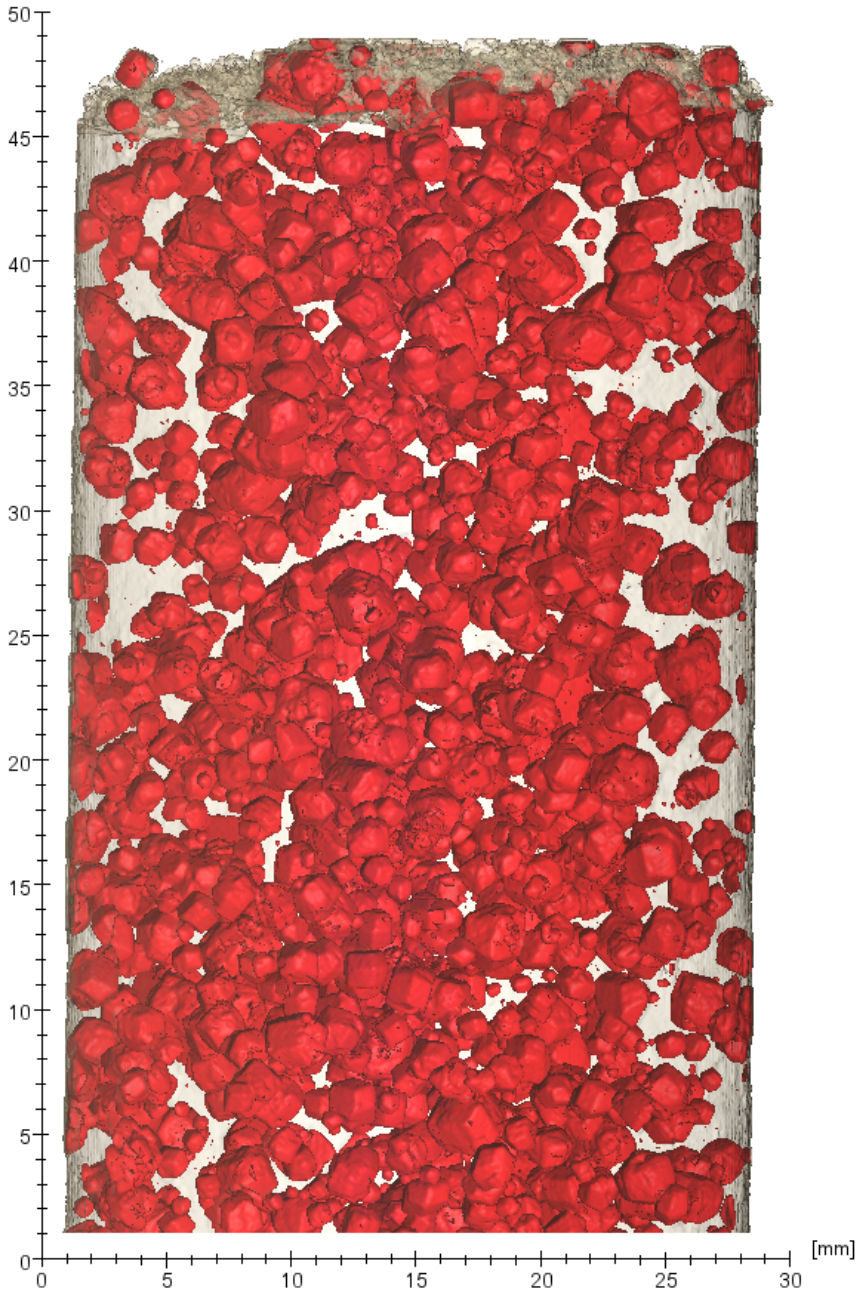
Garnet crystallization modelling with THERIA_G

X-ray micro-computed tomography

CSD (crystal size frequency distribution)



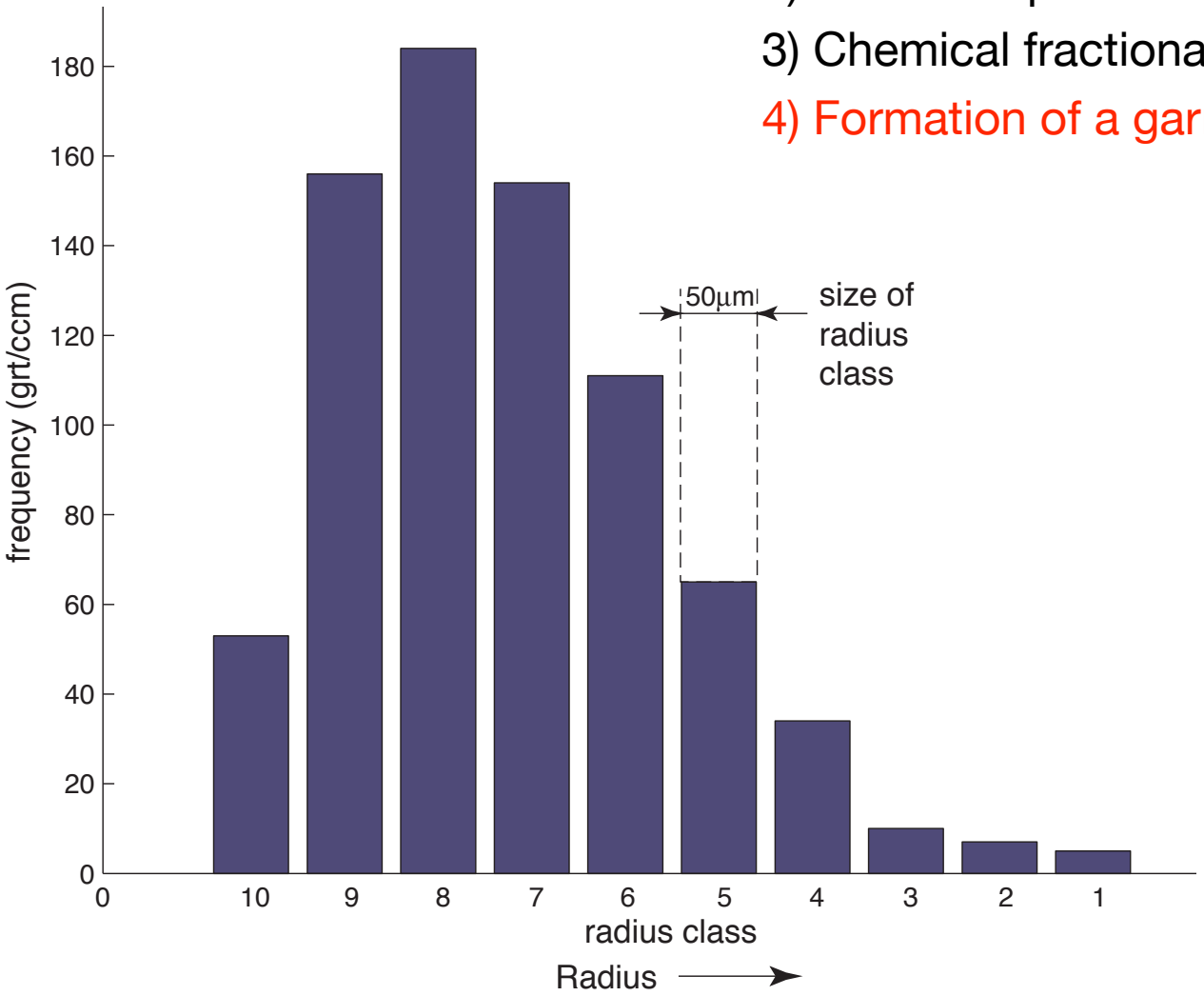
Surface-rendered XR-CT volume



Garnet crystallization modelling with THERIA_G

THERIA_G

Considers: 1) Equilibrium thermodynamics
2) Multi-component diffusion
3) Chemical fractionation
4) Formation of a garnet population



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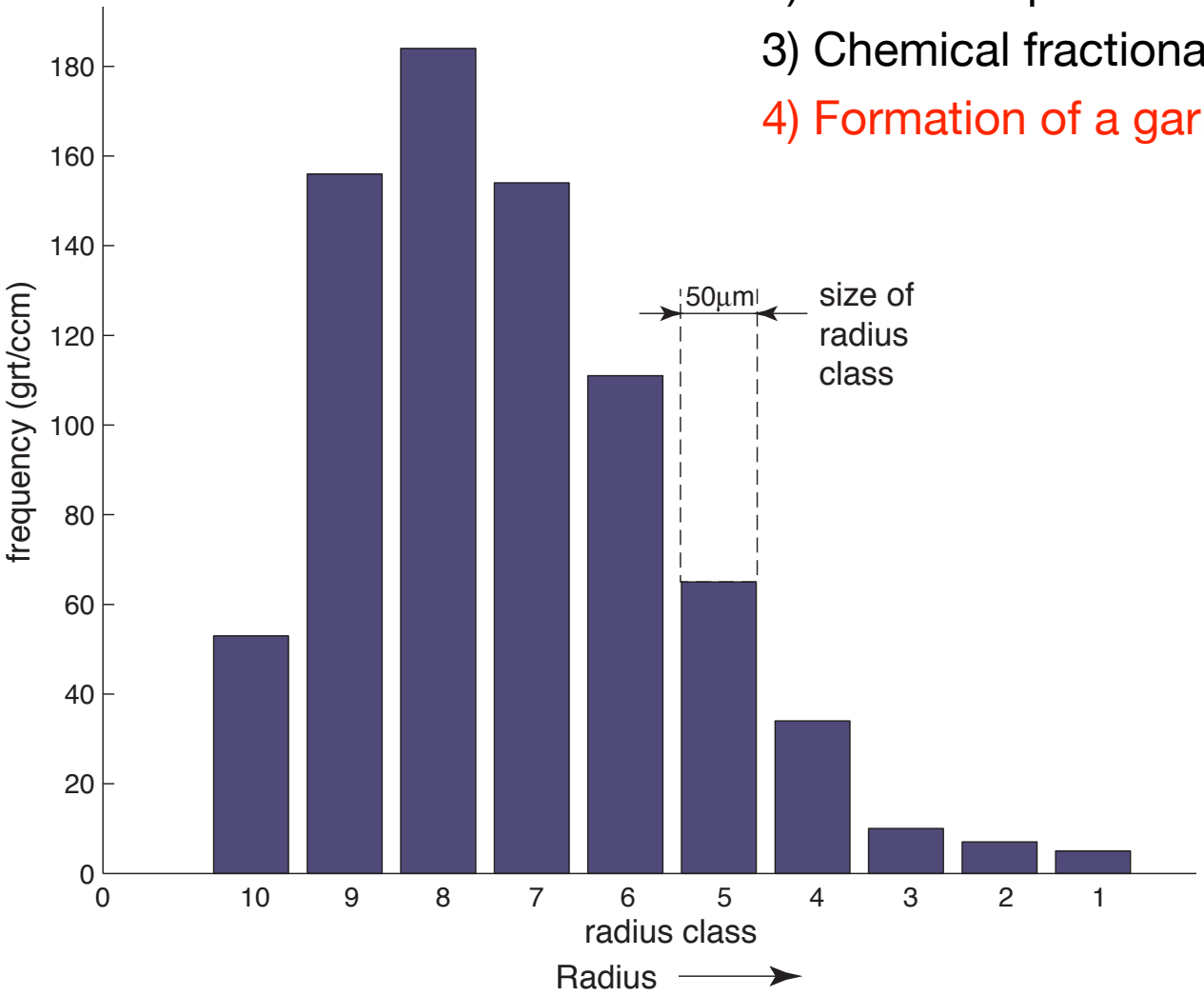

Interface mobility

$$\frac{\mathrm{d}r}{\mathrm{d}t} = M\Delta G_r$$

Driving force for crystal growth

Garnet crystallization modelling with THERIA_G

THERIA_G

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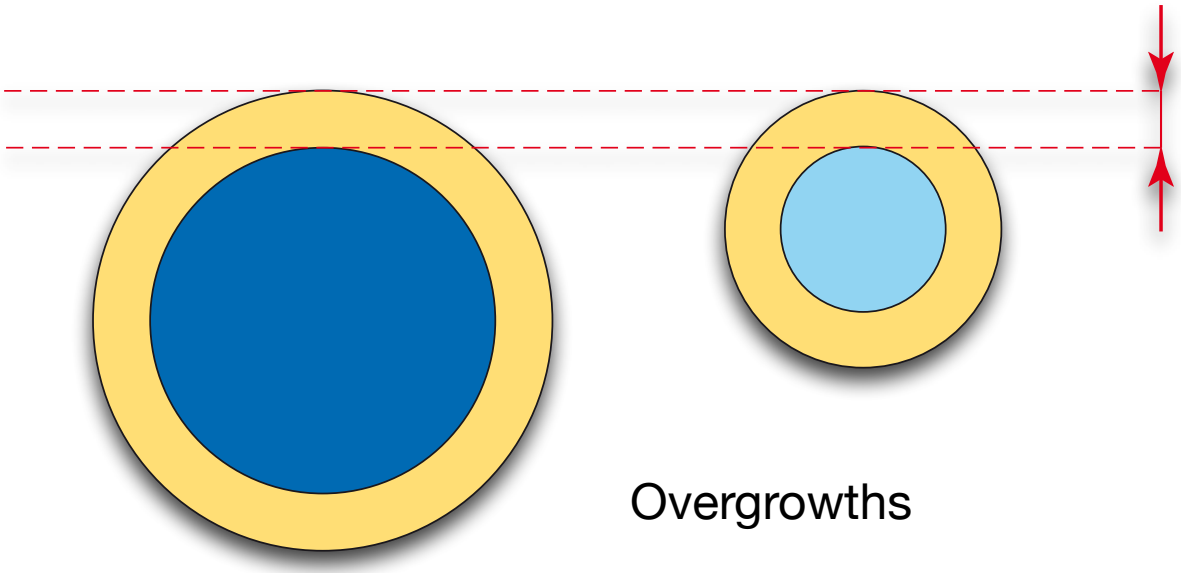

Overgrowths

Interface mobility

$$\frac{\mathrm{d}r}{\mathrm{d}t} = M\Delta G_r$$

Driving force for crystal growth

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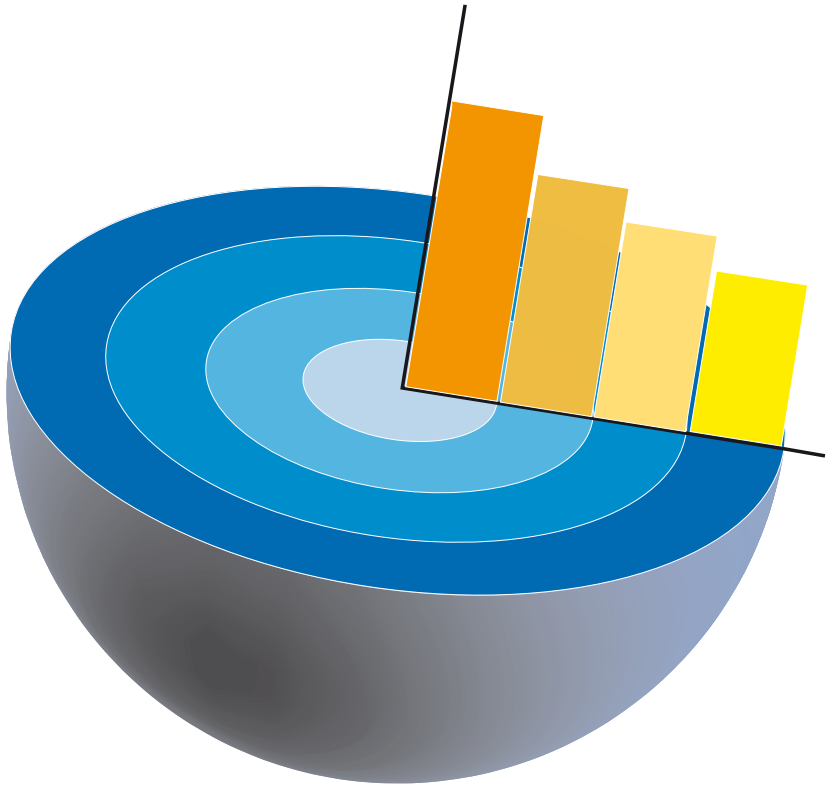


Interface mobility

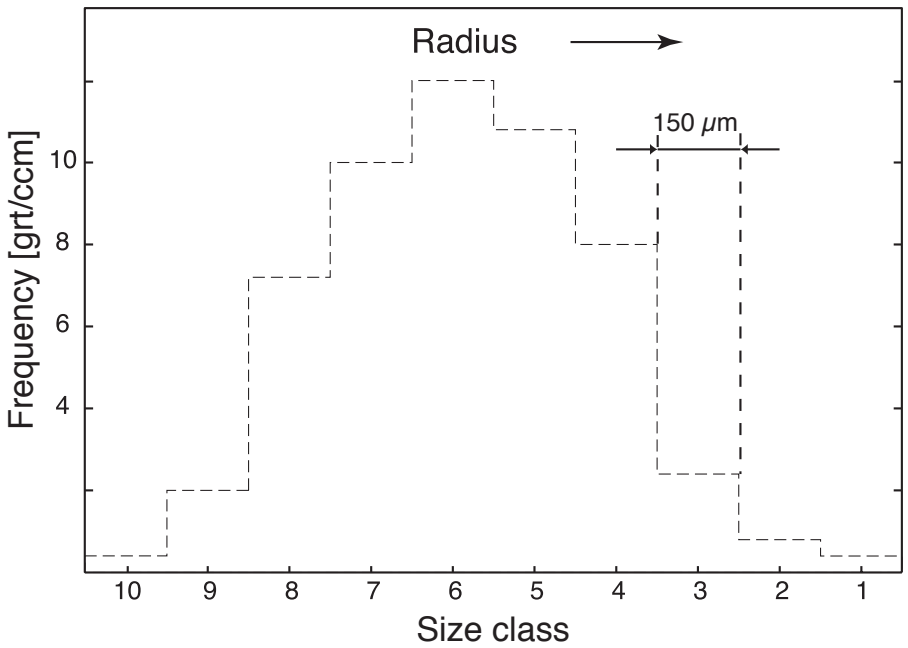
$$\frac{\mathrm{d}r}{\mathrm{d}t} = M\Delta G_r$$

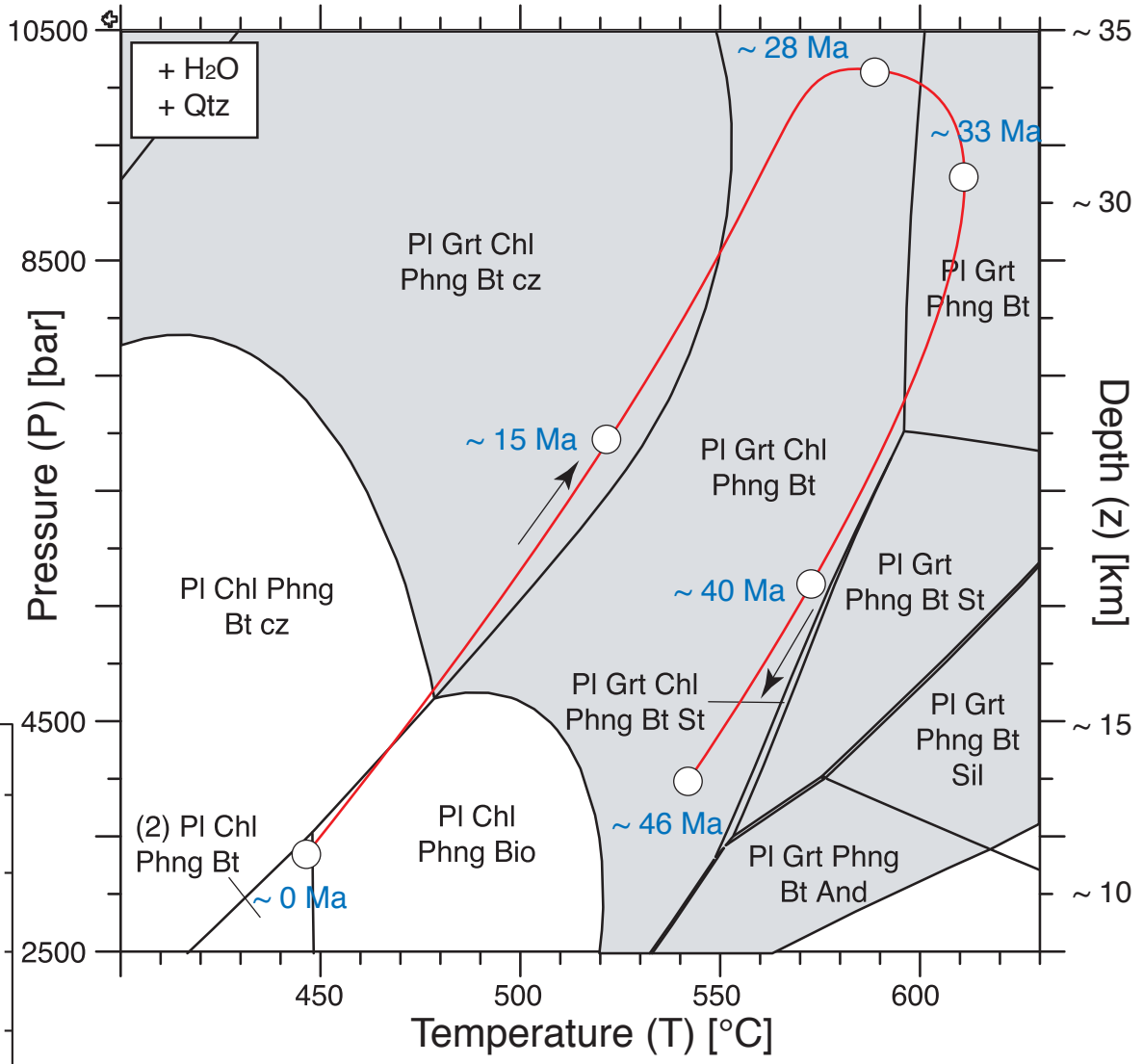
Driving force for crystal growth

Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

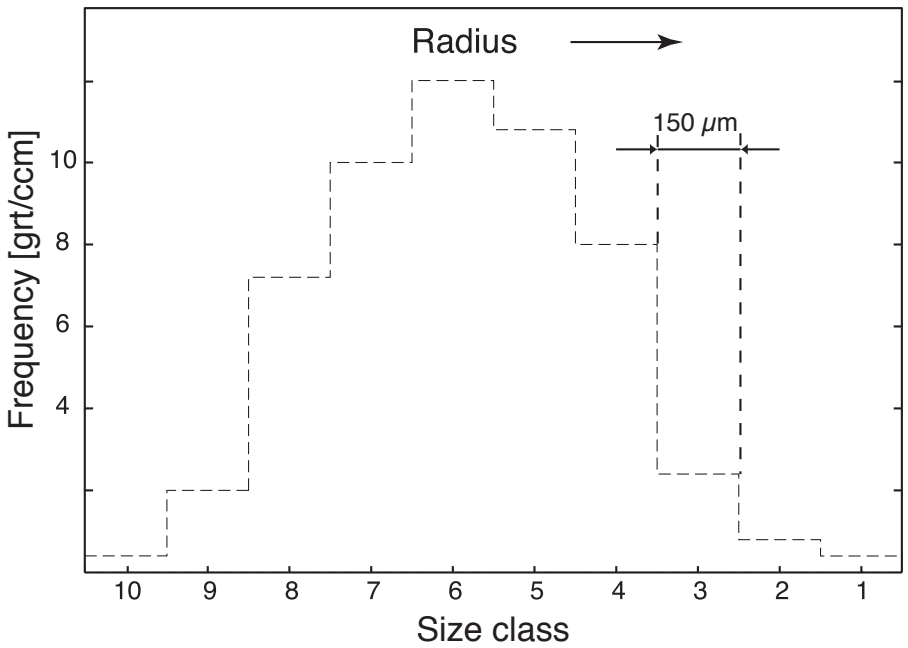


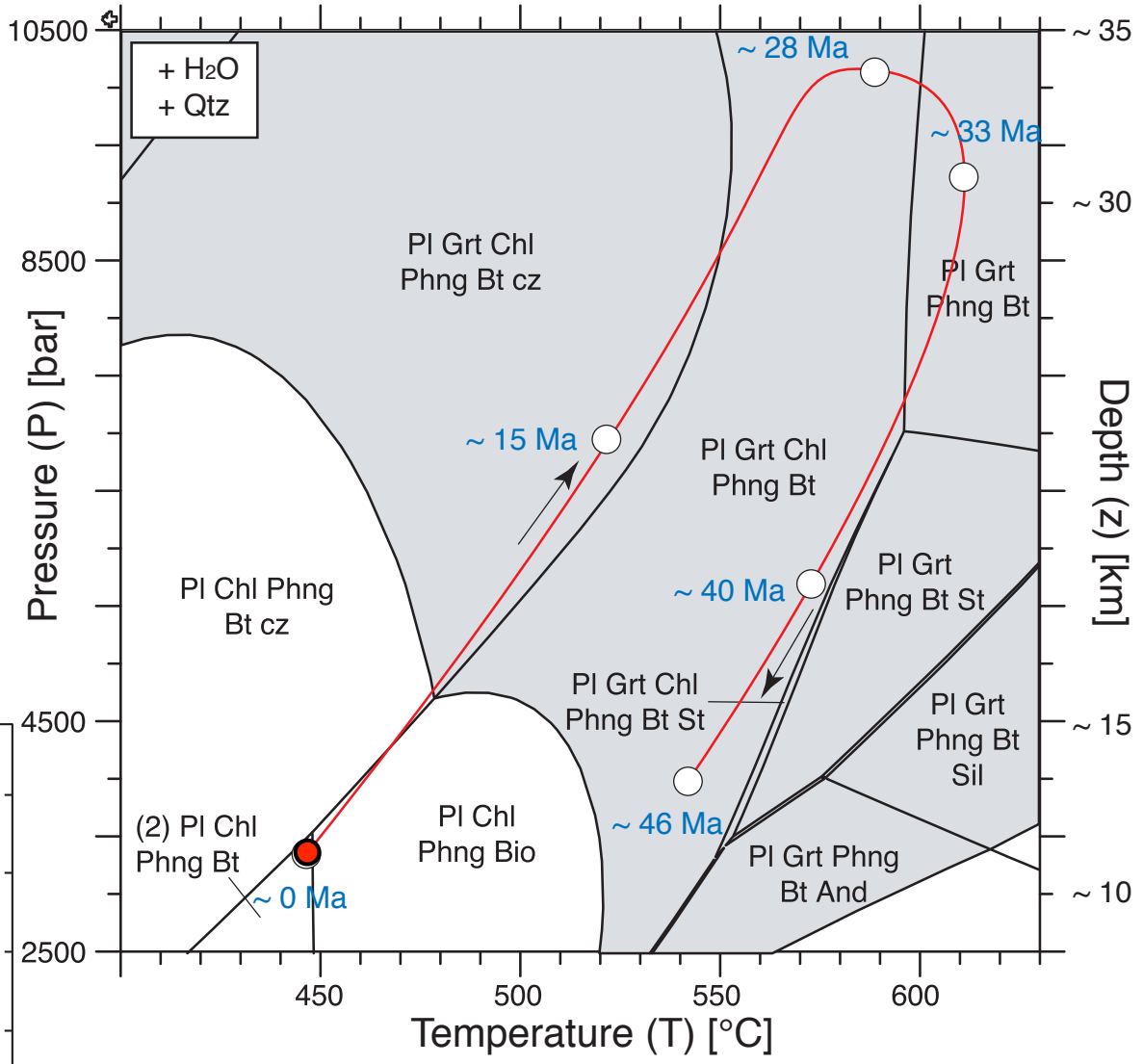


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

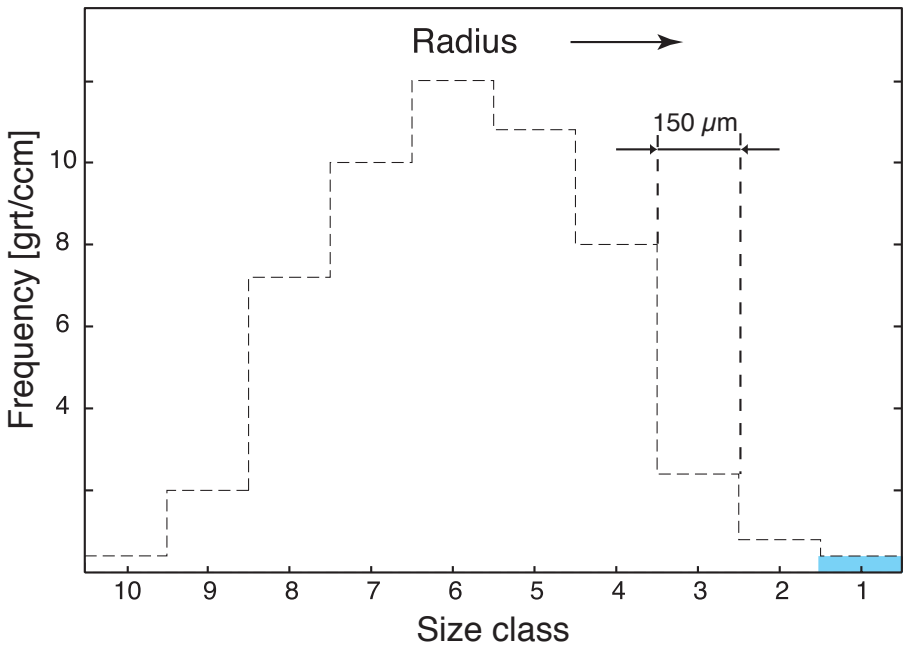


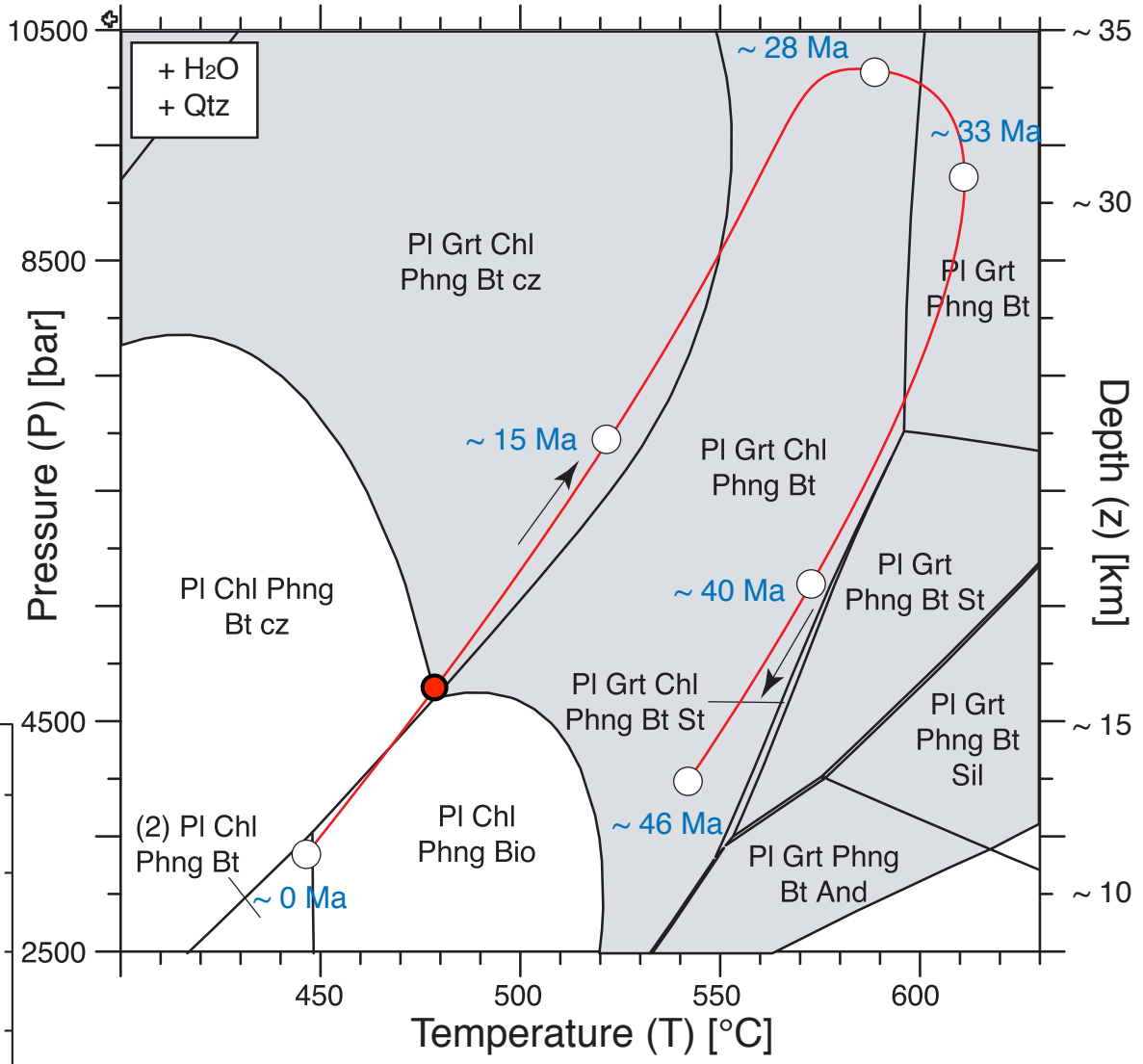


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)





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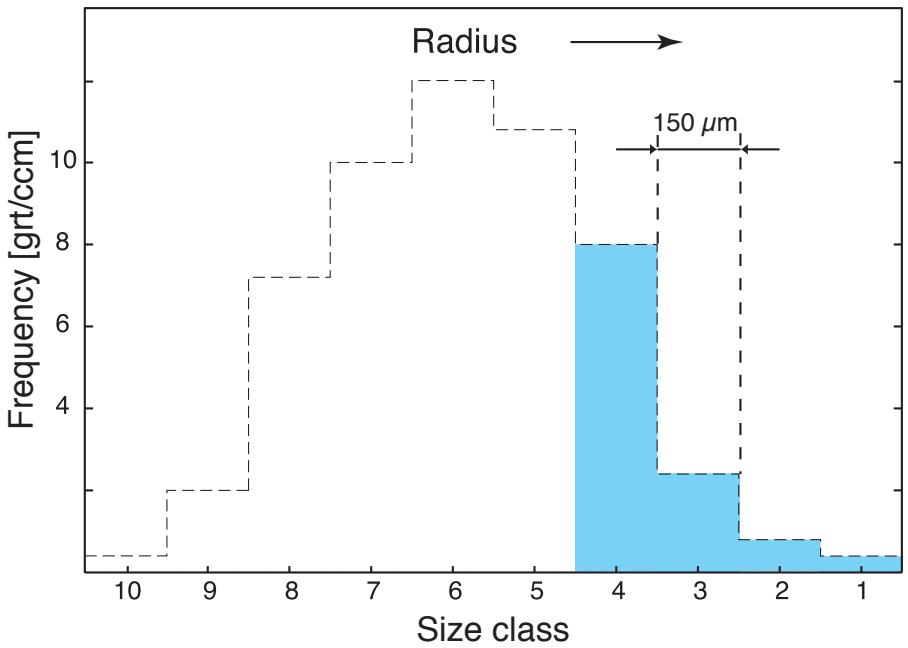
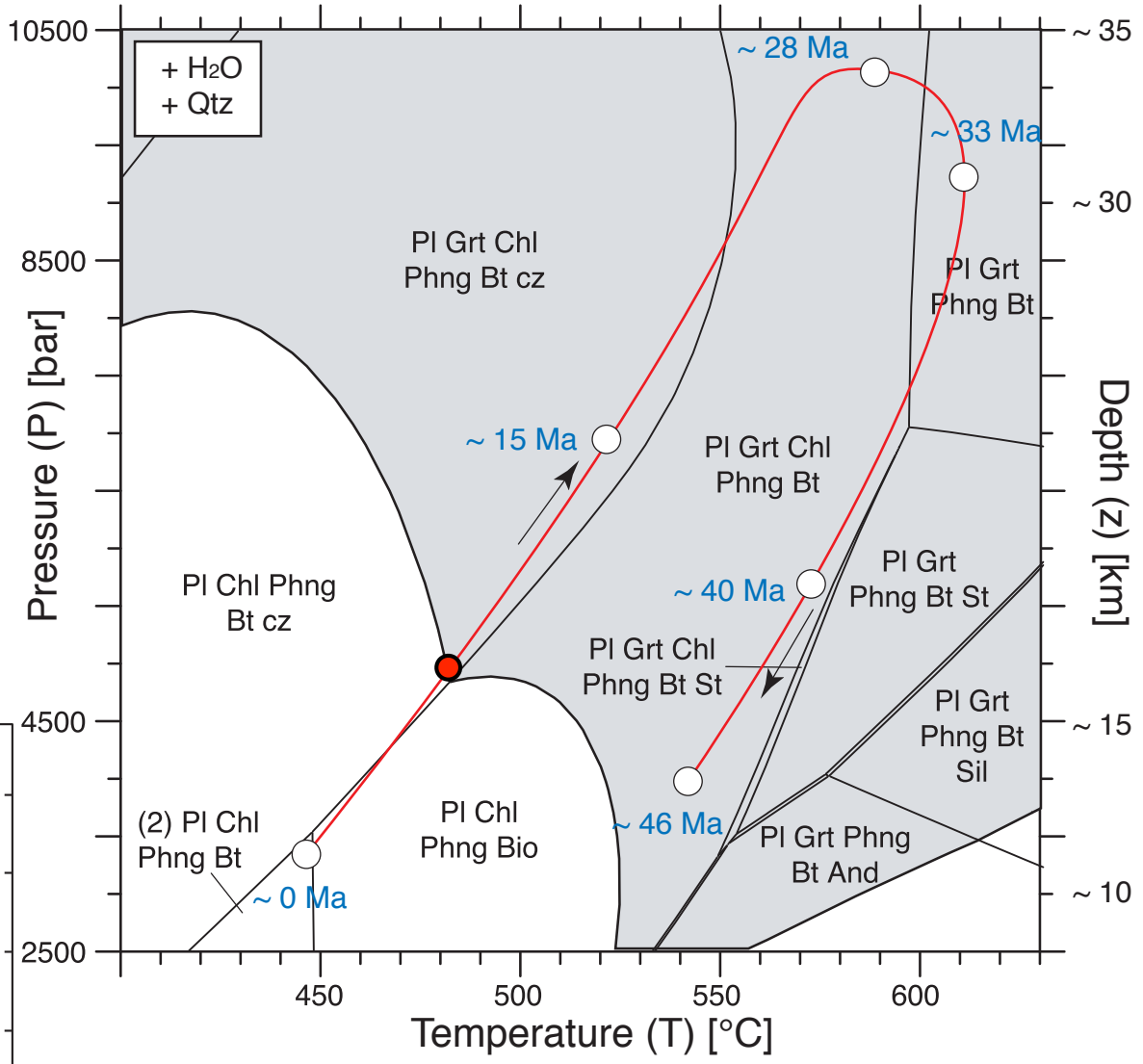
Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

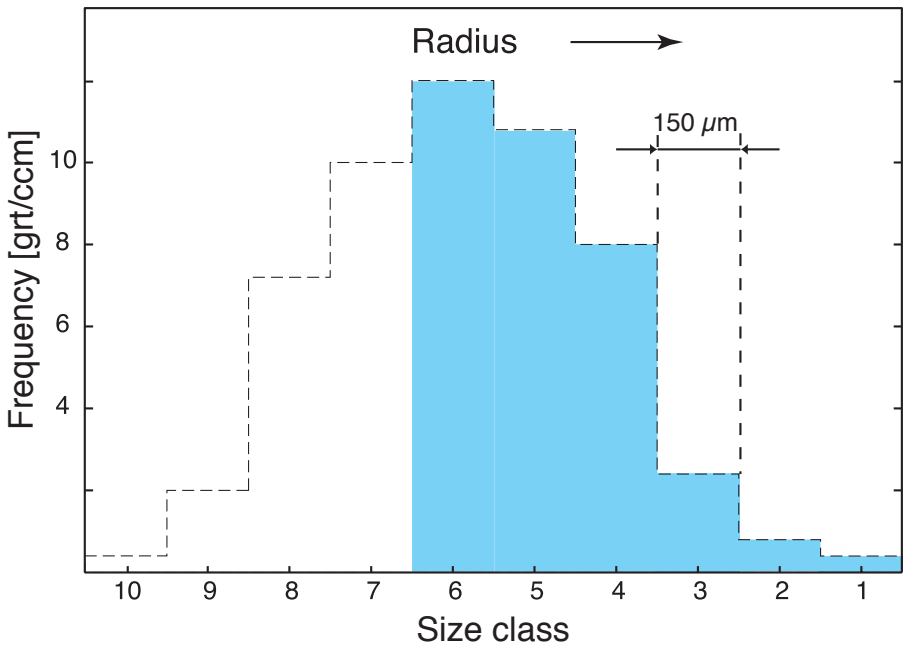


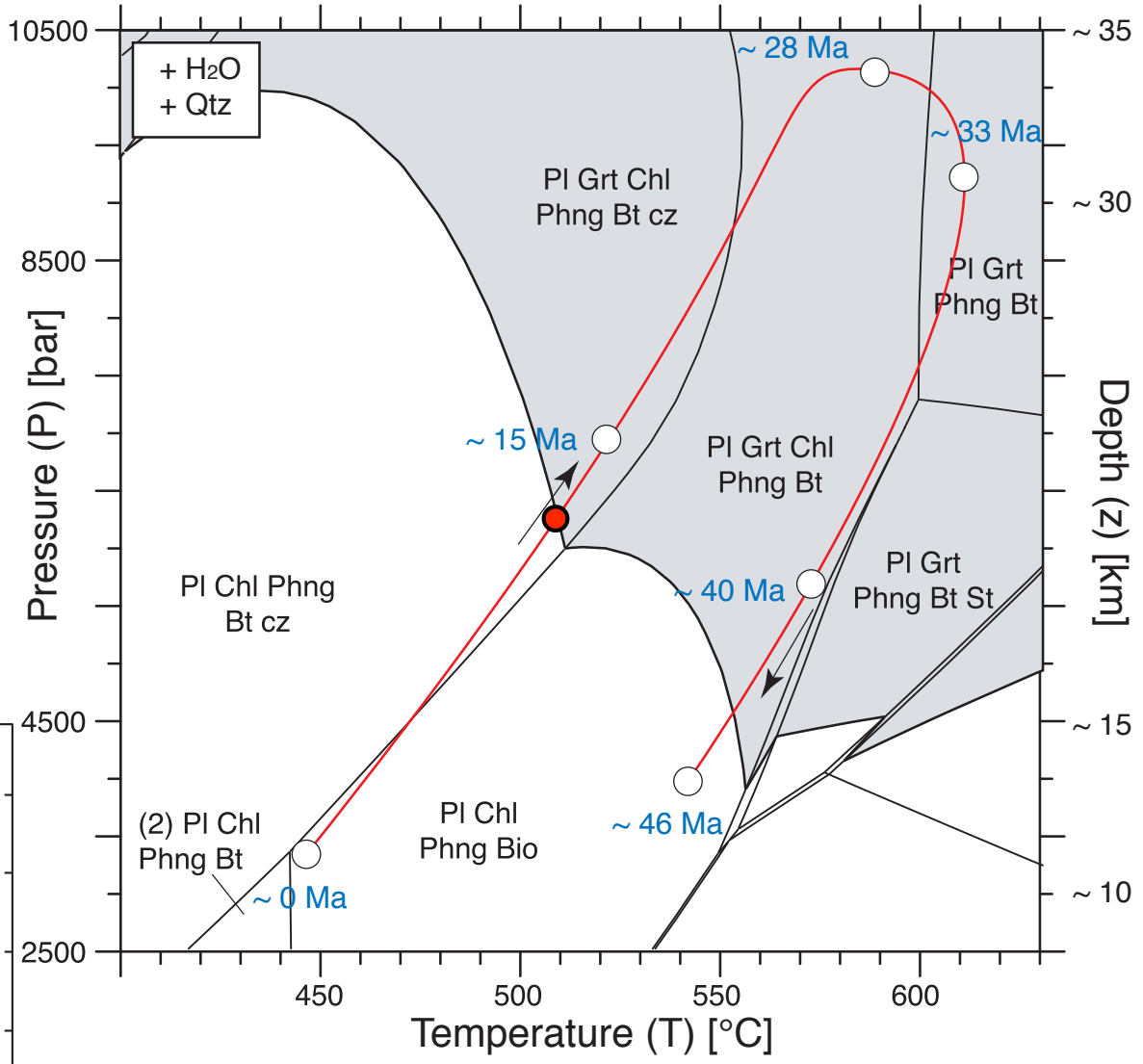


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

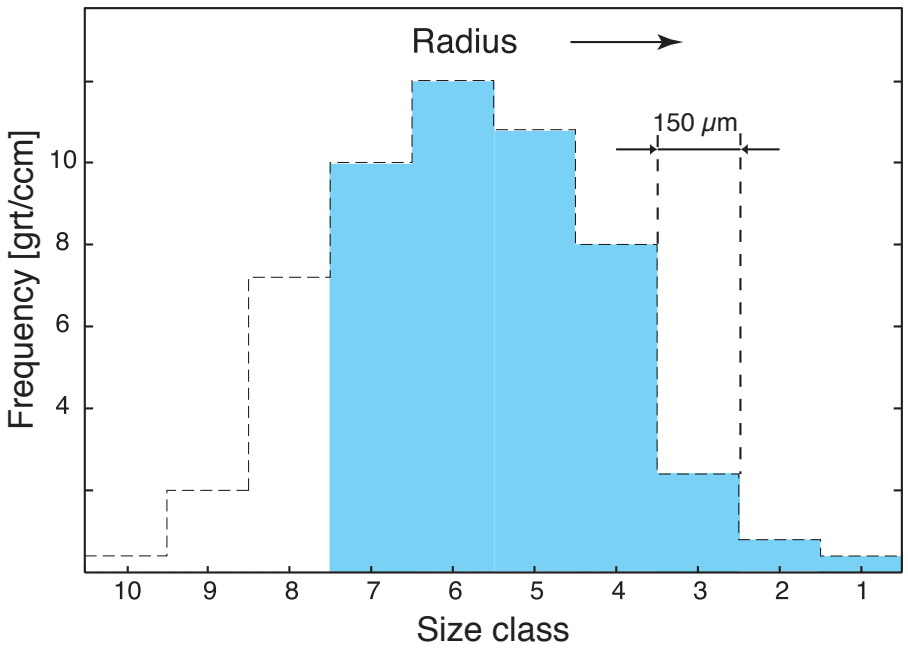


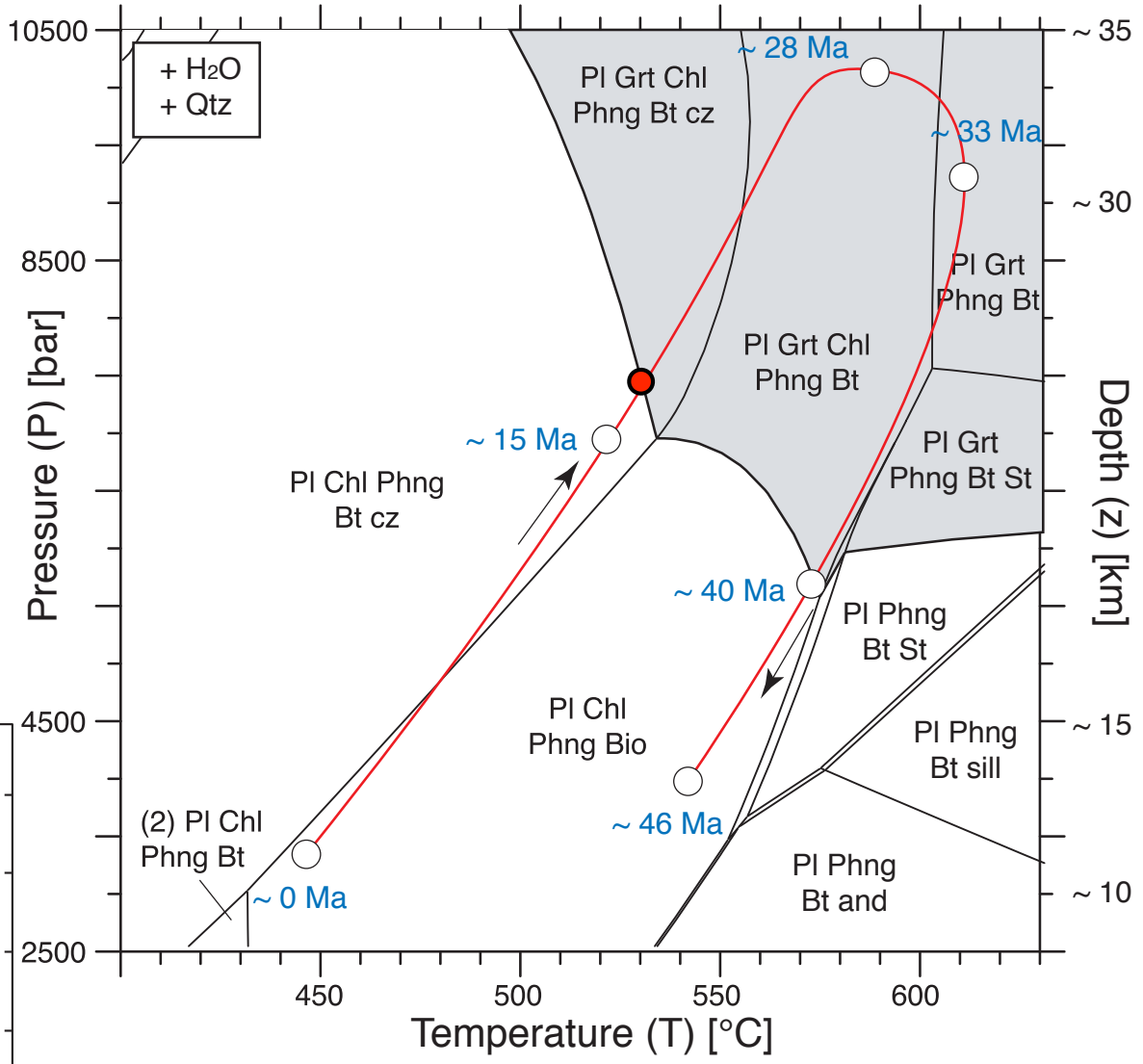


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

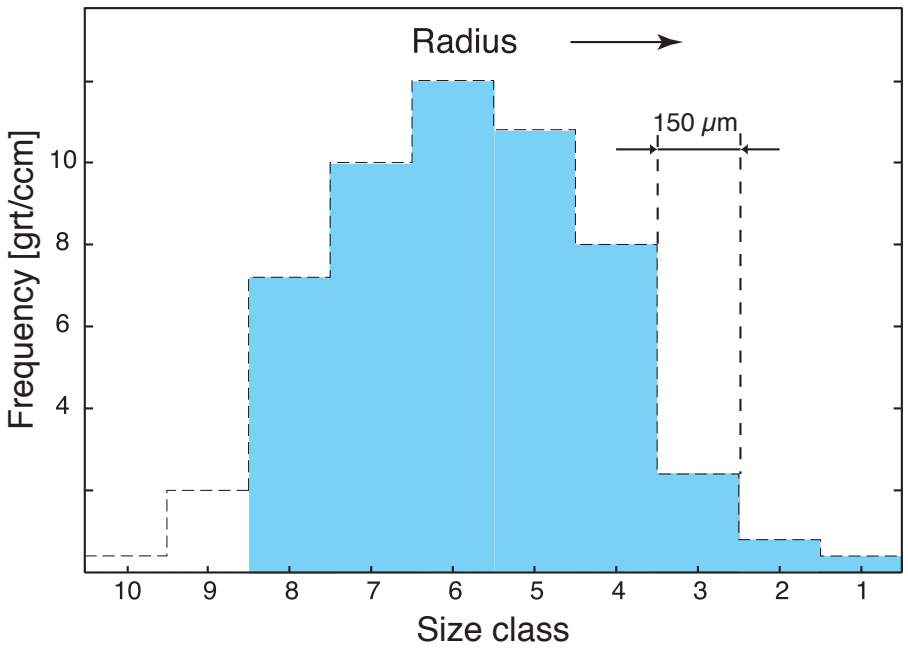


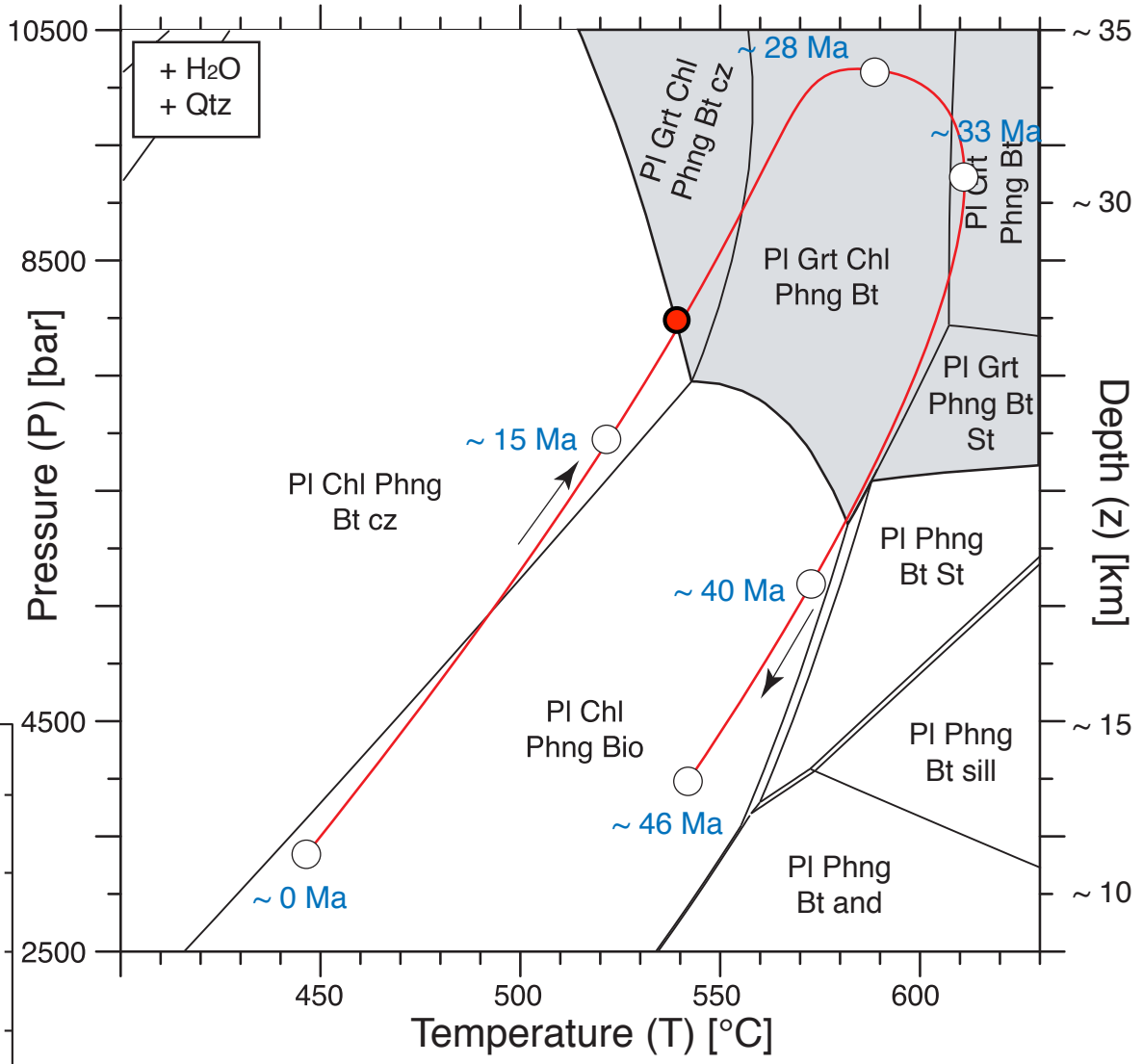


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

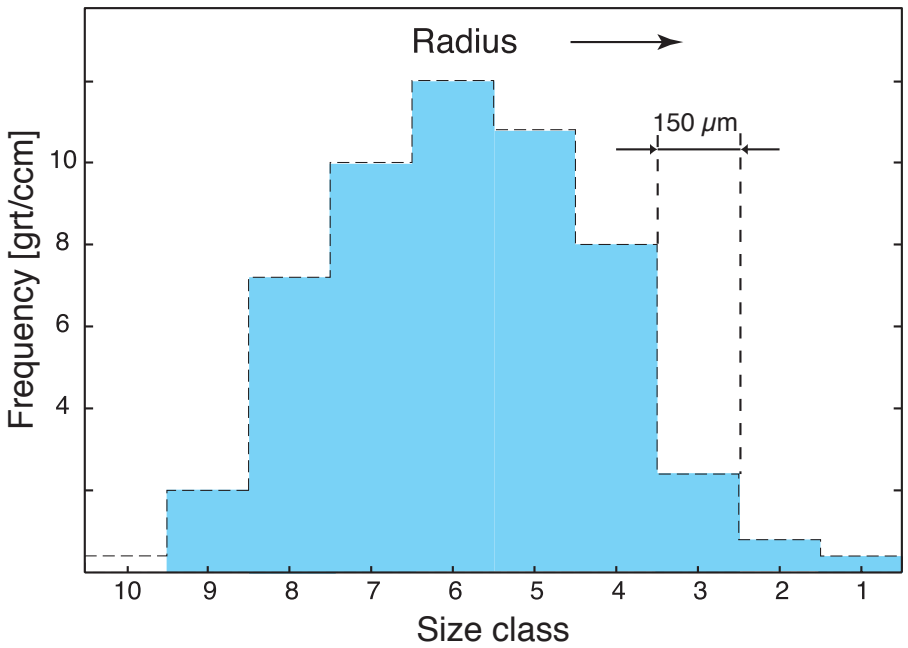


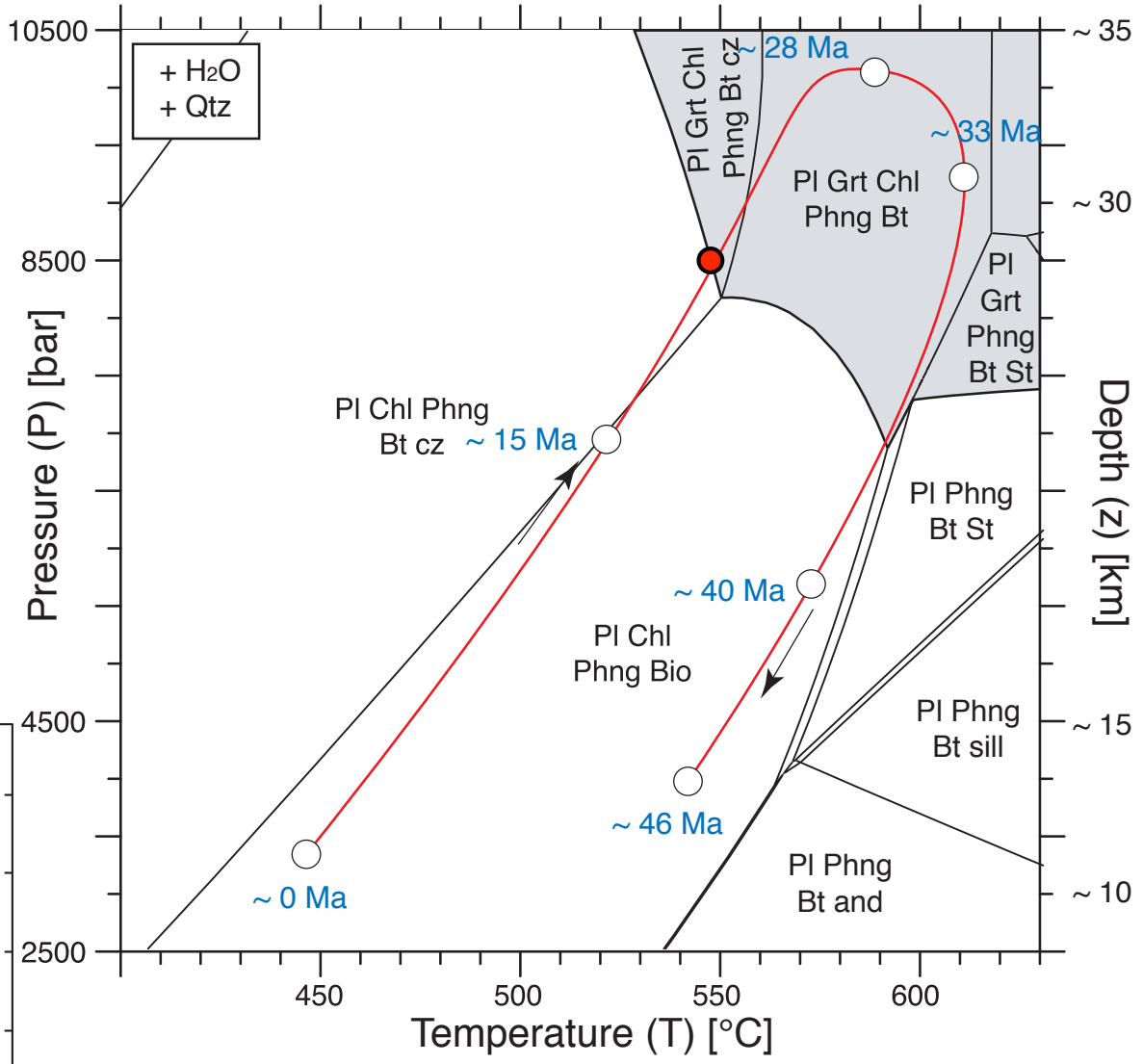


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

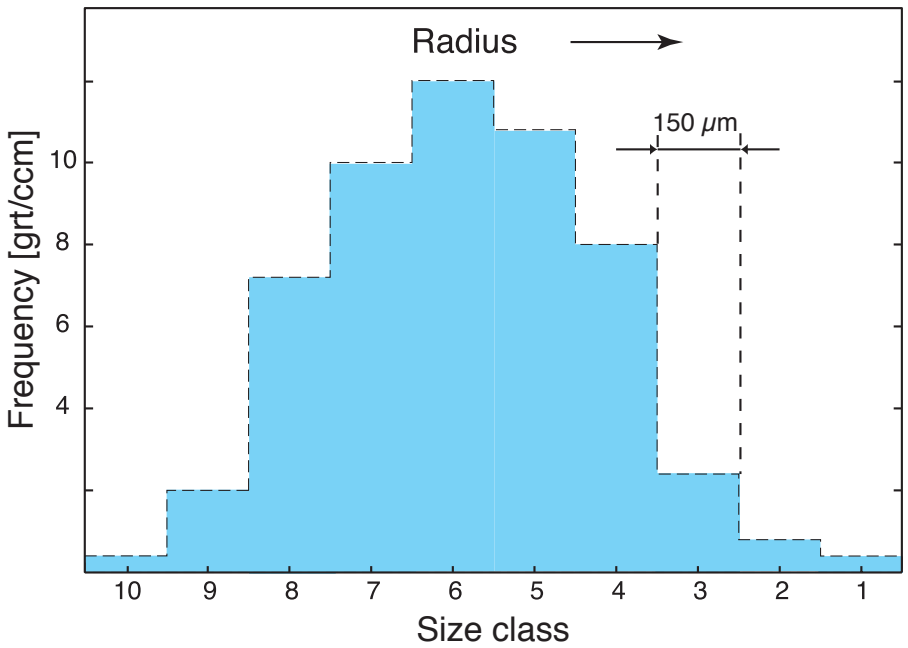


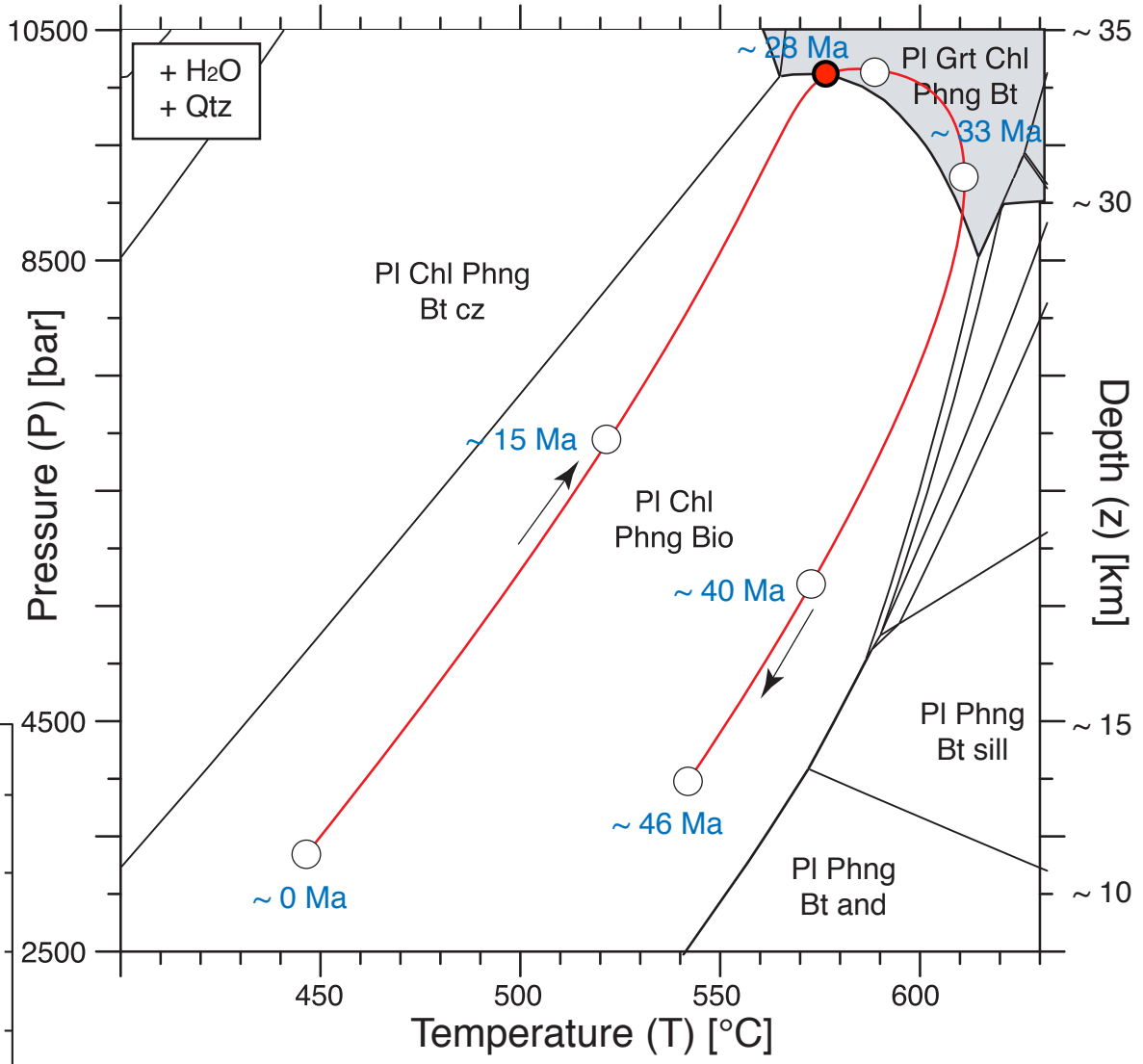


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

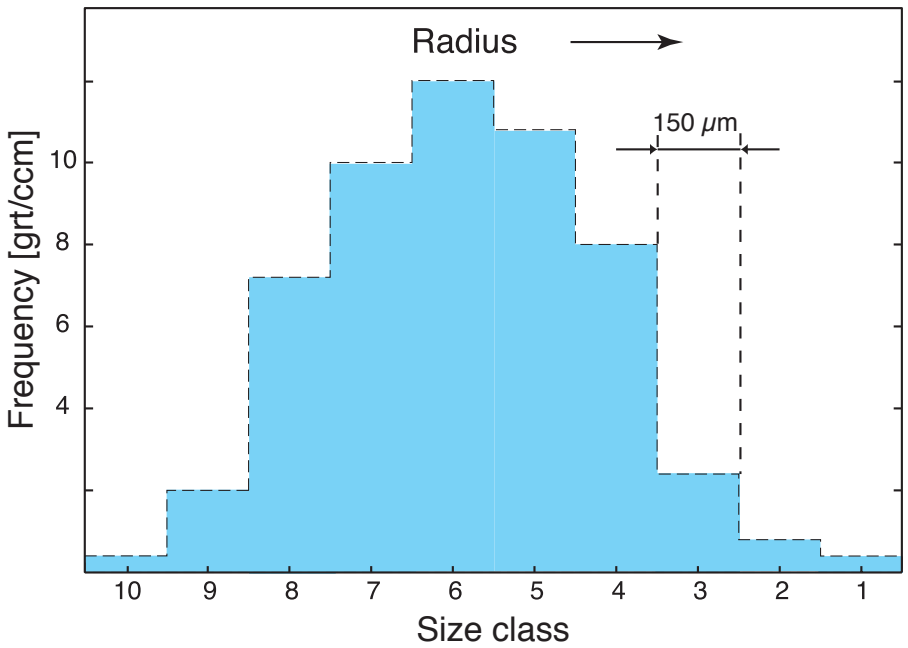


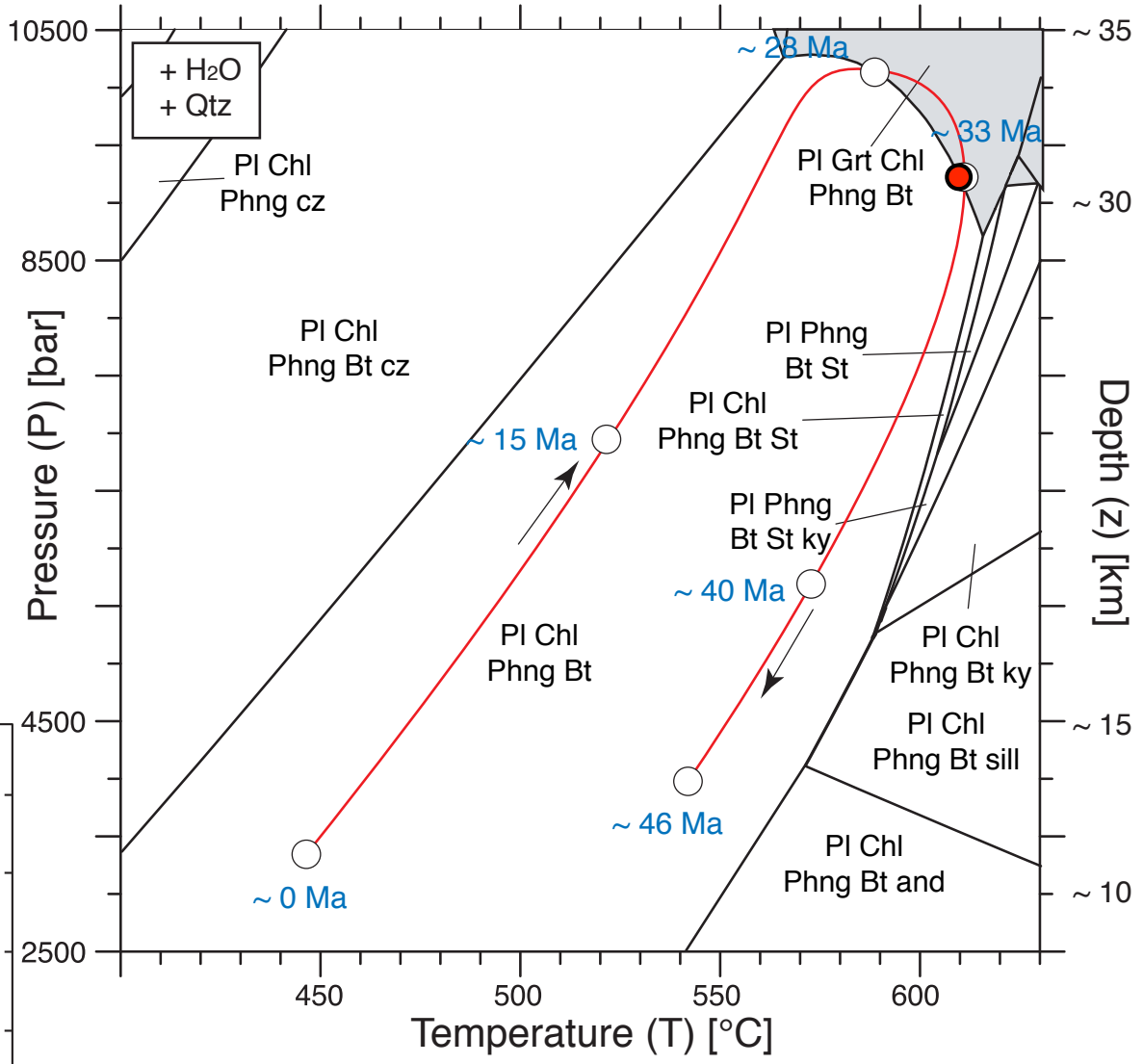


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

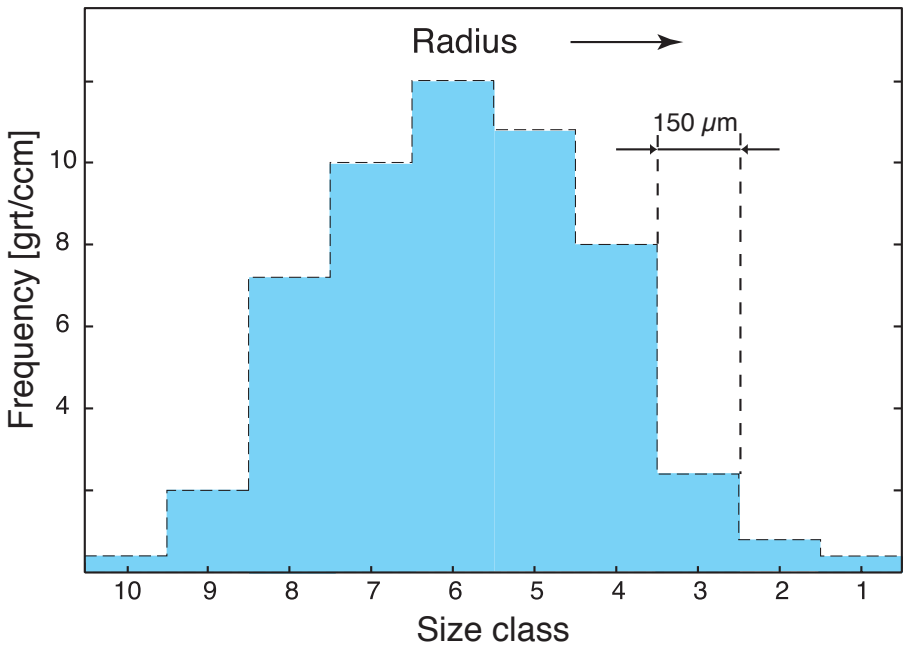


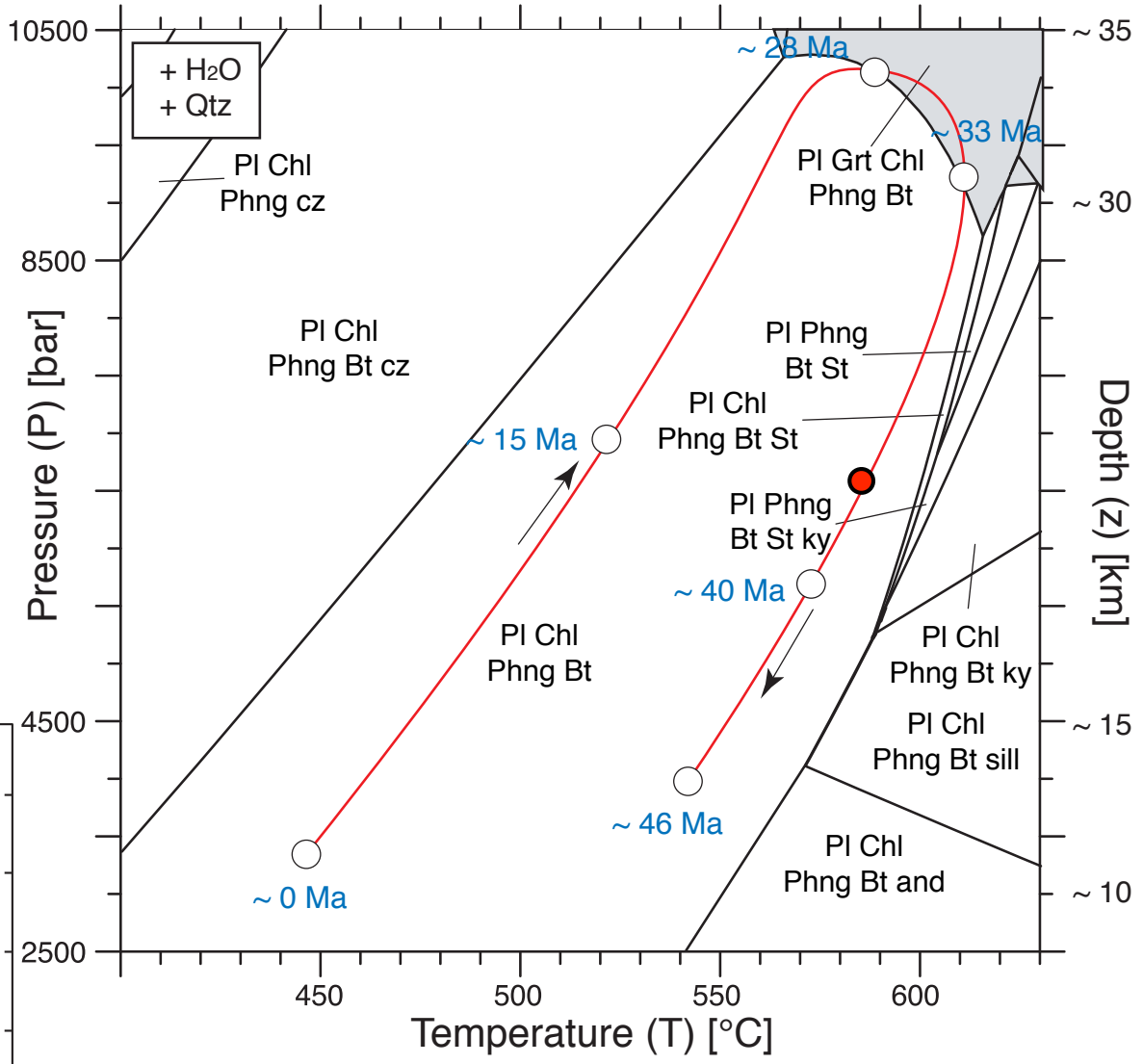


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)

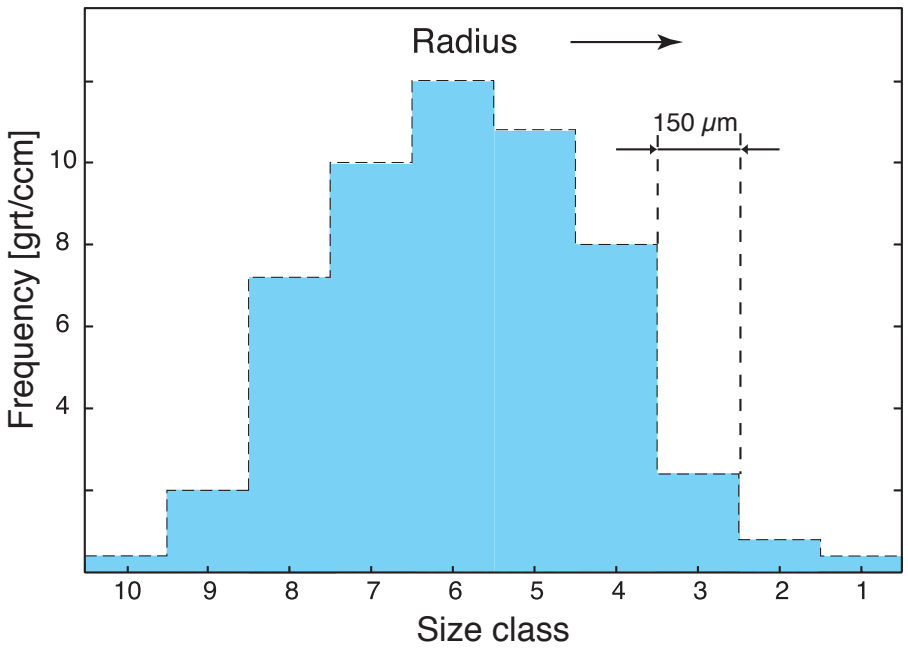


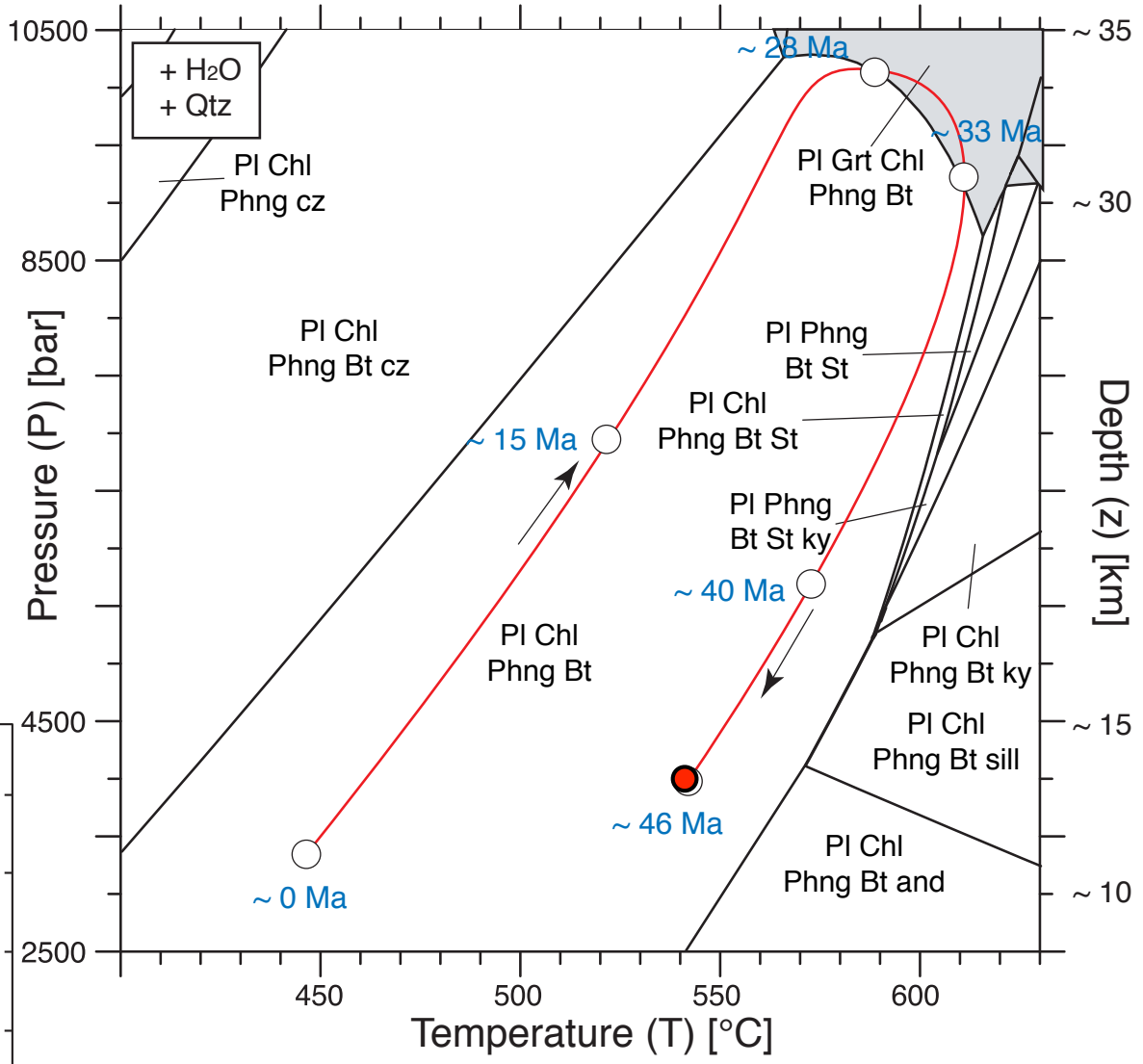


Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

(average metapelite, theoretical CSD)





Garnet crystallization modelling with THERIA_G

Chemical fractionation, nucleation, growth

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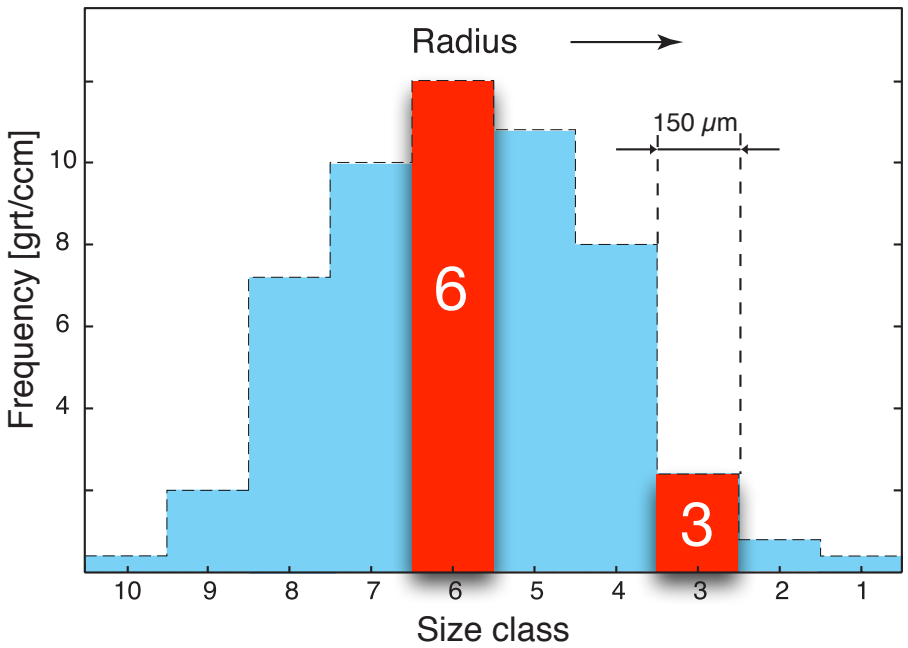

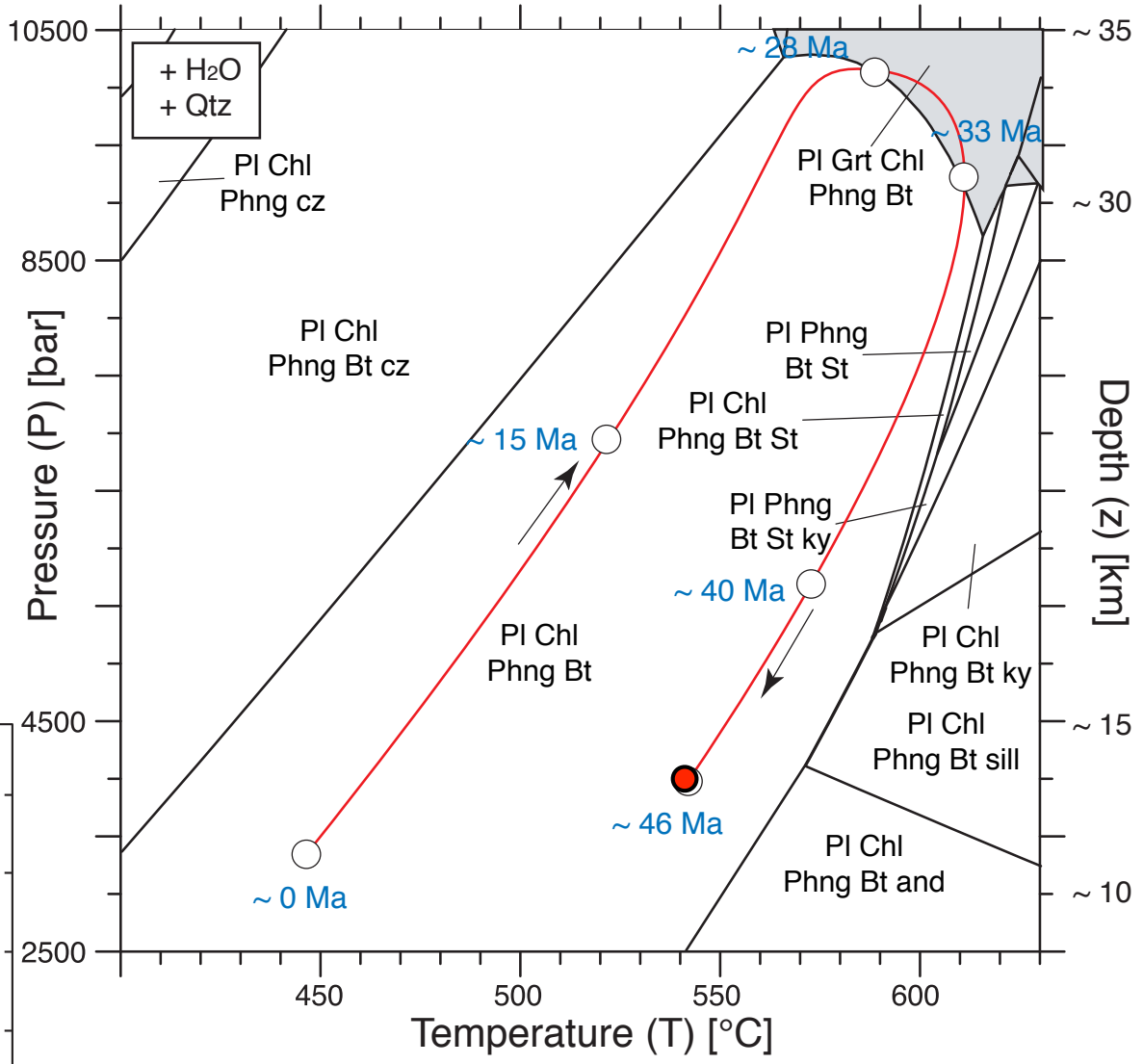

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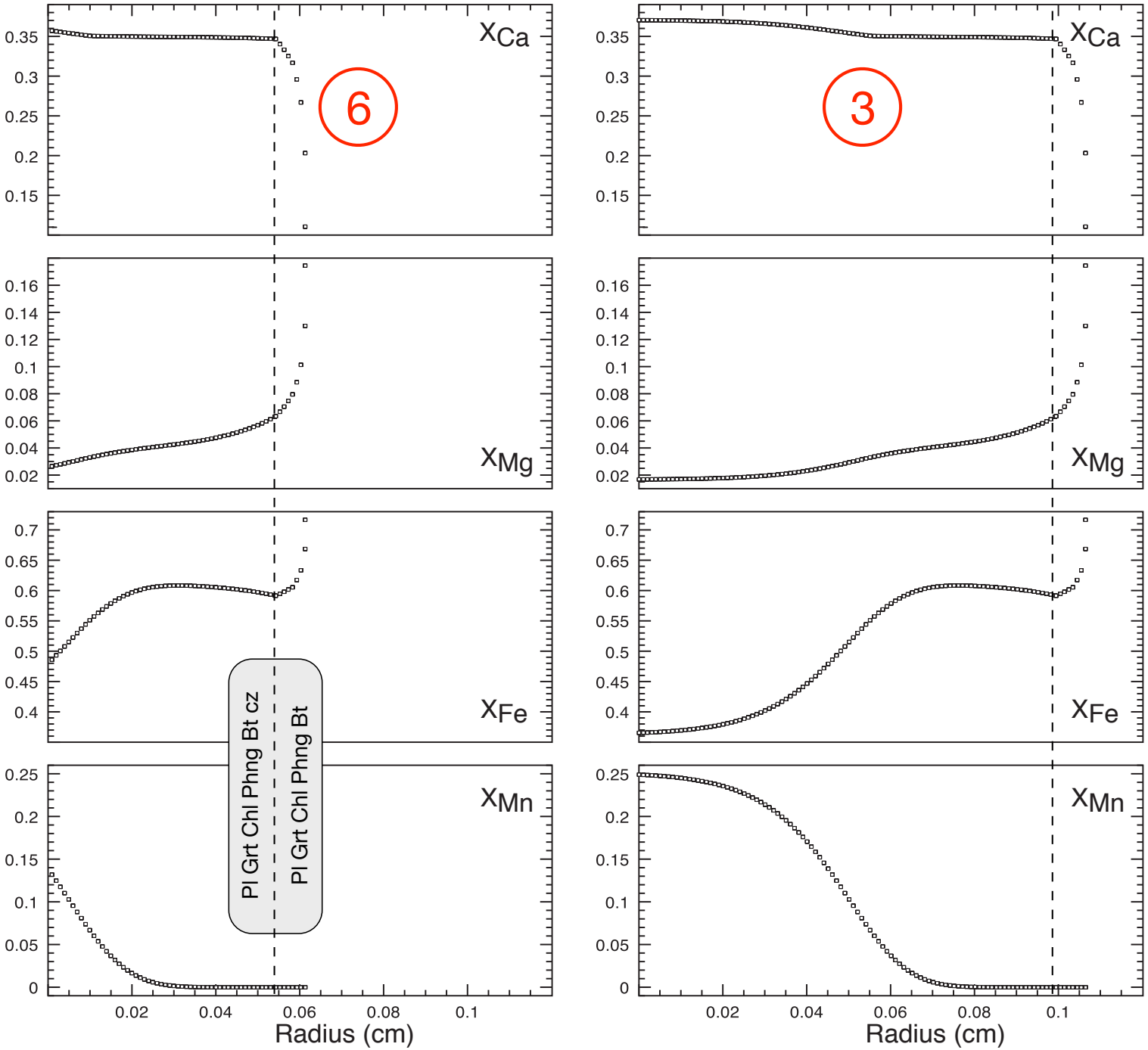
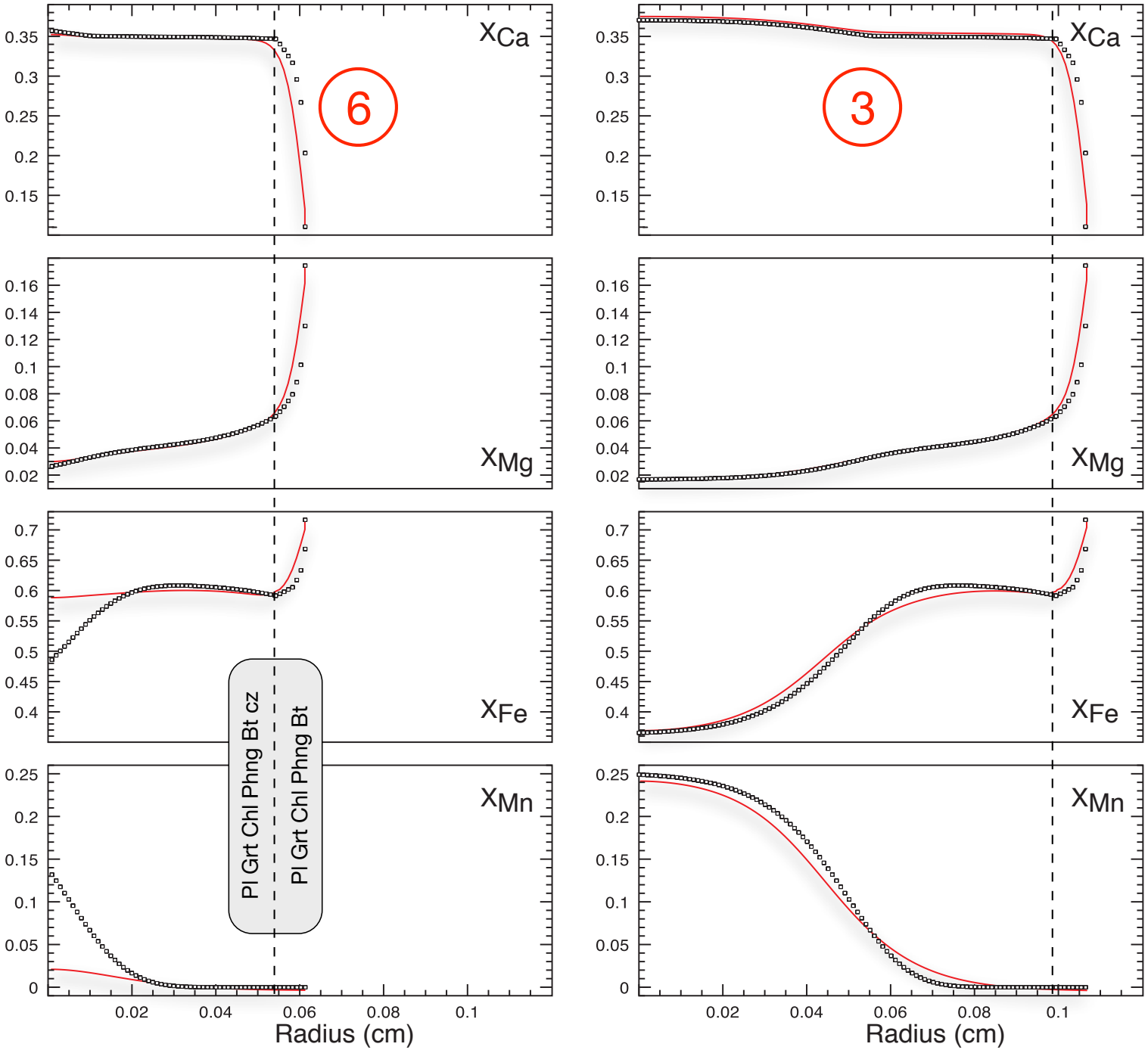
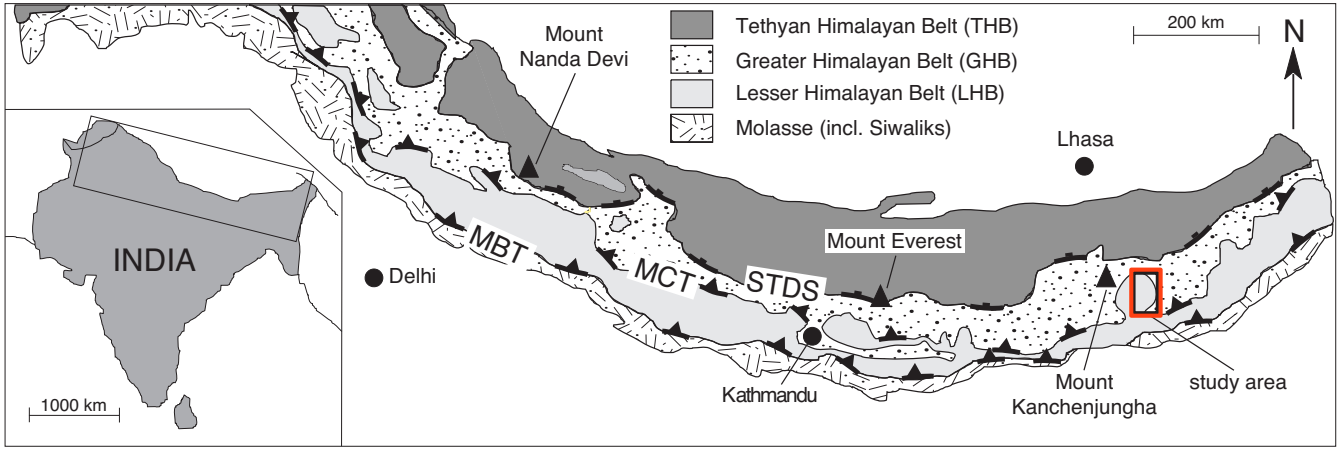


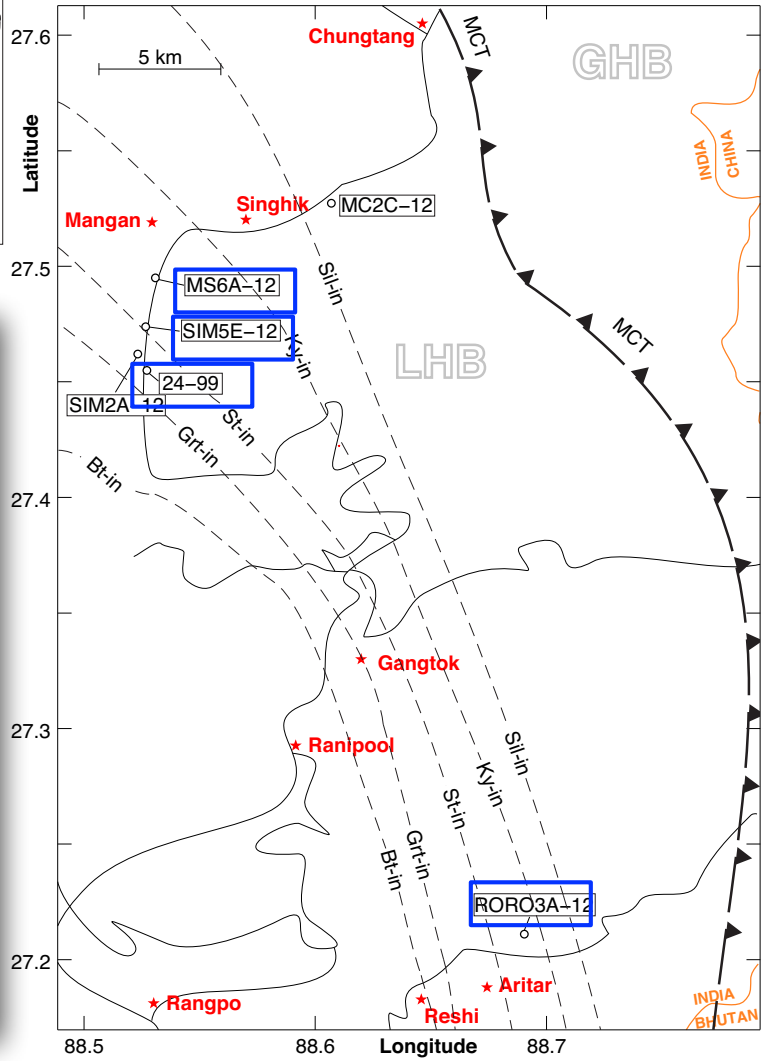
Garnet crystallization modelling with THERIA_G



Garnet crystallization modelling with THERIA_G - Example

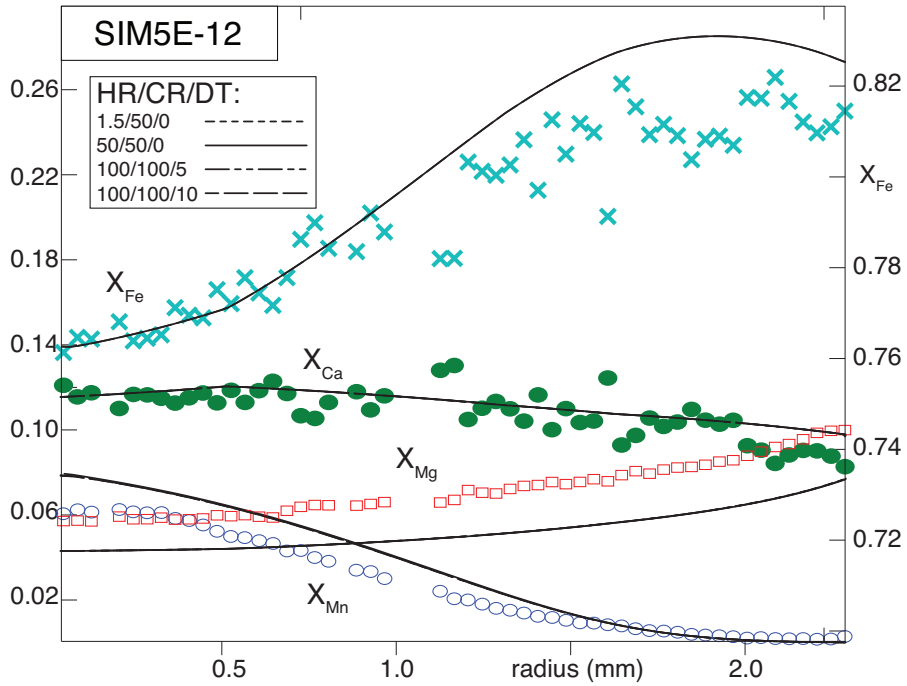
Lesser Himalayan Belt, Sikkim, India

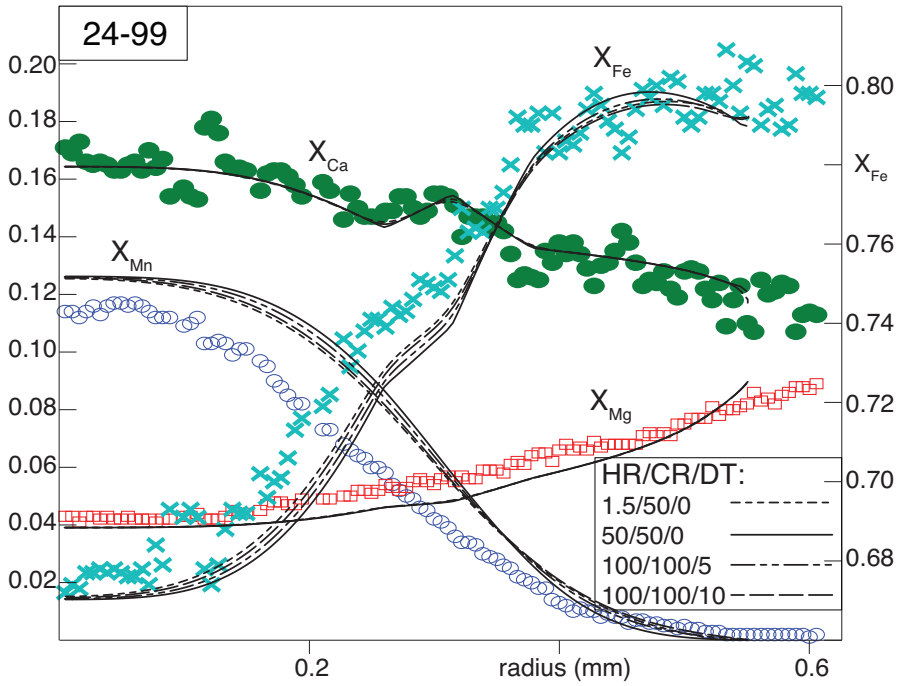


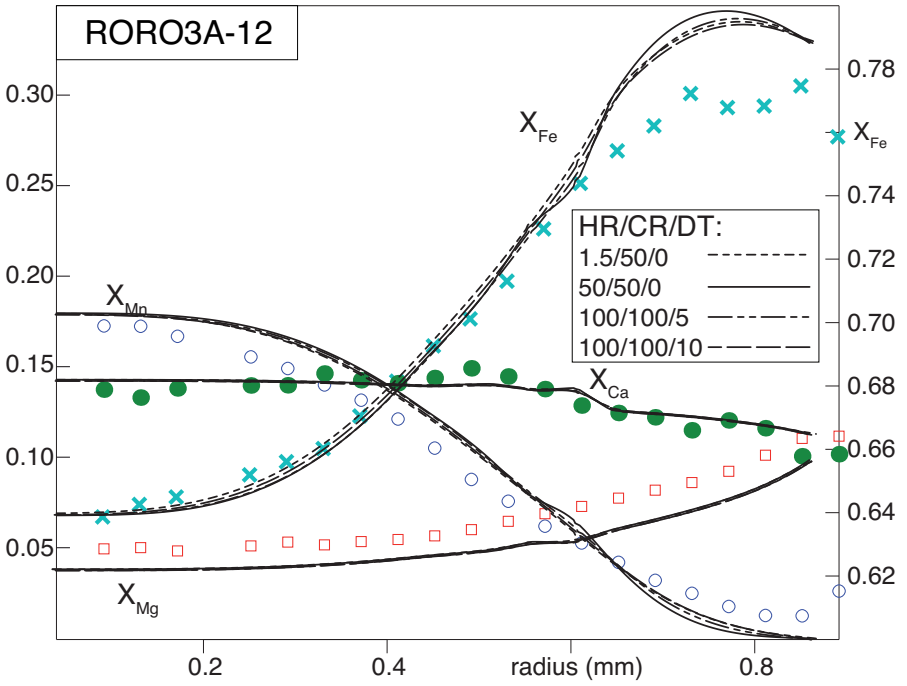


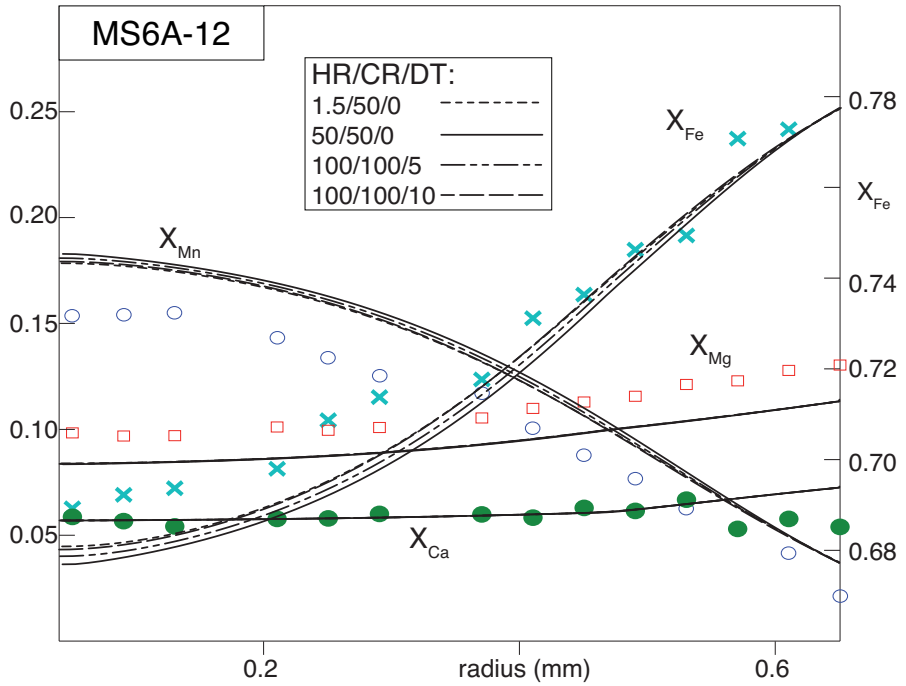
Gaidies et al. (2015)

Garnet crystallization modelling with THERIA_G - Example



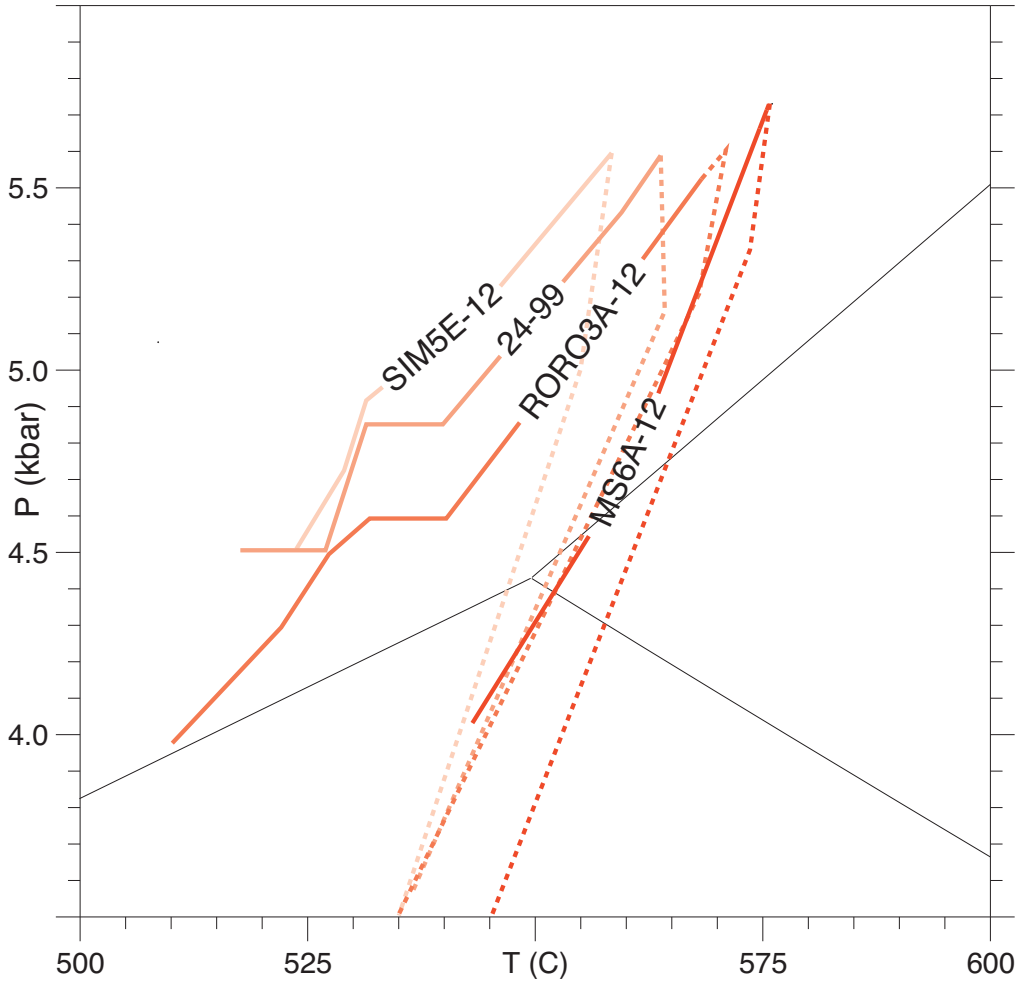




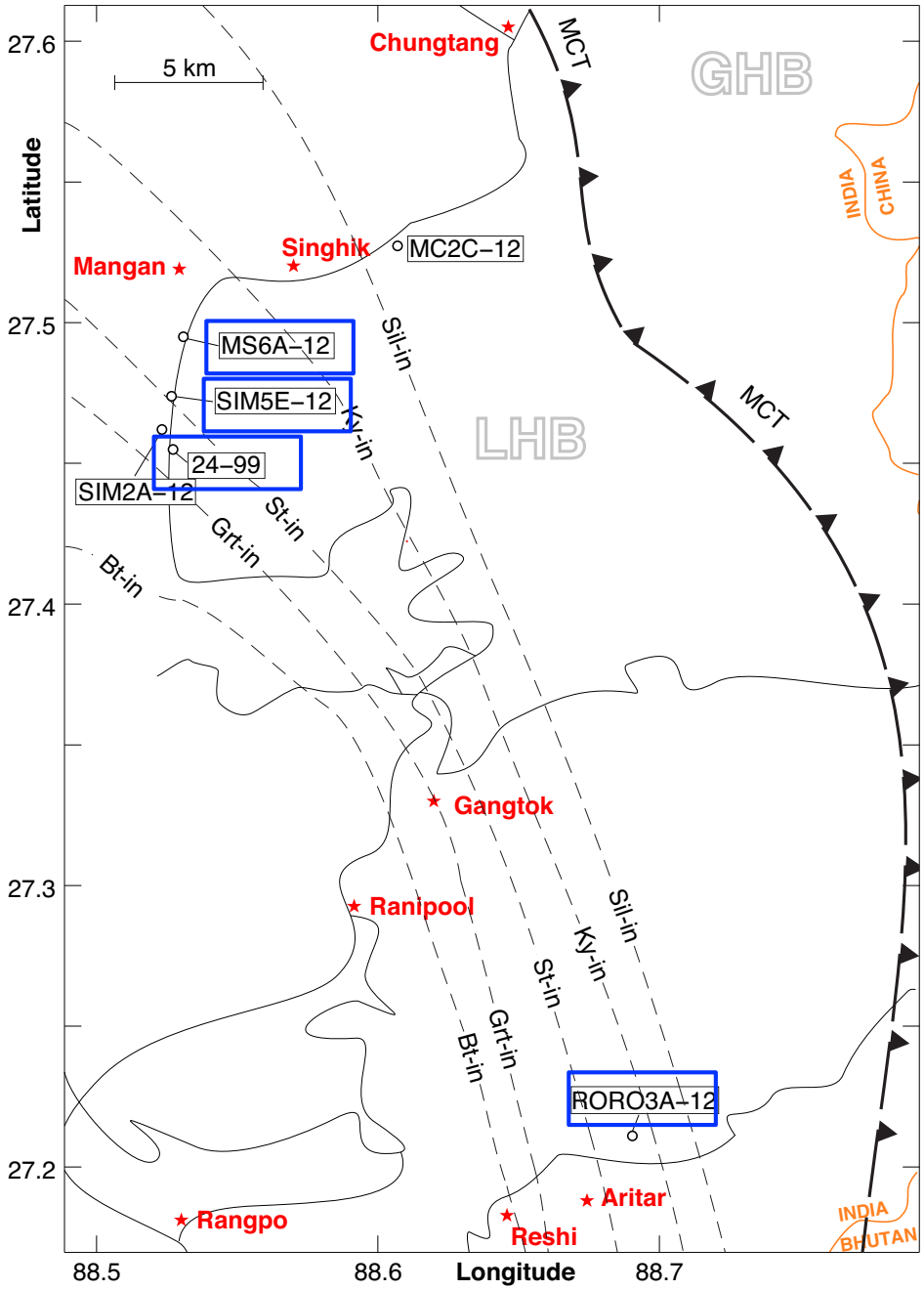


Garnet crystallization modelling with THERIA_G - Example

Lesser Himalayan Belt, Sikkim, India

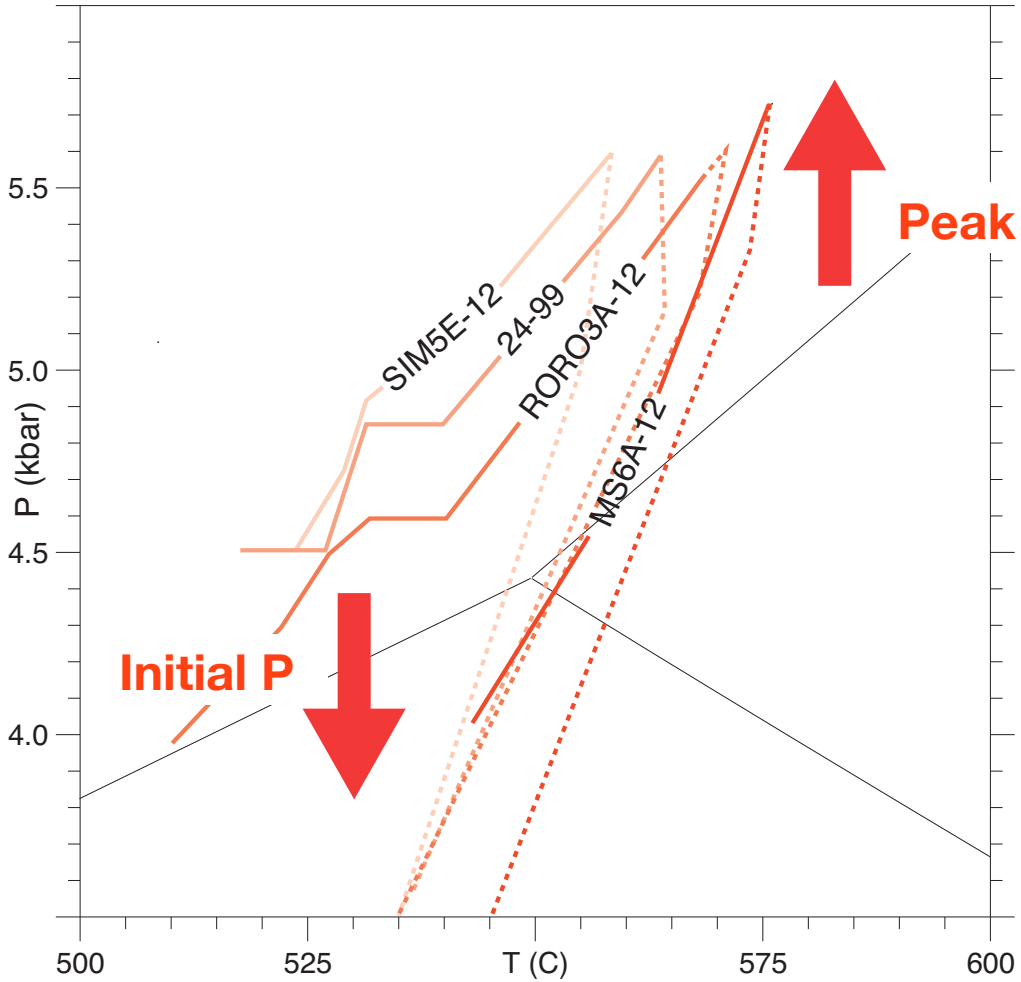


Gaidies et al. (2015)



Garnet crystallization modelling with THERIA_G - Example

Lesser Himalayan Belt, Sikkim, India



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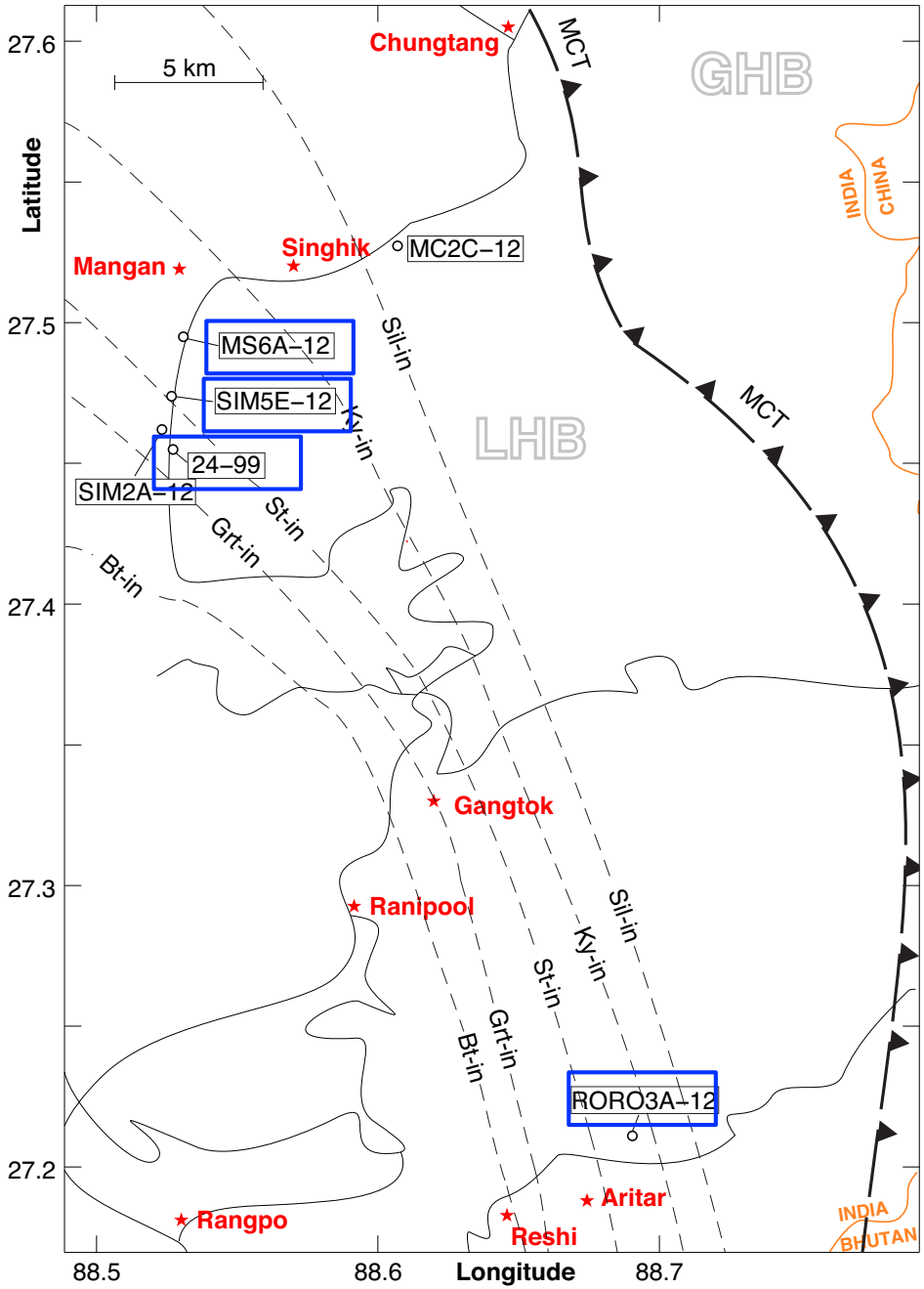
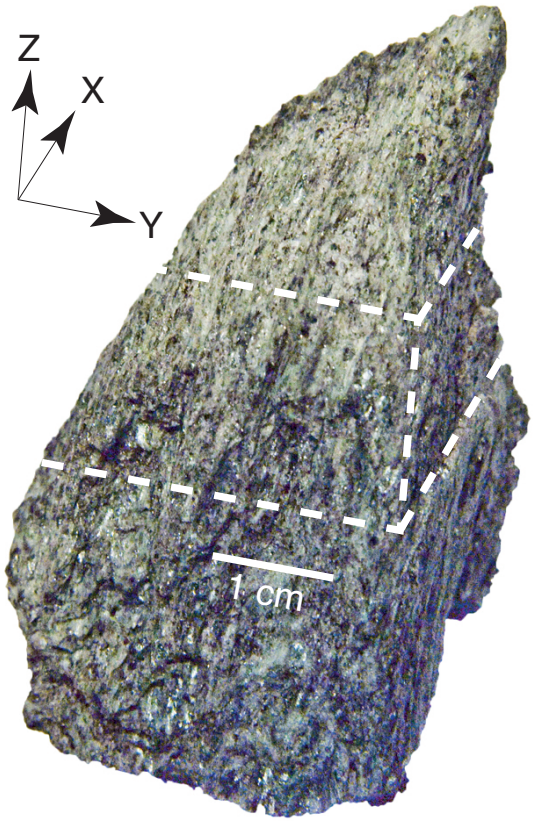
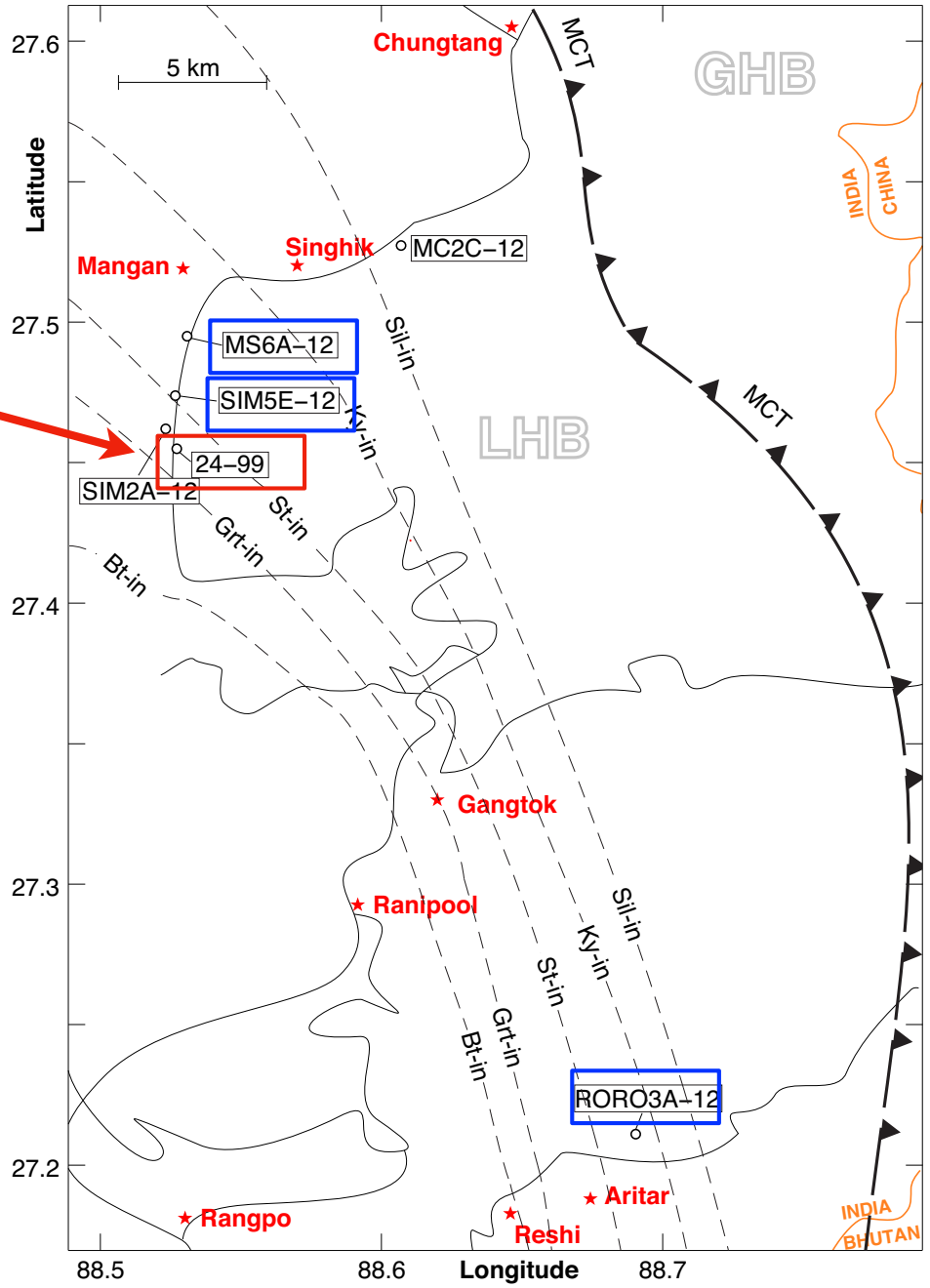
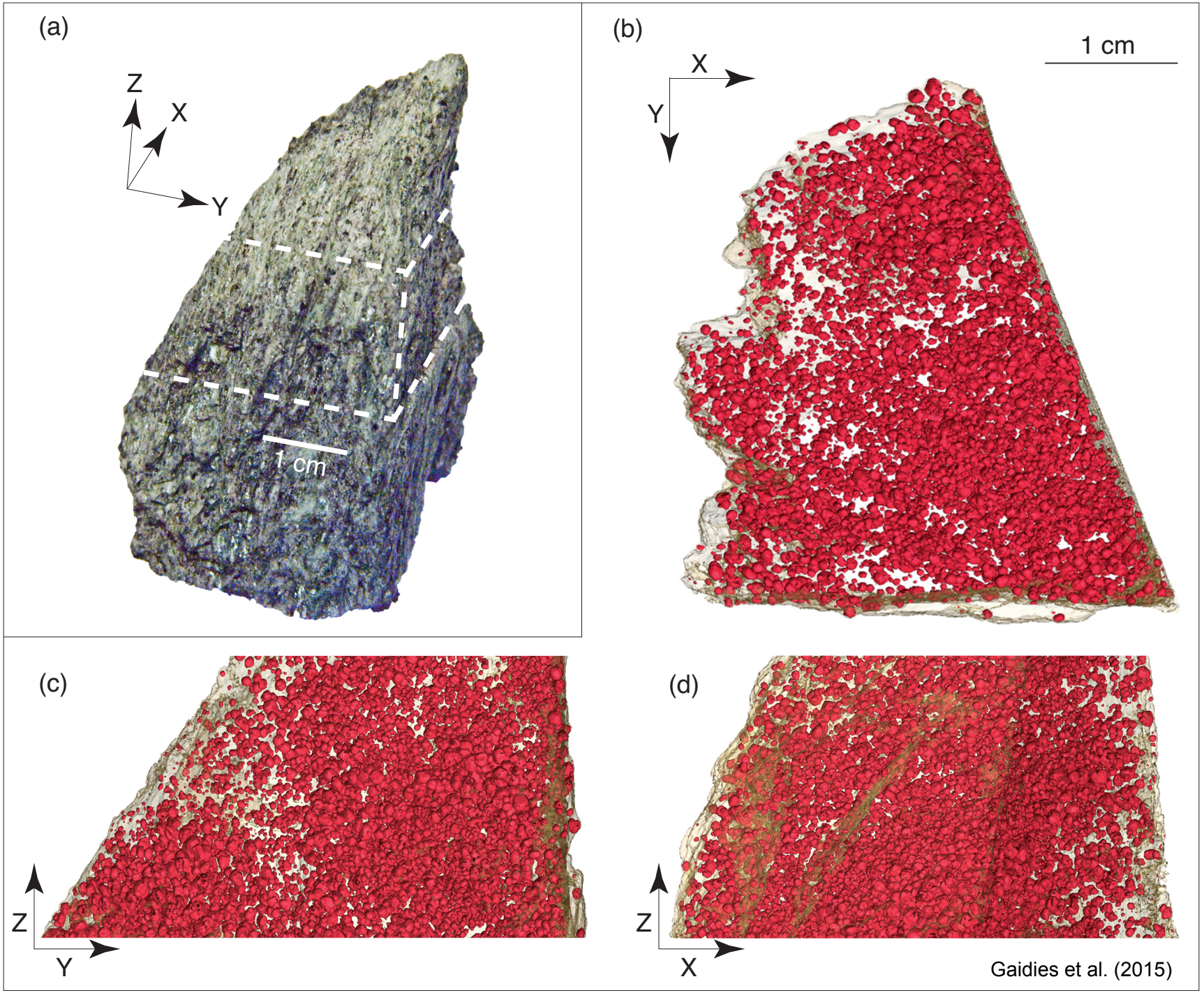


Garnet crystallization modelling with THERIA_G - Example



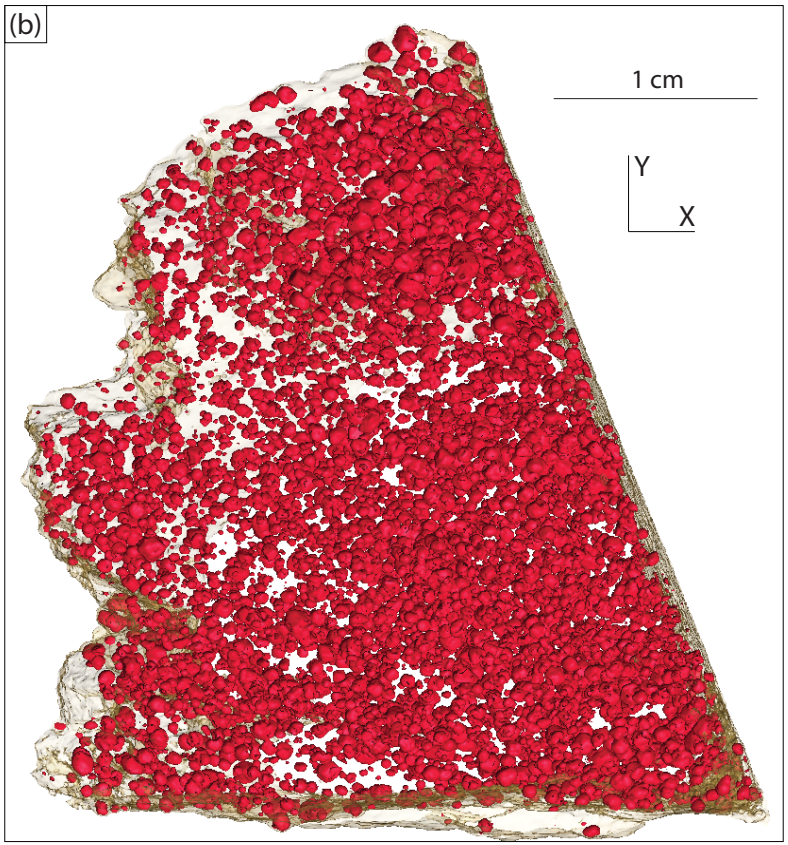


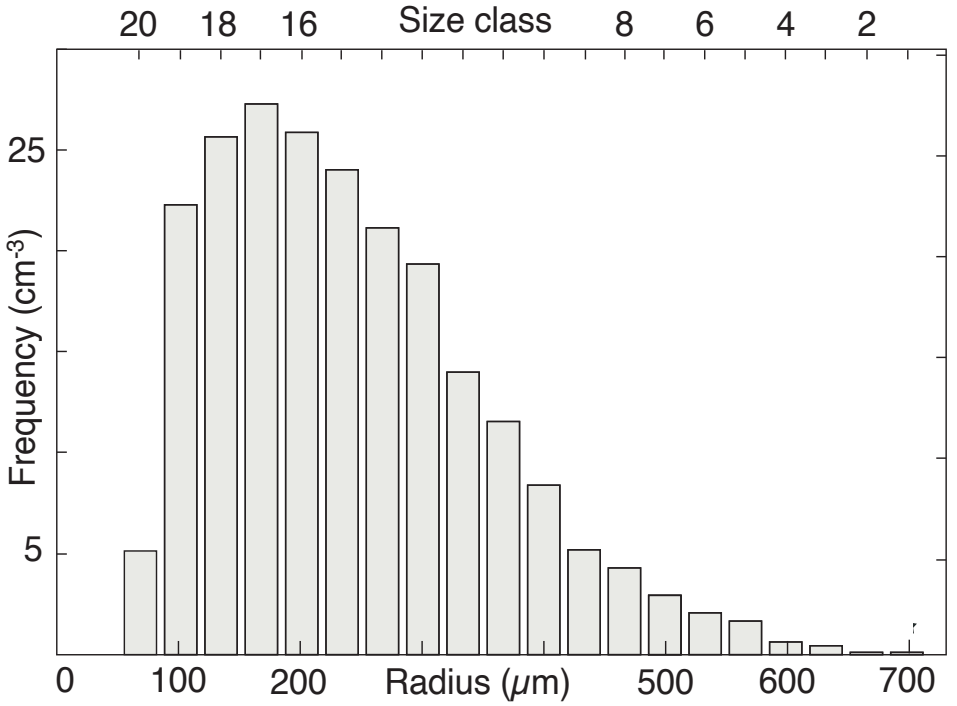
Garnet crystallization modelling with THERIA_G - Example

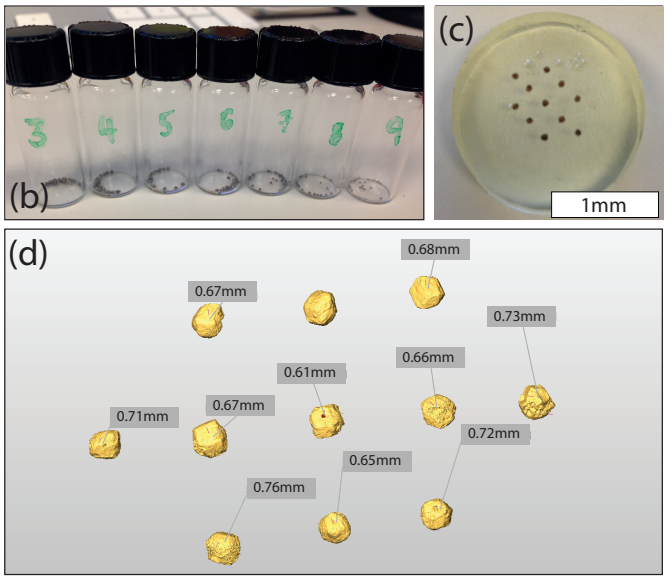


Garnet crystallization modelling with THERIA_G - Example

High-resolution X-ray μ
Computed tomography

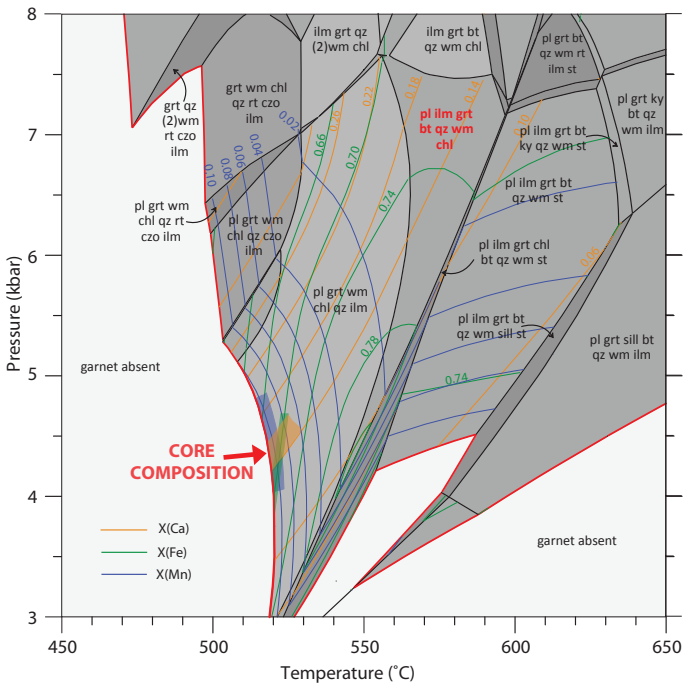




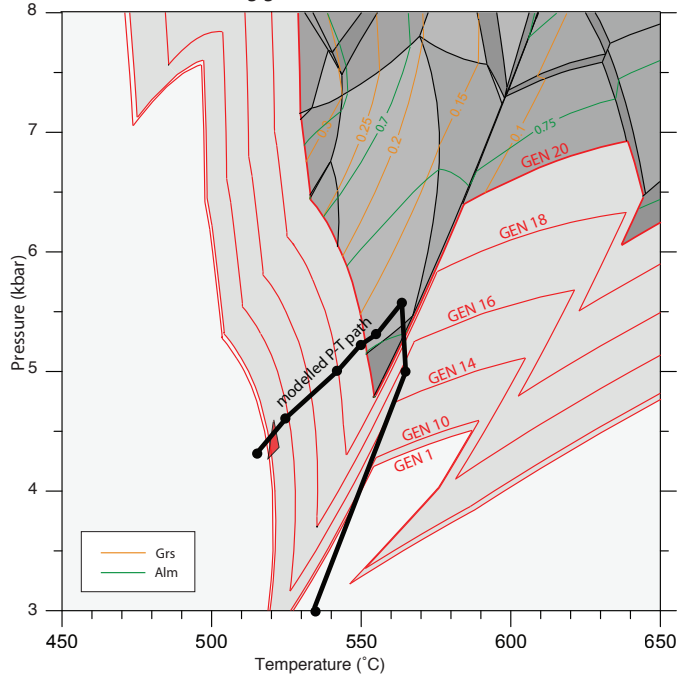


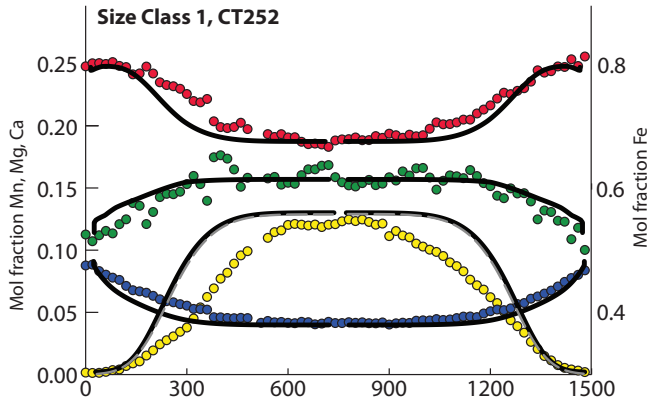
George & Gaidies (2017)

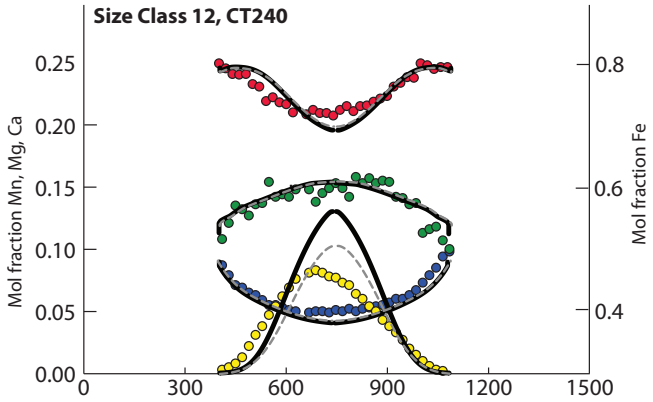
Garnet crystallization modelling with THERIA_G - Example

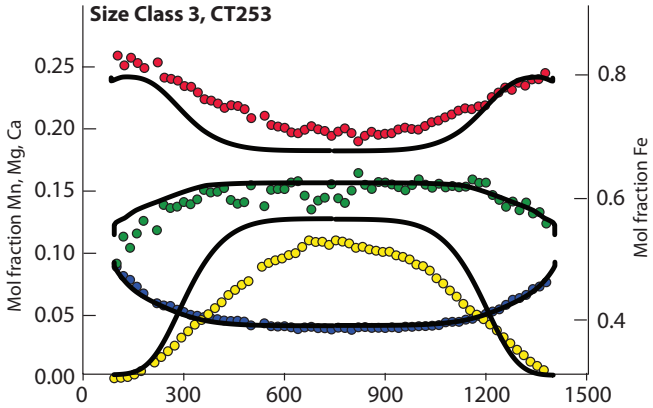


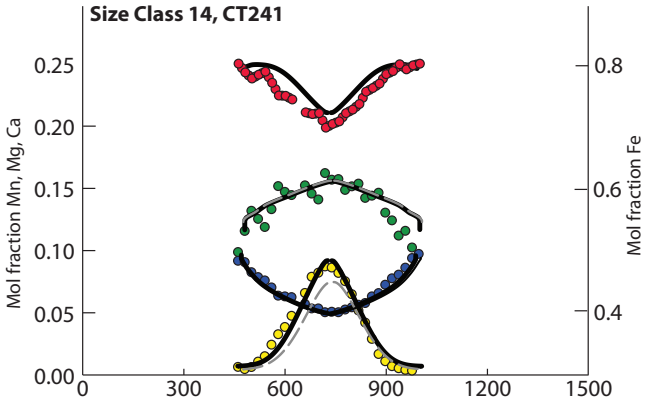
(d) 24-99 fractionating garnet-in

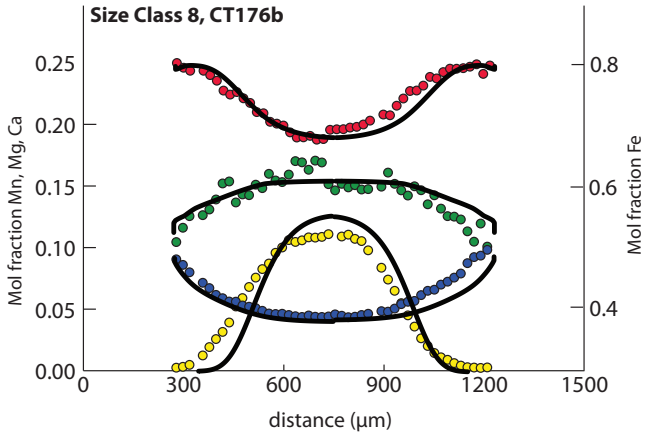


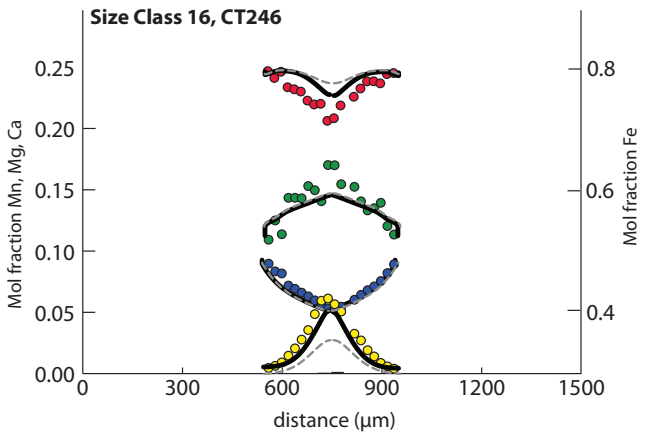






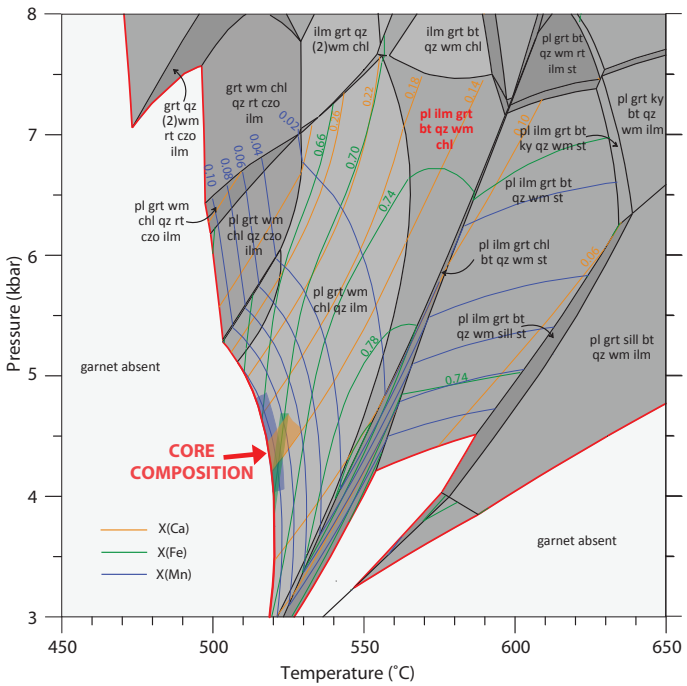




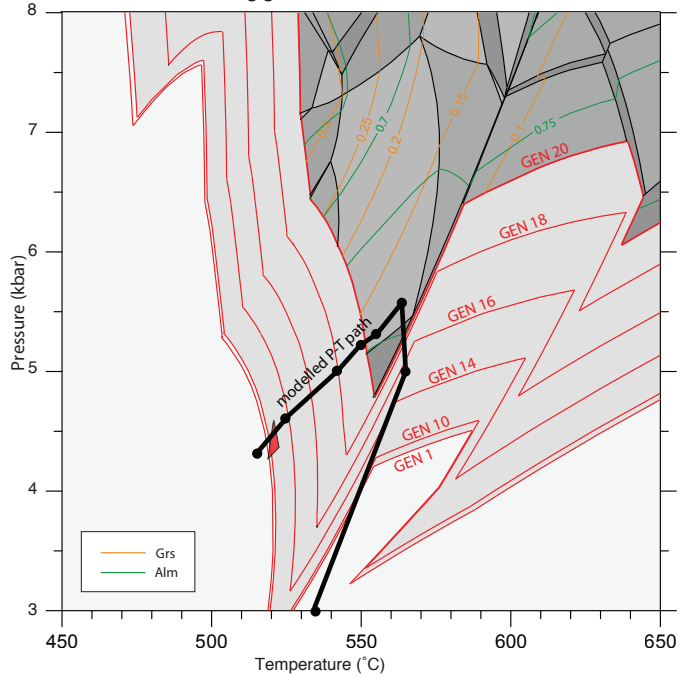


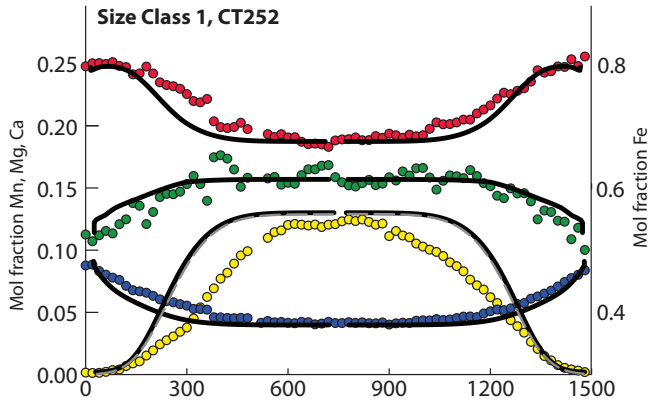
George & Gaidies (2017)

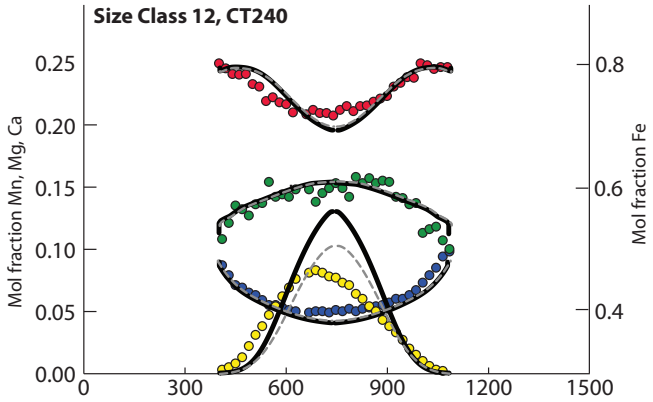
Garnet crystallization modelling with THERIA_G - Example

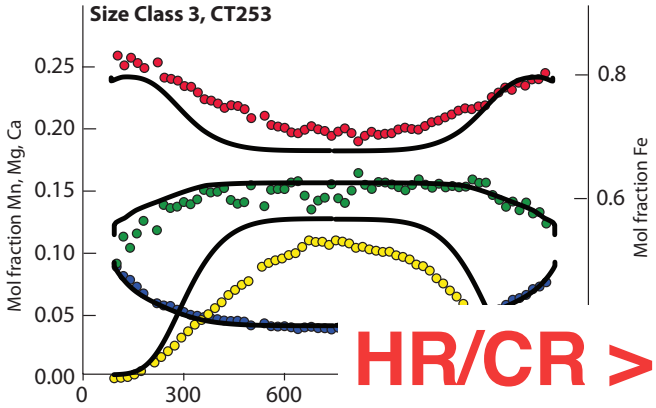


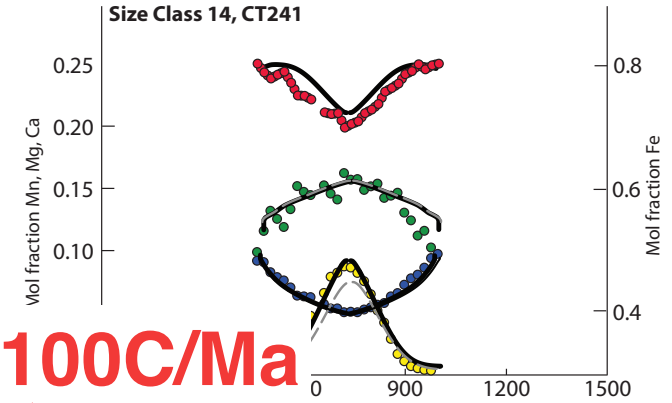
(d) 24-99 fractionating garnet-in



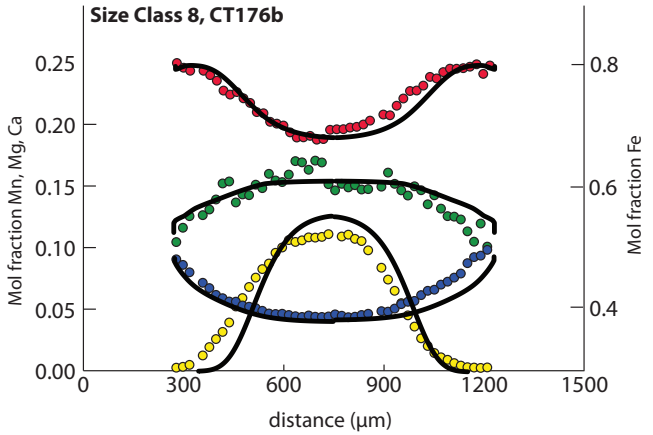


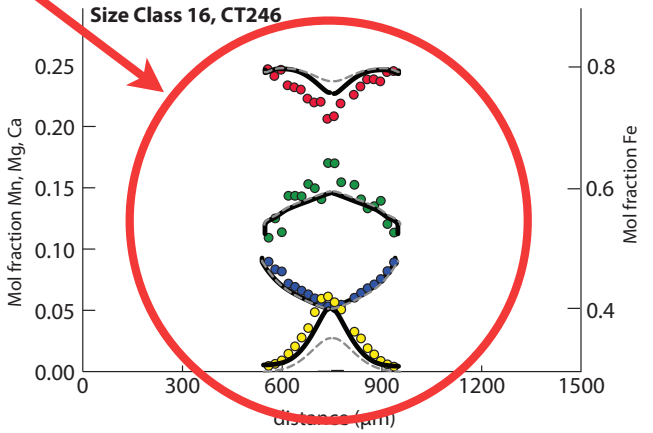






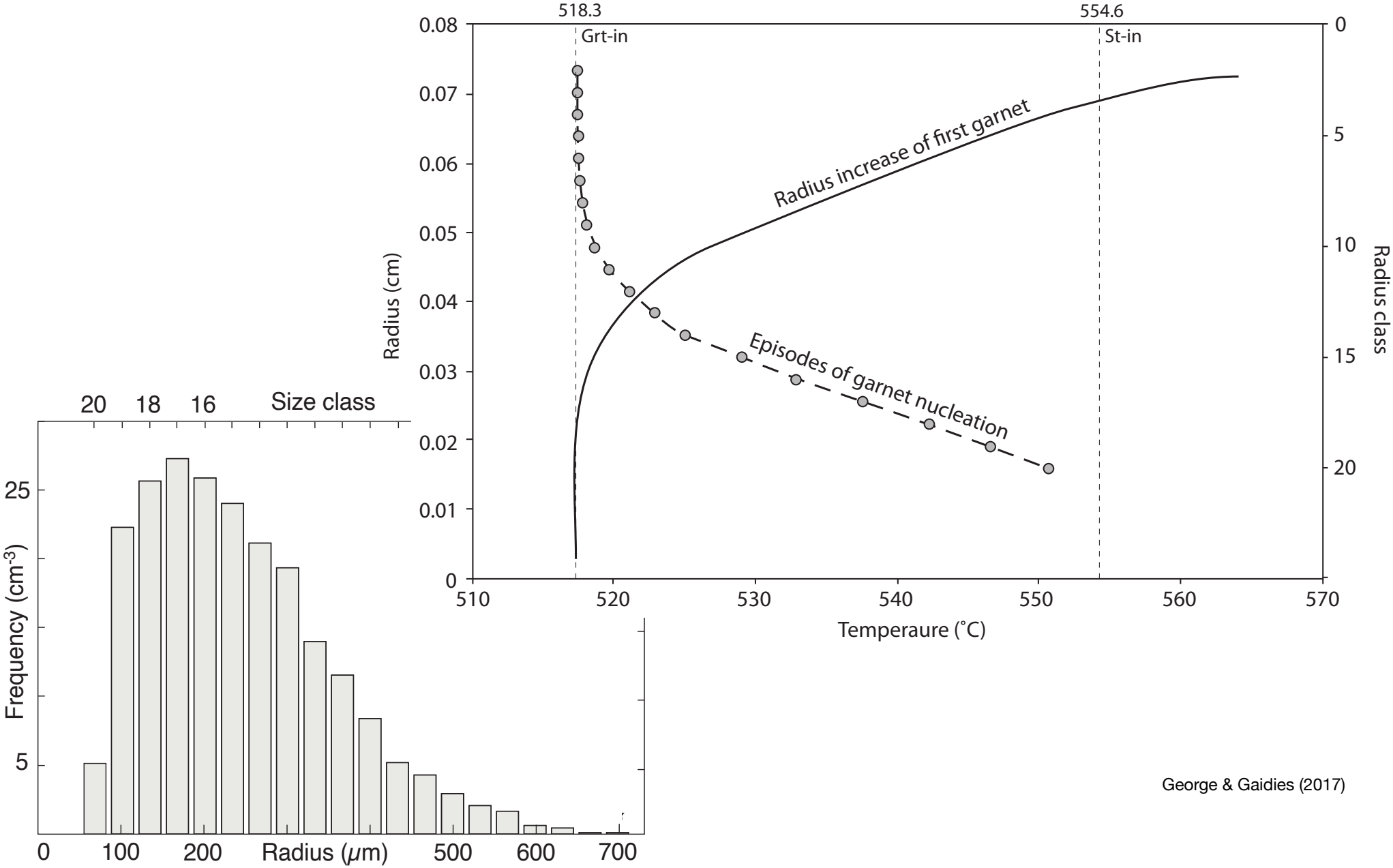
HR/CR > 100C/Ma





George & Gaidies (2017)

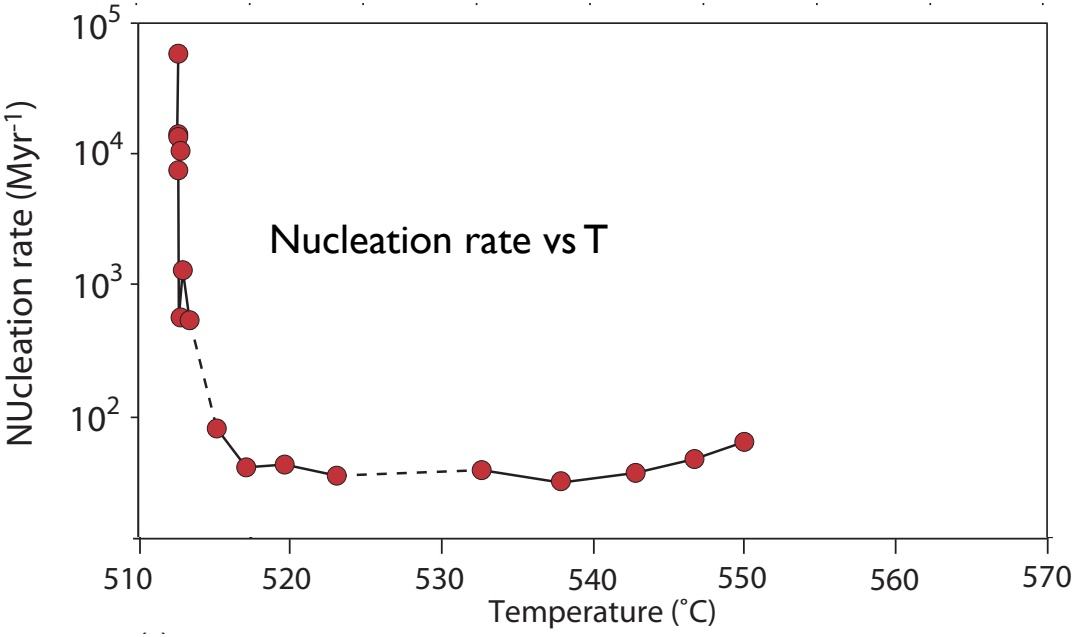
Garnet crystallization modelling with THERIA_G - Example

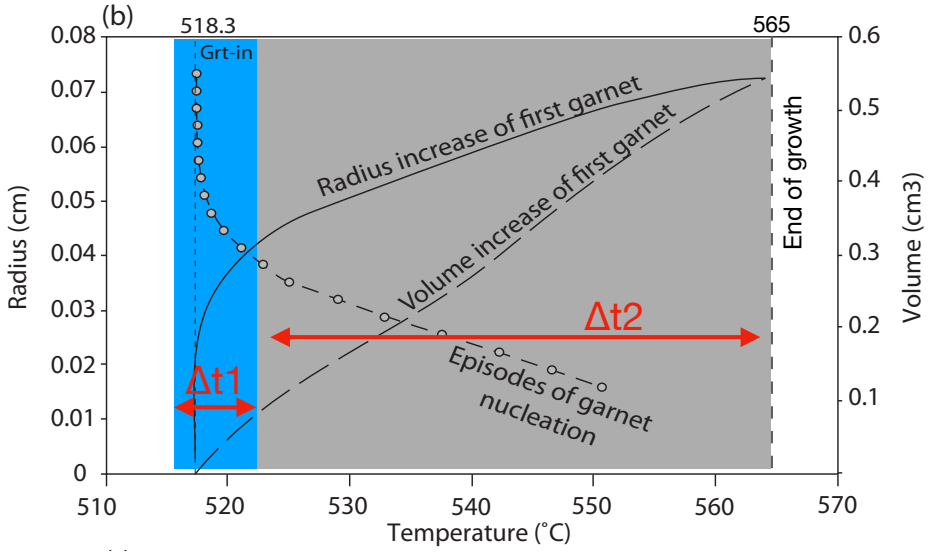


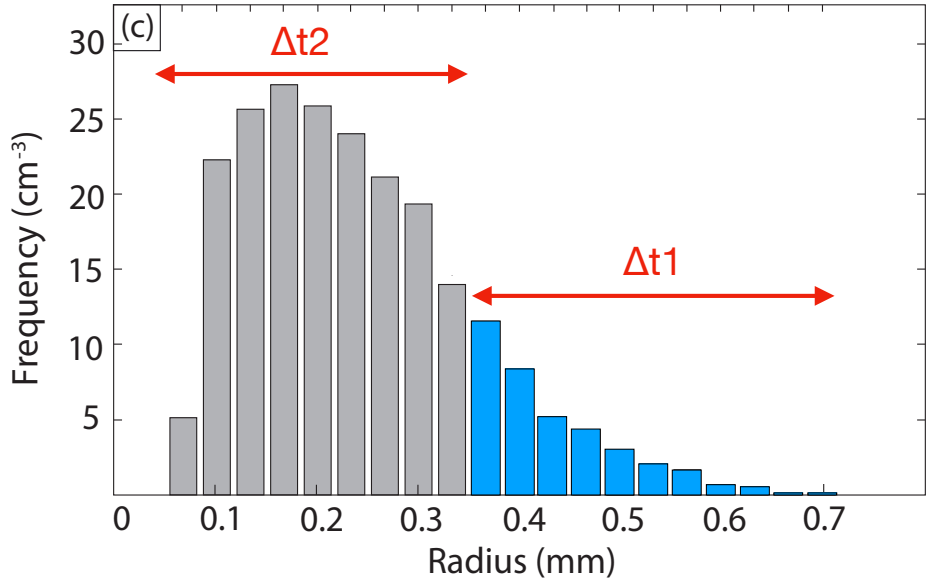
George & Gaidies (2017)

Garnet crystallization modelling with THERIA_G - Example

(George and Gaidies, 2017)

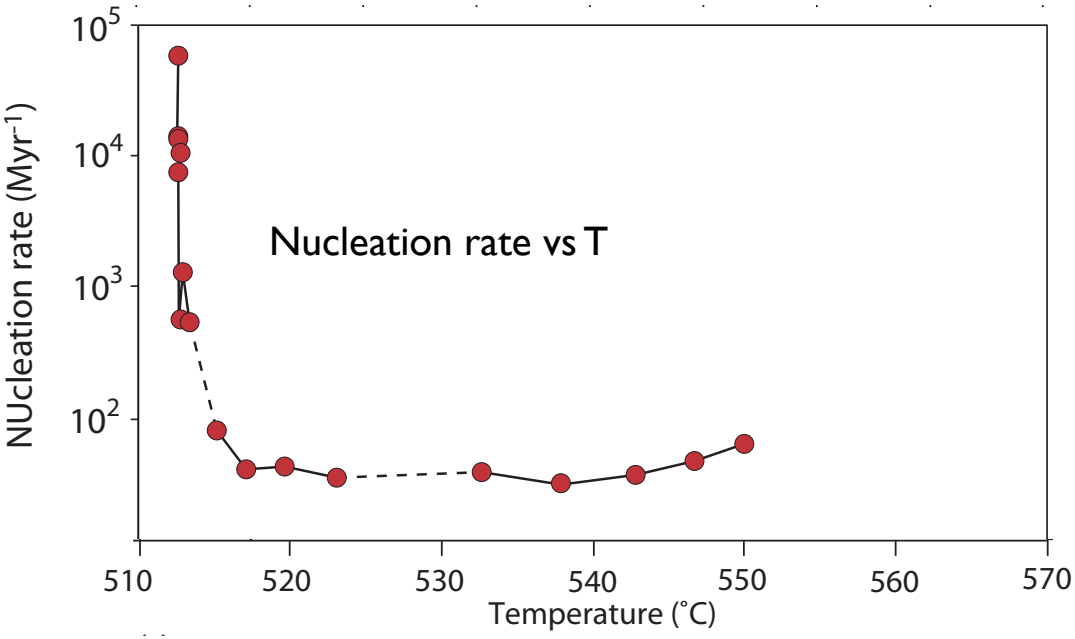


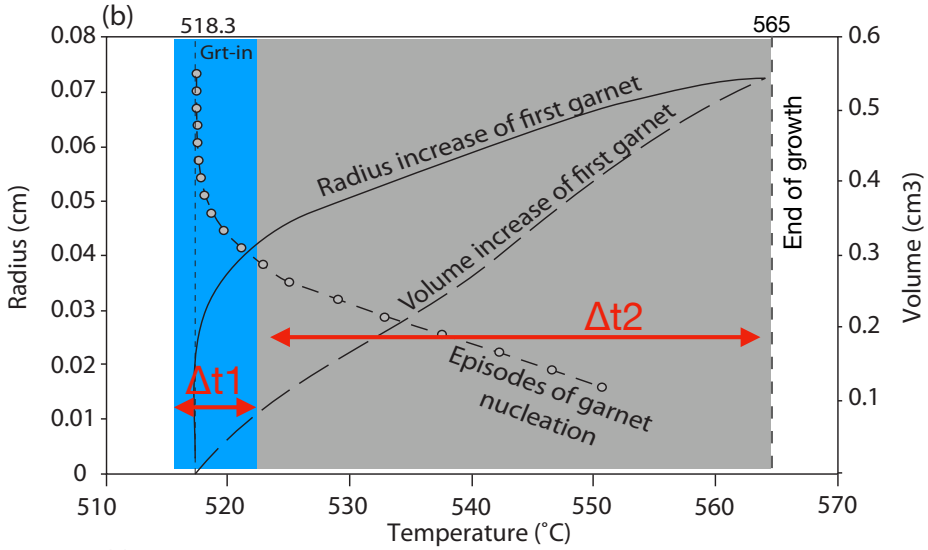


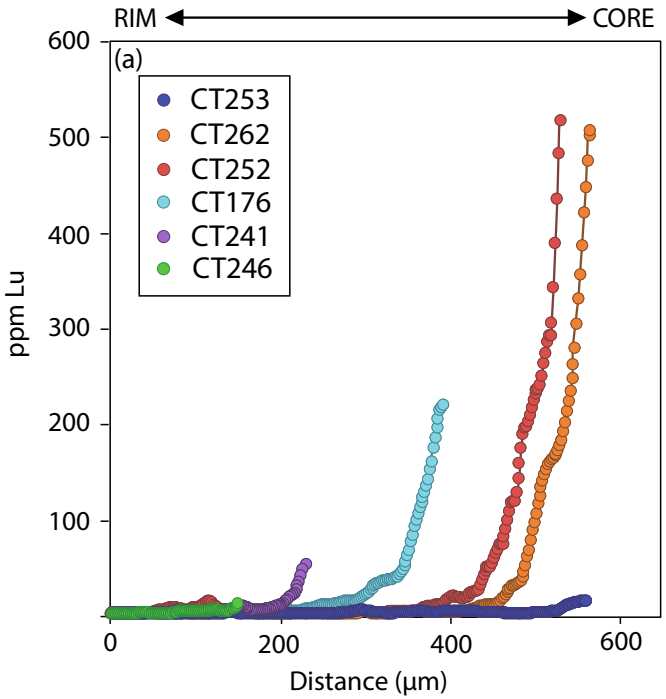


Garnet crystallization modelling with THERIA_G - Example

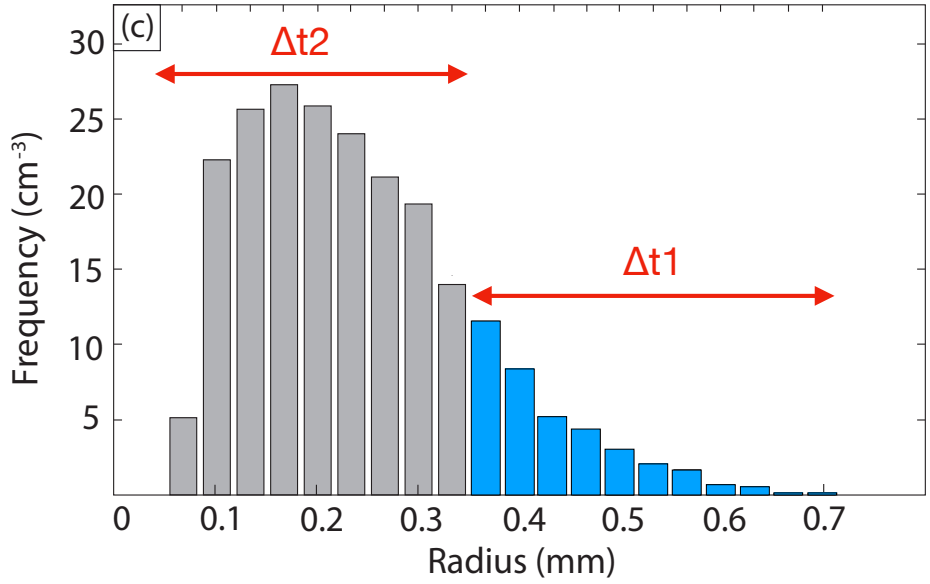
(George and Gaidies, 2017)





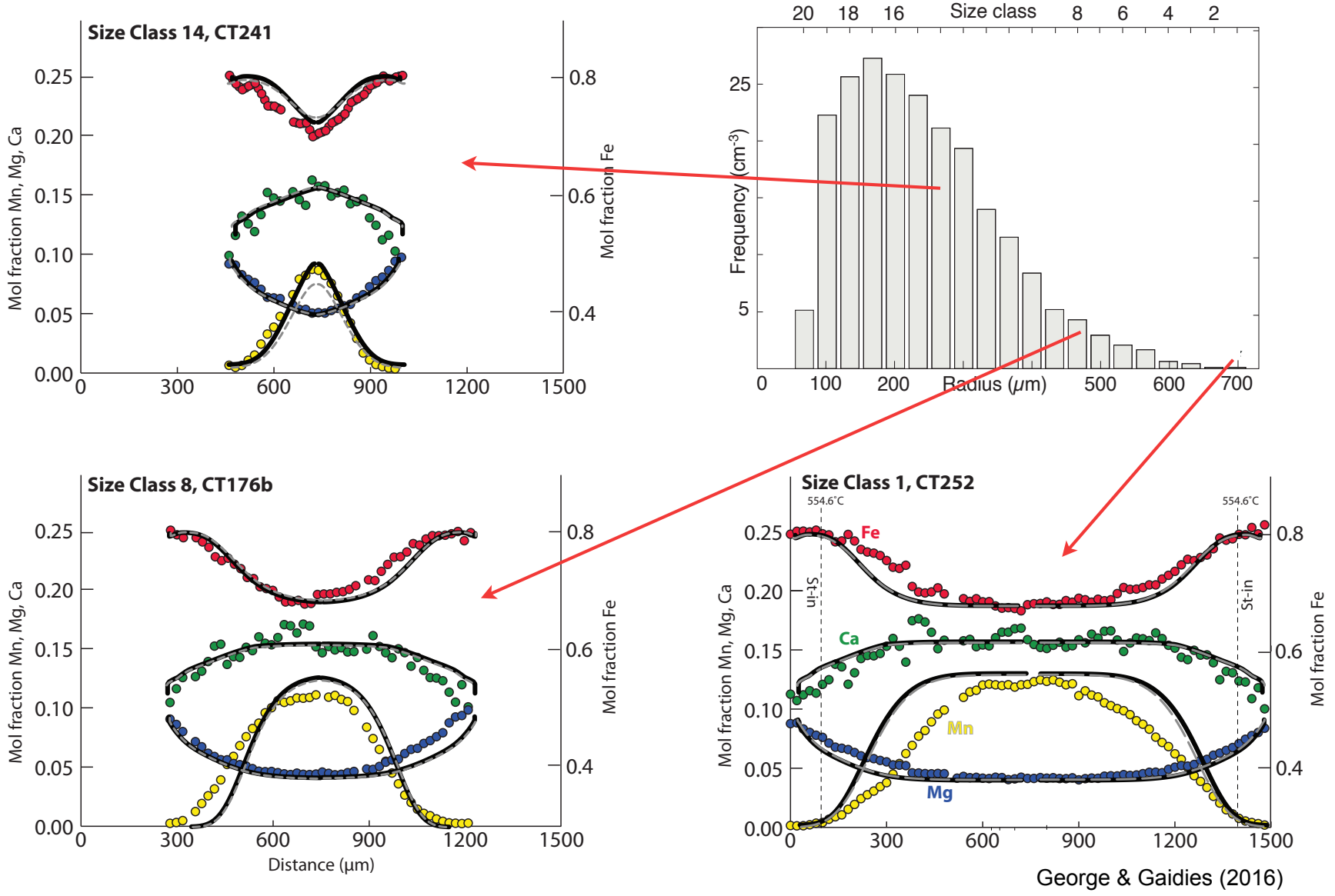


(George et al, 2018)



Theria_G modelling: Input files (in addition to database)

Theria_G (Gaidies et al., 2008) predicts the compositional zoning that develops in a garnet population during growth



George & Gaidies (2016)

Theria_G modelling: Input files (in addition to database)

theriag_PTt.txt:

T (degree C) | P (bar) | Time (Ma; has to start at zero)

515	4300	0
525	4600	0.1
542	5000	0.27
550	5200	0.35
555	5300	0.40
563	5590	0.49
565	5000	0.50
535	3000	0.80

HR=100C/Ma

THERIN.txt:

All four end-members must be present at start of growth

```
0    SI(63.60)TI(0.45)AL(21.65)CA(0.58)MG(2.76)FE(4.76)K(4.50)NA(1.66)MN(0.04)H(100)O(?)
```

Theria_G modelling: Input files

theriag_CSD.txt:

```
5          33.1
0.11
0.11
0.44
0.63
1.66
2.07
2.94
4.30
5.19
8.04
11.56
14.00
19.36
21.15
24.03
25.88
27.29
27.67
22.29
5.14
```

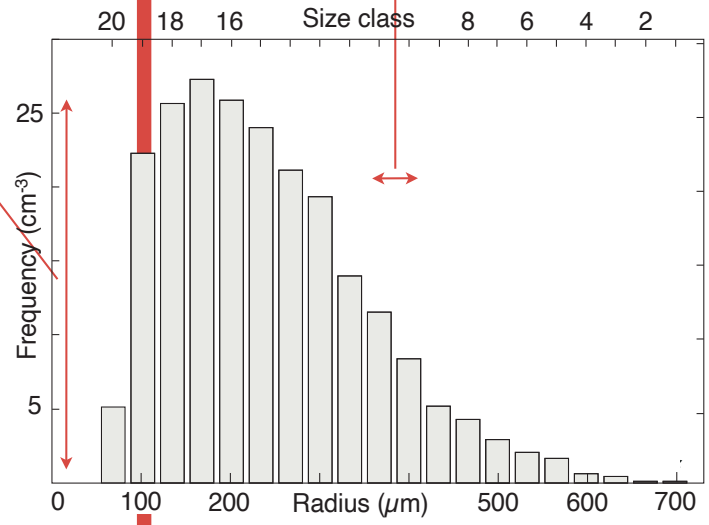
Thickness of garnet shells in µm

Largest grain

Number of garnet crystals in radius class (large to small) per ccm

Smallest grain

Size of radius class in µm = shell thickness plus this number



Theria_G modelling: Input files

Pre-exponential constant | Activation energy | Activation volume

theriag_DIF.txt:

5.1D-4	60569.0D0	6.0D0	Mn
6.4D-4	65824.0D0	5.6D0	Fe
1.1D-3	67997.0D0	5.3D0	Mg

Kinetic parameters of intracrystalline diffusion in garnet (Chakraborty and Ganguly, 1992) at fO2 defined by graphite buffer

Tracer diffusion-coeff. of Ca (D_Ca) is defined as 1/2 D_Fe (Loomis, 82; Florence and Spear, 91)

Theria_G

Mac, Linux:

replace with your Home Directory

(1) Open Terminal

(2) Enter:
`cd /Users/fredsmacbookpro/TheriakDominoMAC/GeochemSoc2020/Working`
or enter (if you followed the installation instructions):
`dom`

(3) Enter:
`theriag`

Windows:

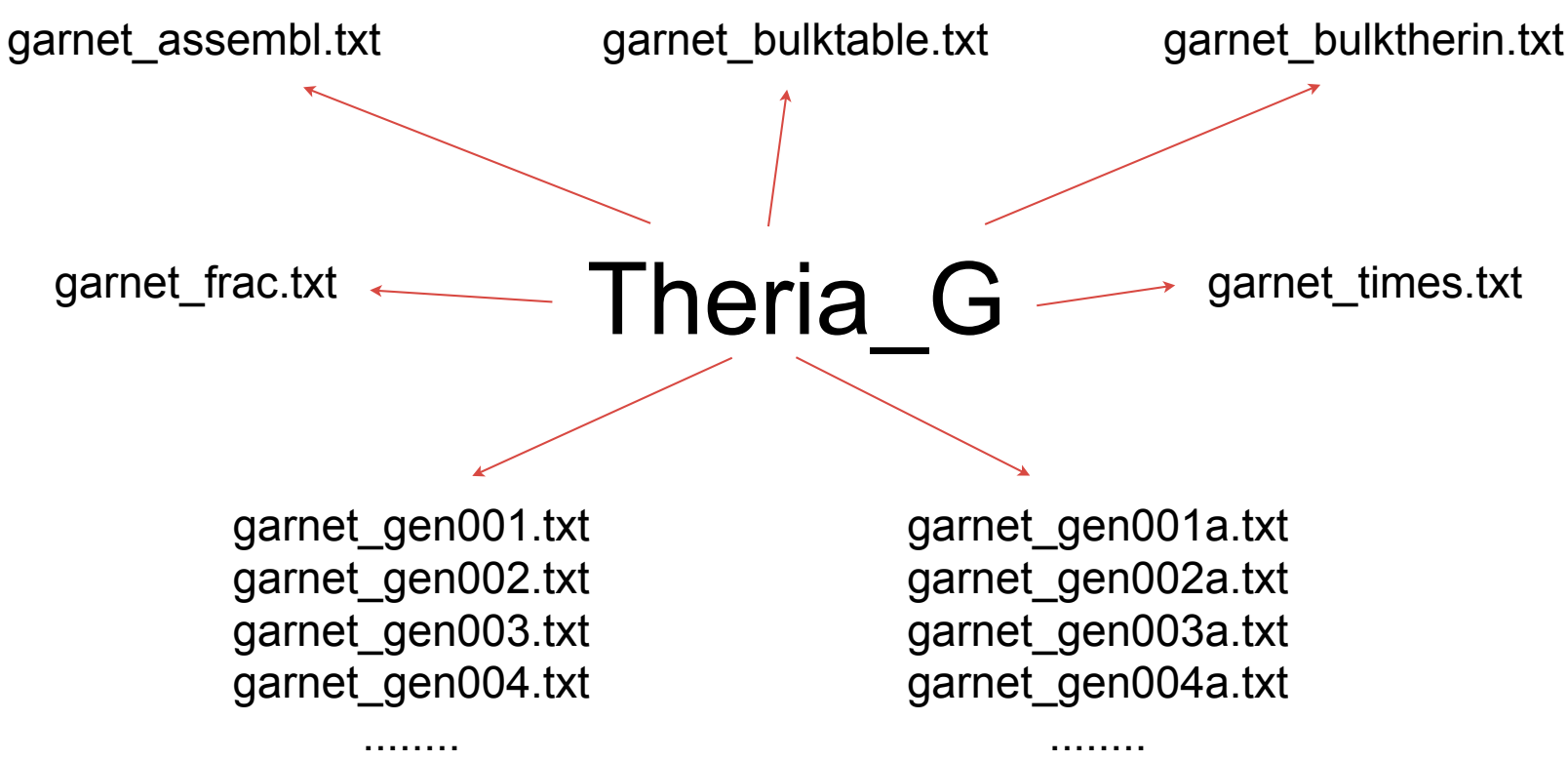
(1) Use File Explorer and navigate to
C:\TheriakDominoWIN\GeochemSoc2020\Working

(2) Double-click start.bat (opens Command Prompt)

(3) Enter:
`theriag`

```
--------------------
database definition
--------------------
Enter [ "?" | CR | "files" | database filename ] < >?
ds5_5.txt
```

Theria_G


garnet_assembl.txt
garnet_bulktable.txt
garnet_bulktherin.txt
garnet_frac.txt
Theria_G
garnet_times.txt
garnet_gen001.txt
garnet_gen002.txt
garnet_gen003.txt
garnet_gen004.txt
.....
garnet_gen001a.txt
garnet_gen002a.txt
garnet_gen003a.txt
garnet_gen004a.txt
.....

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

replace with your Home Directory

Mac, Linux:

(1) Use Finder and navigate to:
`/Users/fredsmacbookpro/TheriakDominoMAC/GeochemSoc2020/Working/NiceRockFromSikkim/4_theriag100`

Windows:

(1) Use File Explorer and navigate to
C:\TheriakDominoWIN\GeochemSoc2020\Working\NiceRockFromSikkim\4_theriag100

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

theriag_PTt.txt:

T (degree C)	P (bar)	Time (Ma; has to start at zero)
515	4300	0
525	4600	0.1
542	5000	0.27
550	5200	0.35
555	5300	0.40
563	5590	0.49
565	5000	0.50
535	3000	0.80

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

replace with your Home Directory

Mac, Linux:

(1) Enter (in Terminal window):

```
cd /Users/fredsmacbookpro/TheriakDominoMAC/GeochemSoc2020/Working/
NiceRockFromSikkim/4_theriag100
```

(2) Enter:

```
plotg
```

Windows:

(1) Use File Explorer and navigate to
C:\TheriakDominoWIN\GeochemSoc2020\Working\NiceRockFromSikkim\4_theriag**100**

(2) Double-click start.bat (opens Command Prompt)

(3) Enter:

```
plotg
```

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

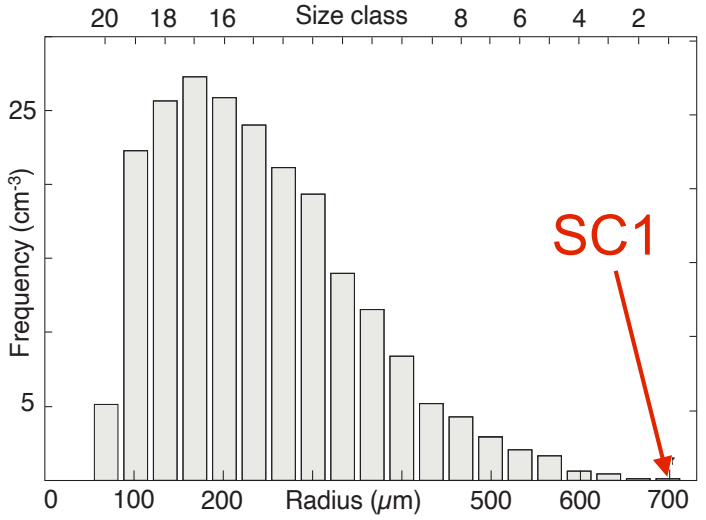
Plot the compositional zoning (spss, grs, py) of the garnet size classes **1**, 10, and 18 that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
1,10
```

for last point along P-T-t path, any large number is fine; plotg will then pick the time closest to this selection

Note, numbers are separated by comma. No spaces!



Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes **1**, 10, and 18 that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
1,10
time is:    0.67141522
```

plotg picks time closest to selection (here last point along P-T-t path)

```
 X-axis                    7                    radius(cm)
 Y-axis                    9,11,12              x(Ca),x(Mg),x(Mn)
 X-min   X-max             0      0.08          limits [mol
 Y-min   Y-max             0      0.18          -fraction]
```

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes **1**, 10, and 18 that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
1,10
time is:    0.67141522

 X-axis                          7                    radius(cm)
 Y-axis                          9,11,12              x(Ca),x(Mg),x(Mn)
 X-min   X-max                   0      0.08          limits [mol
 Y-min   Y-max                   0      0.18          -fraction]
```

plotg picks time closest to selection (here last point along P-T-t path)

plotg creates **xyplot** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Mac, Linux:

(1) Enter:

```
guzzler
```

Windows:

(1) Enter:

```
guzzler
```

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes **1**, 10, and 18 that is predicted to develop during the metamorphism of the sample.

guzzler ==> clean

```
Enter [ "?" | CR | graphics file name ] < >?
xyplot
```

accept all the remaining offers (hit return key four times)

guzzler creates **clean** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Mac, Linux:

(1) Enter:

```
explot
```

Windows:

(1) Enter:

```
explot
```

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

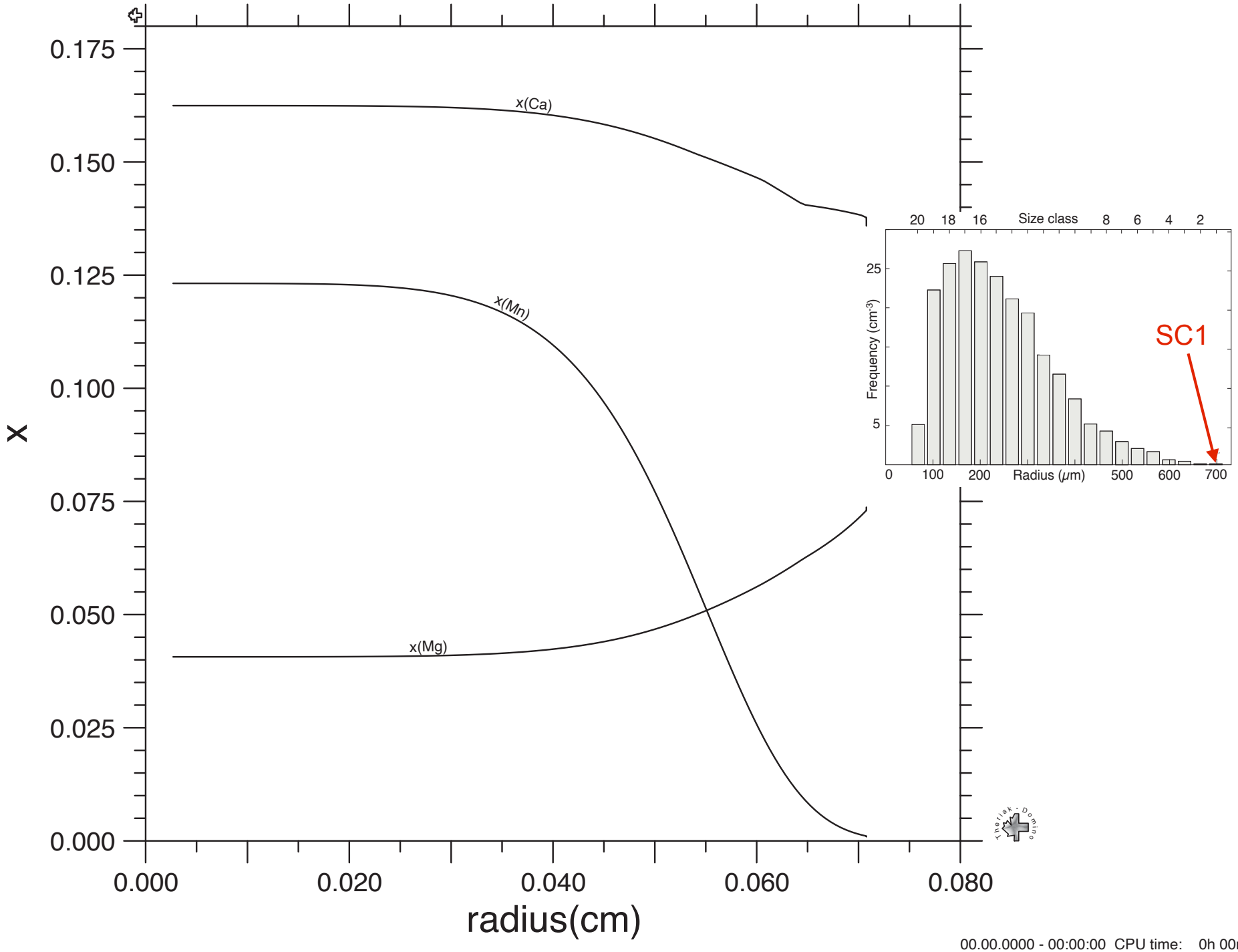
Plot the compositional zoning (spss, grs, py) of the garnet size classes **1**, 10, and 18 that is predicted to develop during the metamorphism of the sample.

explot ==> plot.ps plot.svg

```
Enter [ "?" | CR | graphics file name ] <>?
clean
```

explot creates **plot.ps** and **plot.svg** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)



00.00.0000 - 00:00:00 CPU time: 0h 00m

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

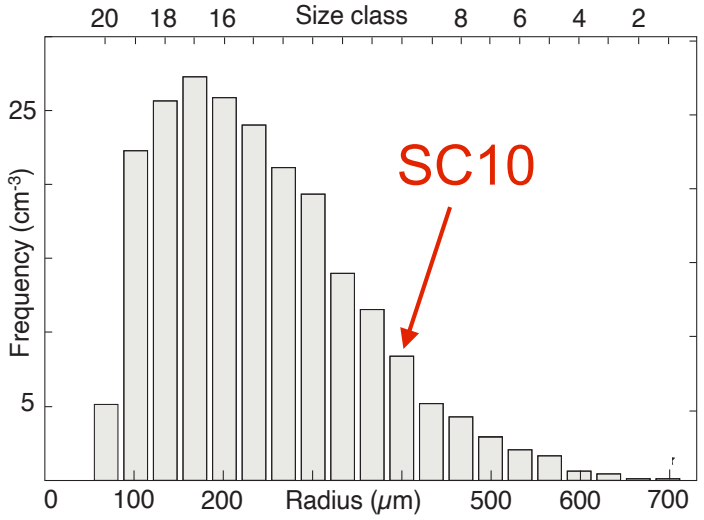
Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, **10**, and 18 that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
10,10
```

for last point along P-T-t path, any large number is fine; plotg will then pick the time closest to this selection

Note, numbers are separated by comma. No spaces!



Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, **10**, and 18 that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
10,10
time is:    0.67141522

 X-axis                          7                    radius(cm)
 Y-axis                          9,11,12              x(Ca),x(Mg),x(Mn)
 X-min   X-max                   0      0.08          limits [mol
 Y-min   Y-max                   0      0.18          -fraction]
```

plotg picks time closest to selection (here last point along P-T-t path)

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, **10**, and 18 that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
10,10
time is:    0.67141522

 X-axis                                  7                    radius(cm)
 Y-axis                                  9,11,12              x(Ca),x(Mg),x(Mn)
 X-min   X-max                           0      0.08          limits [mol
 Y-min   Y-max                           0      0.18          -fraction]
```

plotg picks time closest to selection (here last point along P-T-t path)

plotg creates **xyplot** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Mac, Linux:

(1) Enter:

```
guzzler
```

Windows:

(1) Enter:

```
guzzler
```

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, **10**, and 18 that is predicted to develop during the metamorphism of the sample.

guzzler ==> clean

```
Enter [ "?" | CR | graphics file name ] < >?
xyplot
```

accept all the remaining offers (hit return key four times)

guzzler creates **clean** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Mac, Linux:

(1) Enter:

```
explot
```

Windows:

(1) Enter:

```
explot
```

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

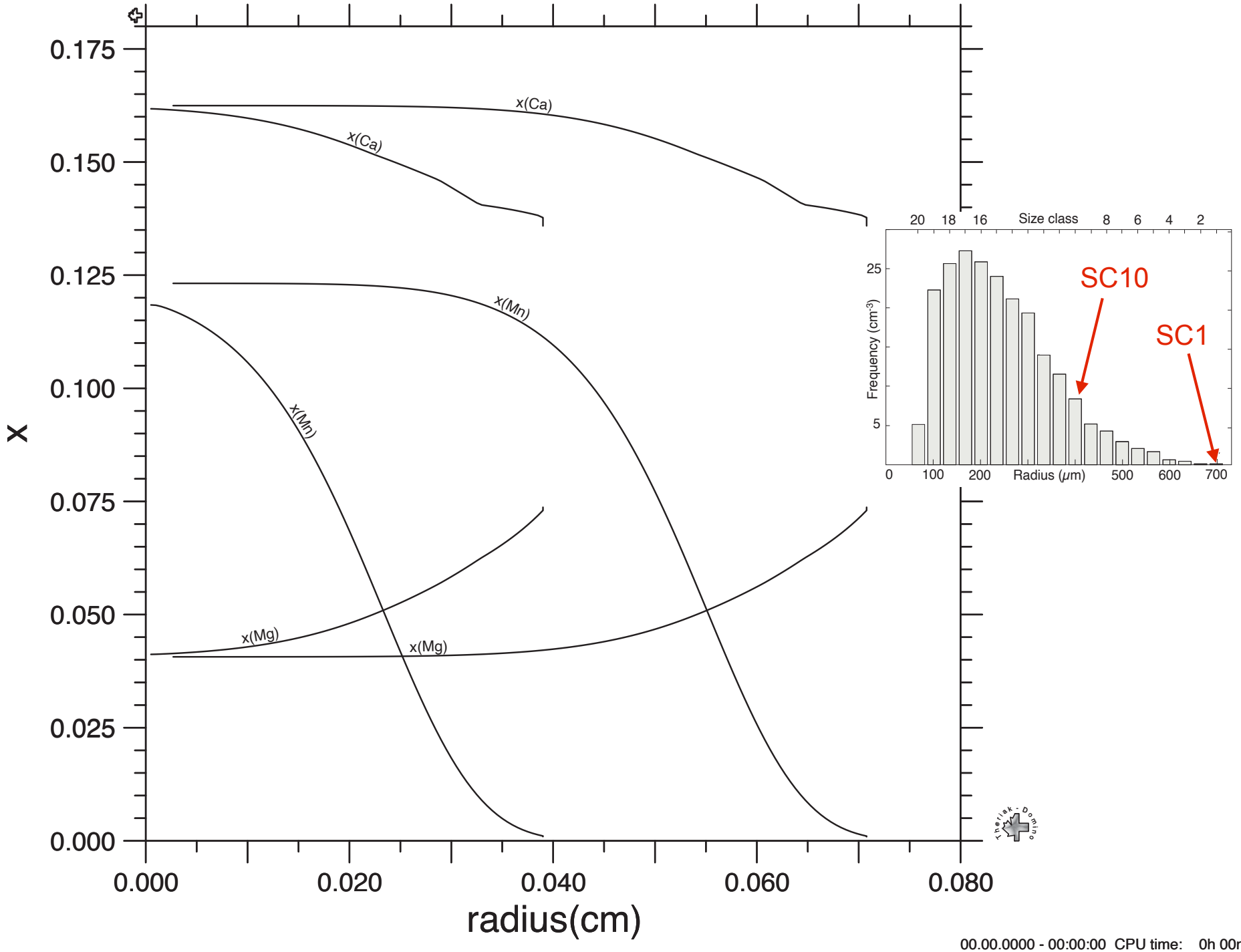
Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, **10**, and 18 that is predicted to develop during the metamorphism of the sample.

explot ==> plot.ps plot.svg

```
Enter [ "?" | CR | graphics file name ] <>?
clean
```

explot creates **plot.ps** and **plot.svg** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)



00.00.0000 - 00:00:00 CPU time: 0h 00m

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

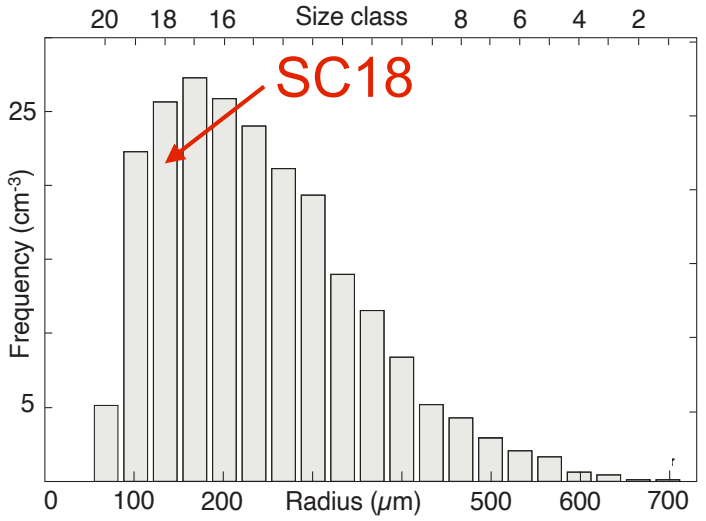
Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, 10, and **18** that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
18,10
```

for last point along P-T-t path, any large number is fine; plotg will then pick the time closest to this selection

Note, numbers are separated by comma. No spaces!



Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, 10, and **18** that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
18,10
time is:   0.67141522

 X-axis                          7                    radius(cm)
 Y-axis                          9,11,12              x(Ca),x(Mg),x(Mn)
 X-min   X-max                   0      0.08          limits [mol
 Y-min   Y-max                   0      0.18          -fraction]
```

plotg picks time closest to selection (here last point along P-T-t path)

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, 10, and **18** that is predicted to develop during the metamorphism of the sample.

plotg ==> xyplot

```
enter generation nr, and time(my) (use generation = 0 for CSD)
18,10
time is:   0.67141522
```

plotg picks time closest to selection (here last point along P-T-t path)

```
 X-axis                    7                    radius(cm)
 Y-axis                    9,11,12              x(Ca),x(Mg),x(Mn)
 X-min   X-max             0      0.08          limits [mol
 Y-min   Y-max             0      0.18          -fraction]
```

plotg creates **xyplot** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Mac, Linux:

(1) Enter:

```
guzzler
```

Windows:

(1) Enter:

```
guzzler
```

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, 10, and **18** that is predicted to develop during the metamorphism of the sample.

guzzler ==> clean

```
Enter [ "?" | CR | graphics file name ] < >?
xyplot
```

accept all the remaining offers (hit return key four times)

guzzler creates **clean** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

Mac, Linux:

(1) Enter:

```
explot
```

Windows:

(1) Enter:

```
explot
```

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

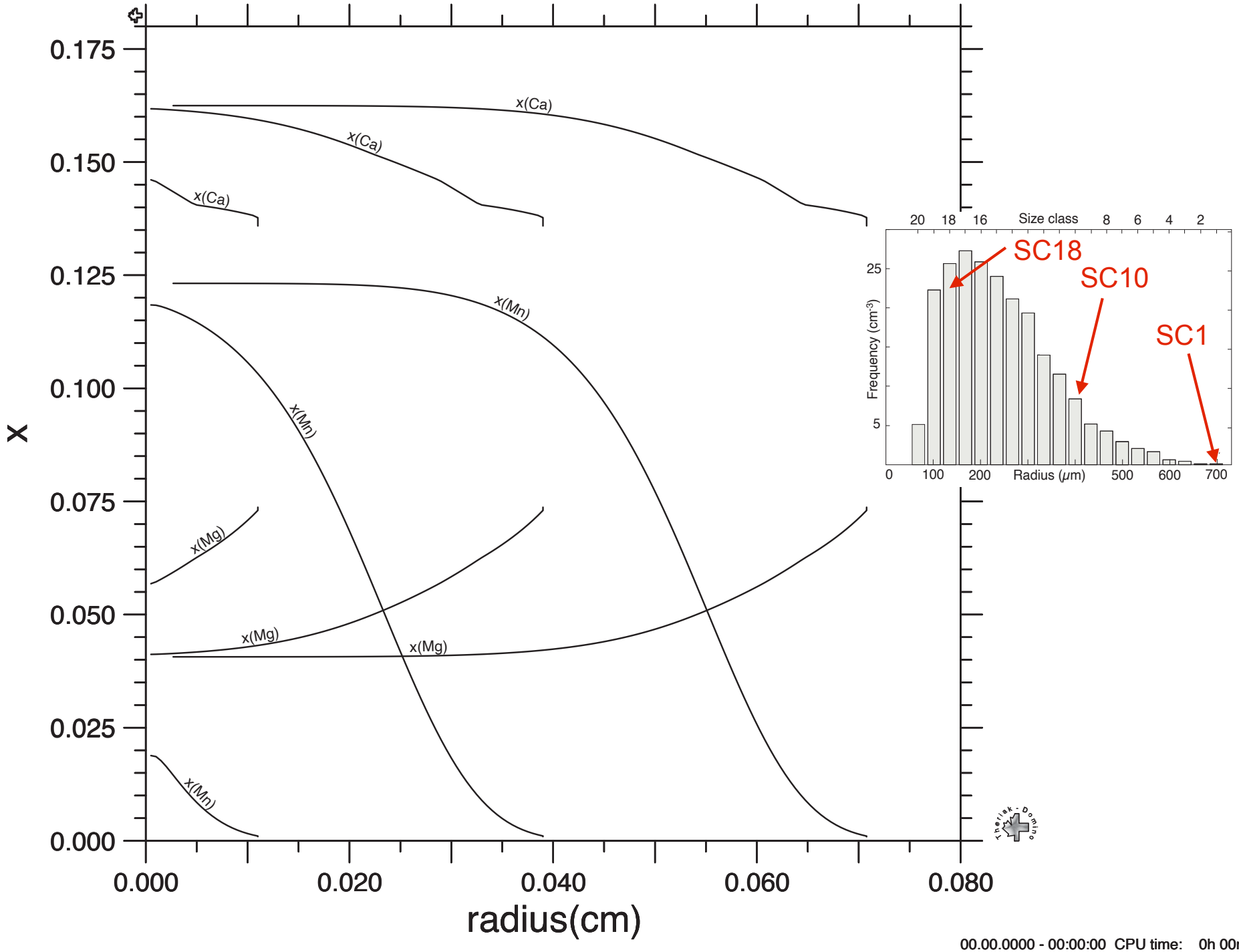
Plot the compositional zoning (spss, grs, py) of the garnet size classes 1, 10, and **18** that is predicted to develop during the metamorphism of the sample.

explot ==> plot.ps plot.svg

```
Enter [ "?" | CR | graphics file name ] <>?
clean
```

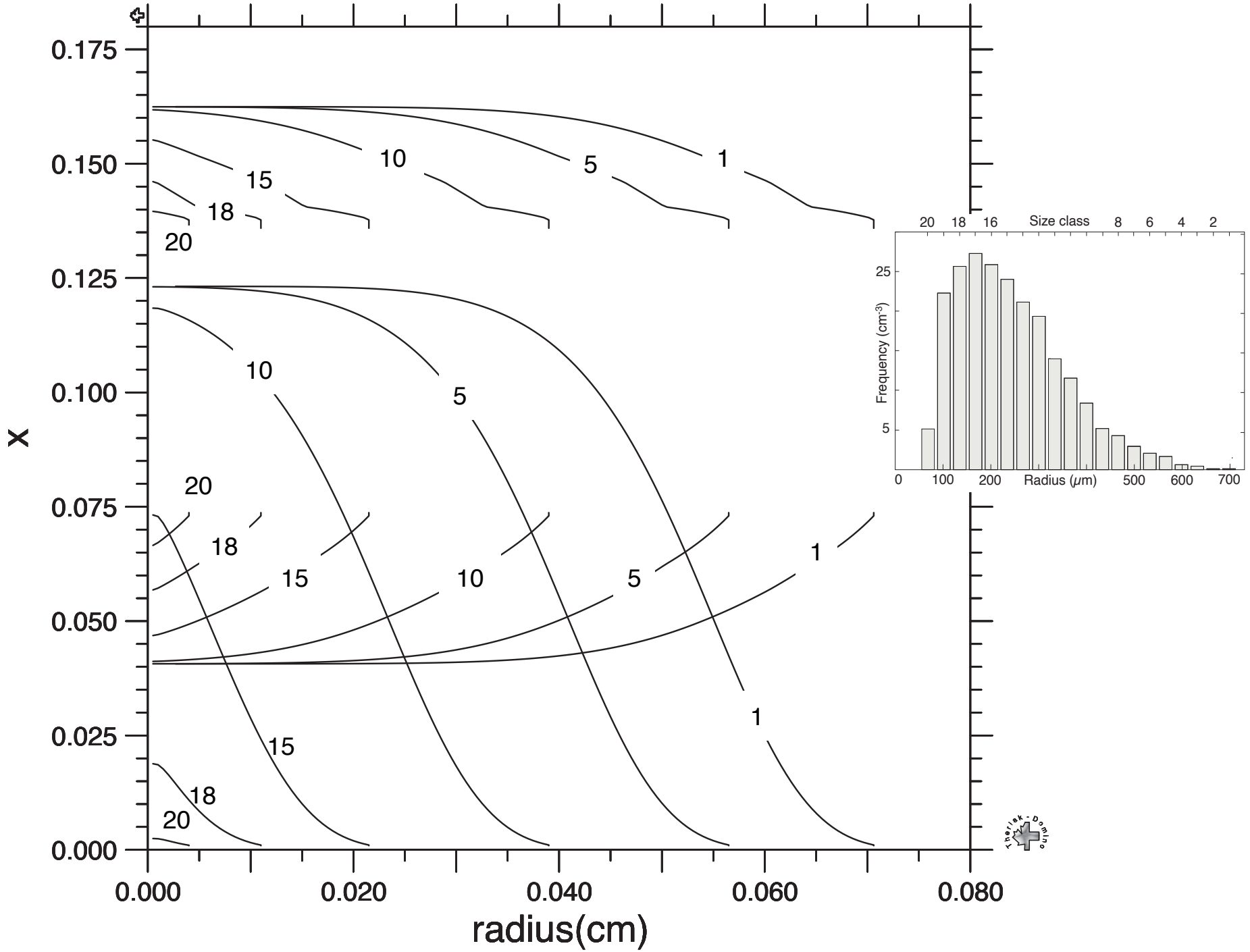
explot creates **plot.ps** and **plot.svg** in working directory

Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)

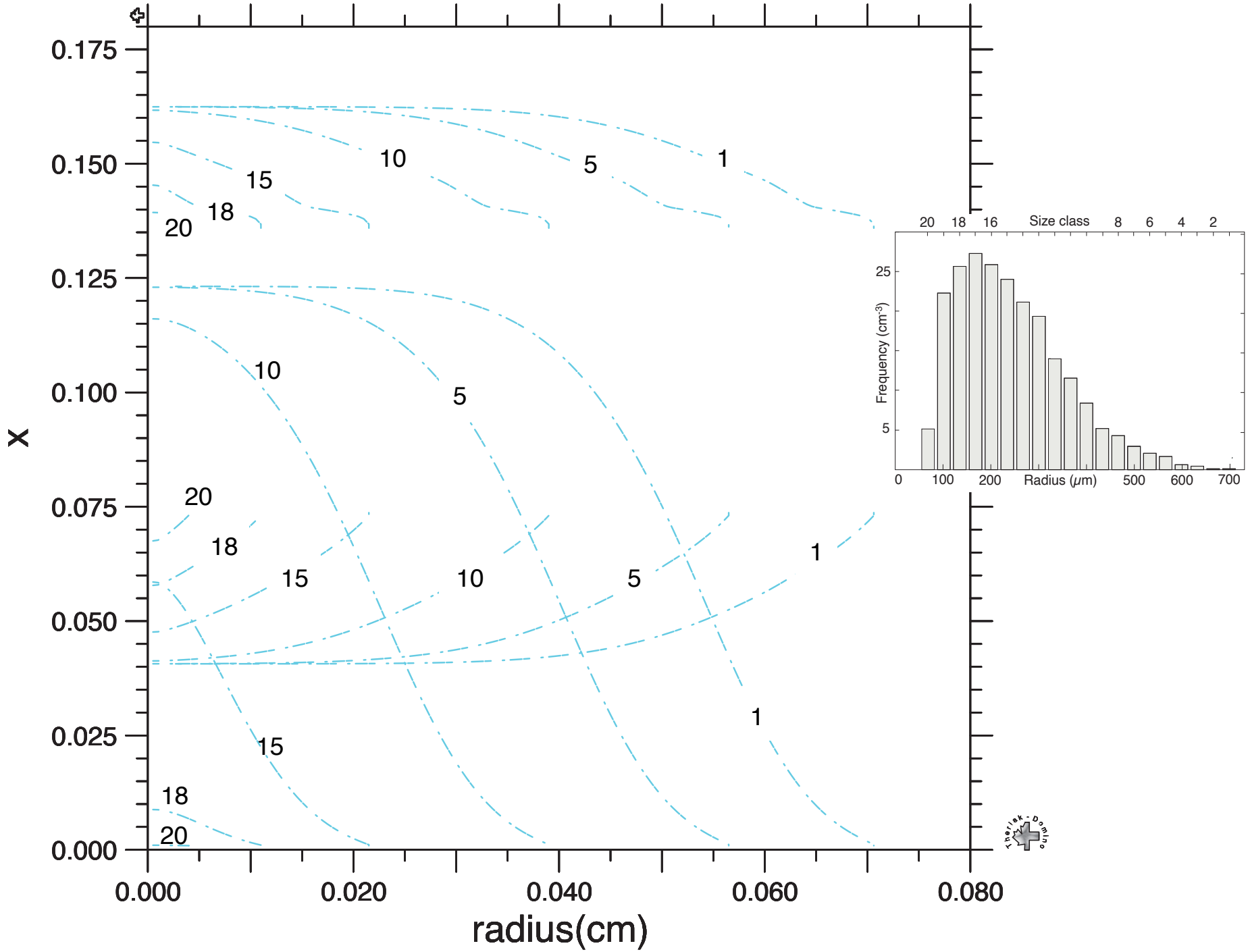


00.00.0000 - 00:00:00 CPU time: 0h 00m

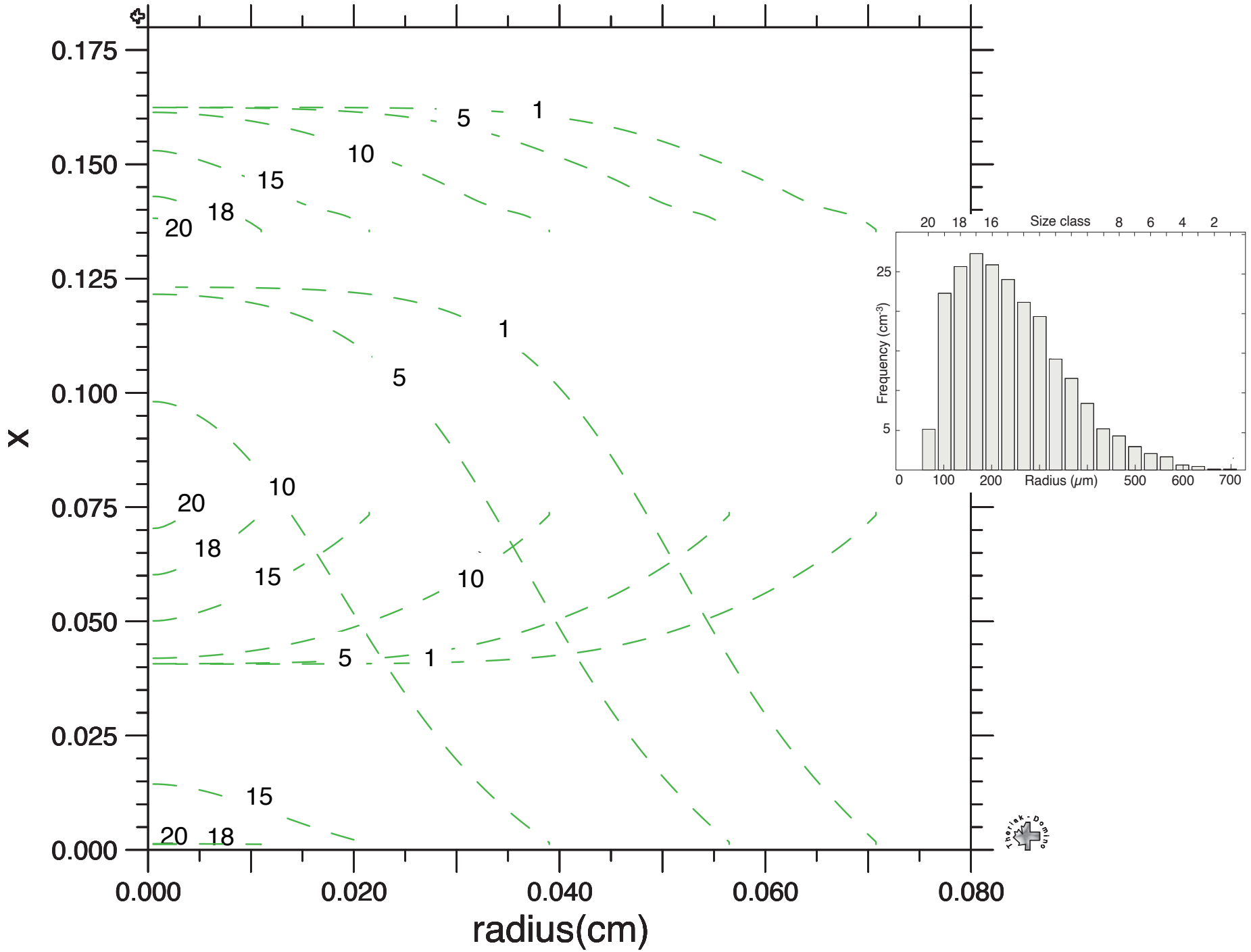
Theria_G modelling. Case 1: 100 C/Ma (folder: theriag100)



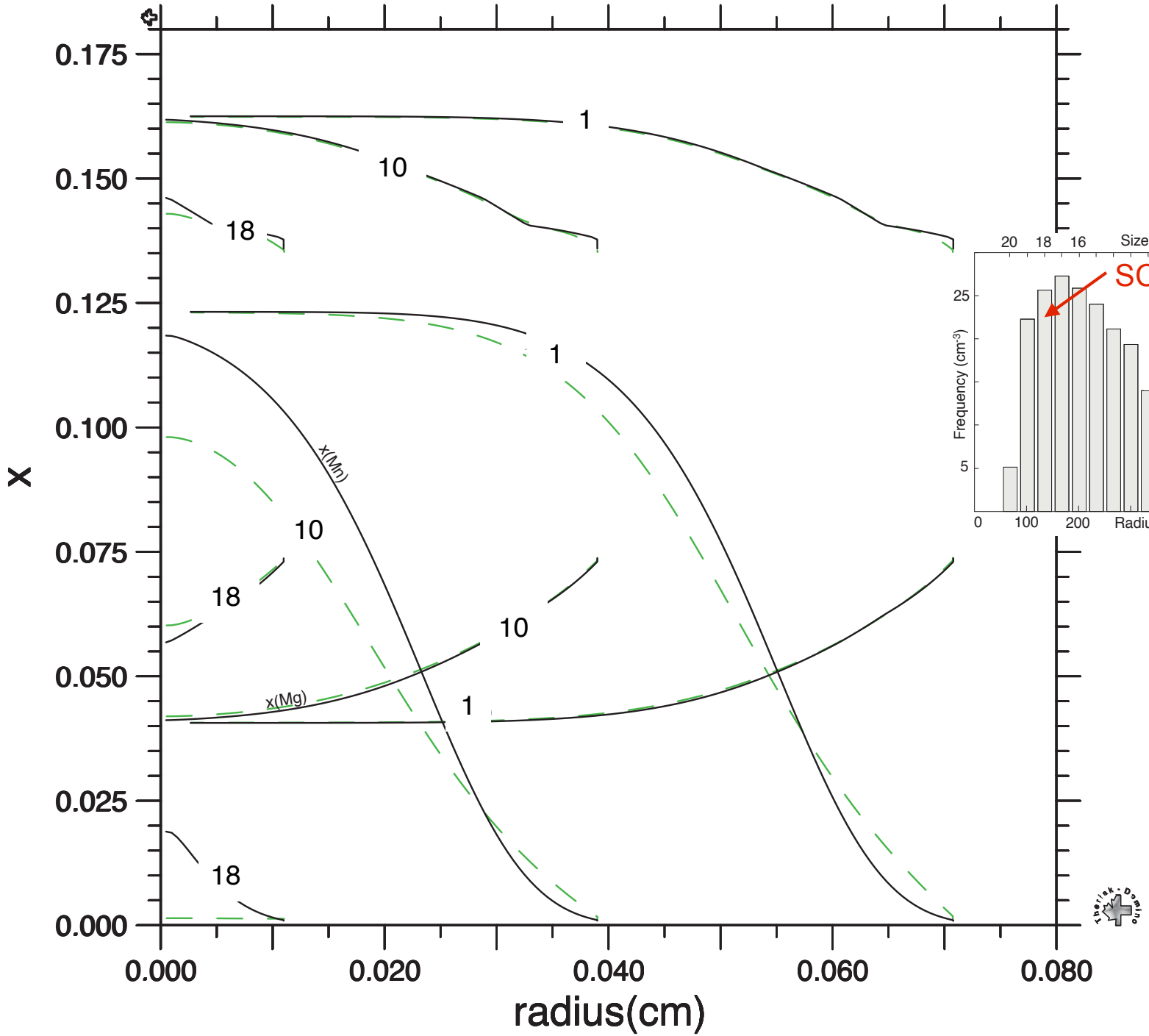
Theria_G modelling. Case 2: 10 C/Ma (folder: theriag10)



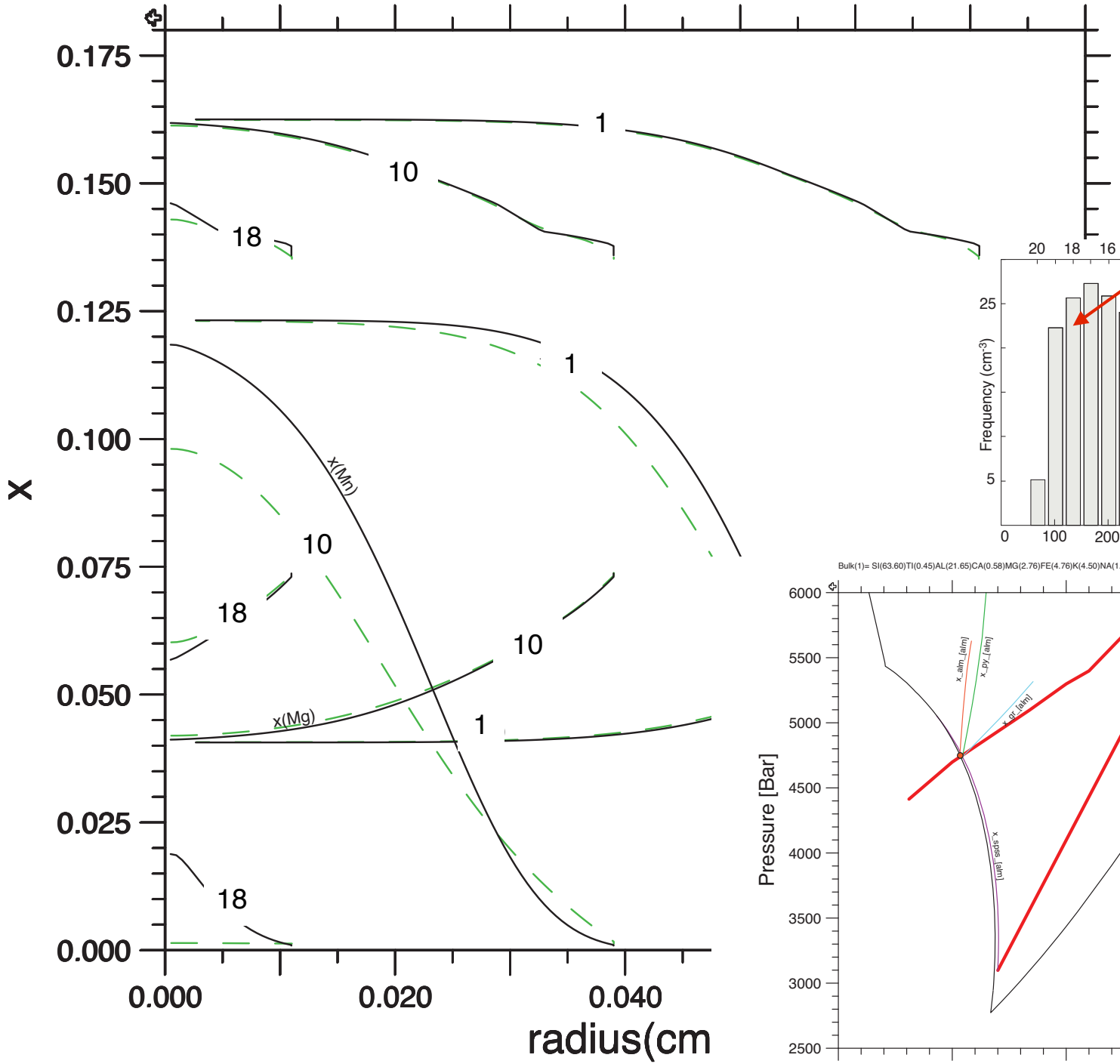
Theria_G modelling. Case 3: 1 C/Ma (folder: theriag1)

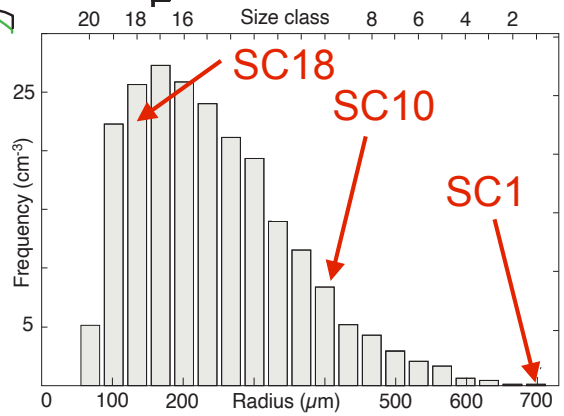


Theria_G modelling. 100 C/Ma vs 1 C/Ma

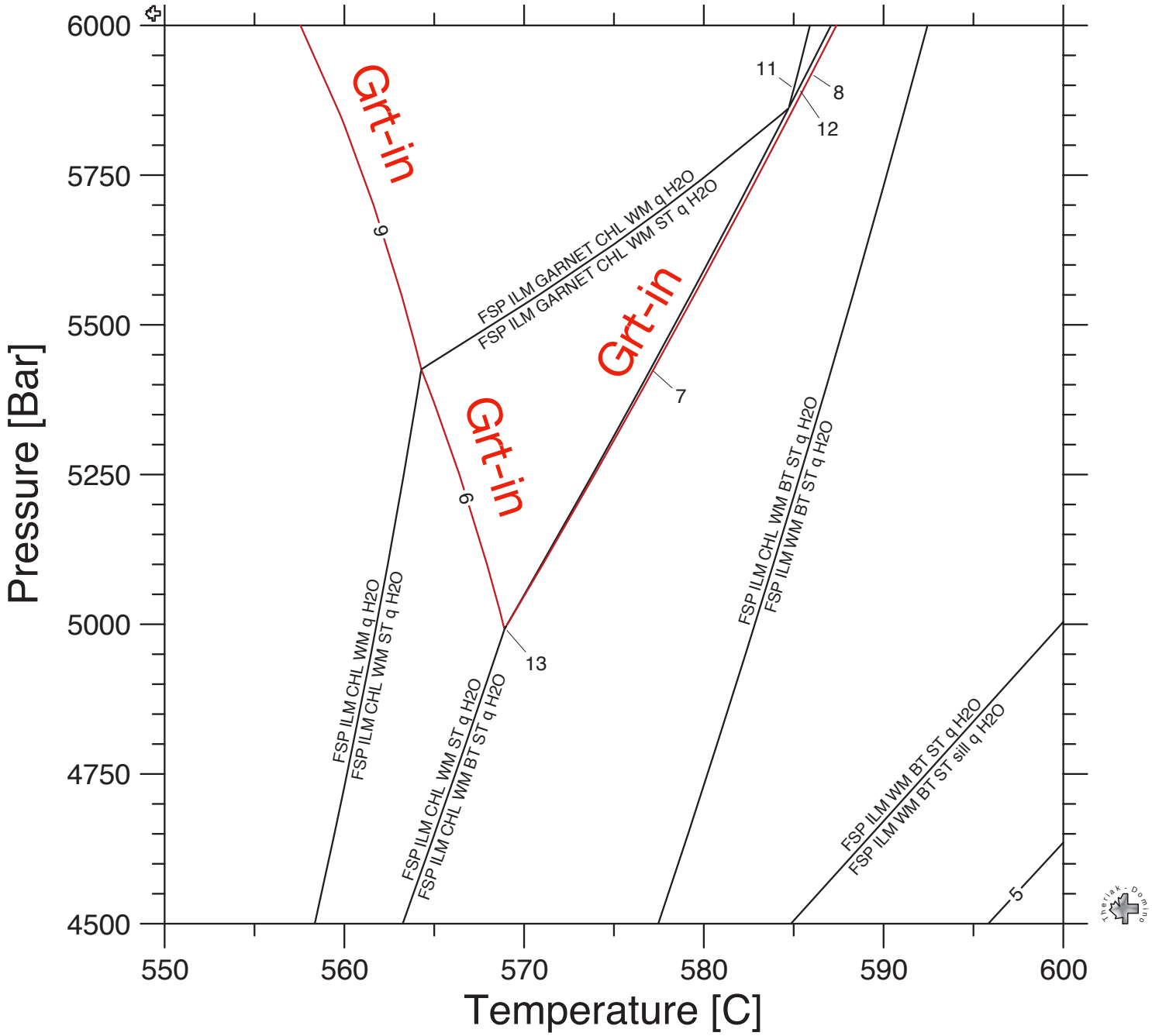


Theria_G modelling. 100 C/Ma vs 1 C/Ma

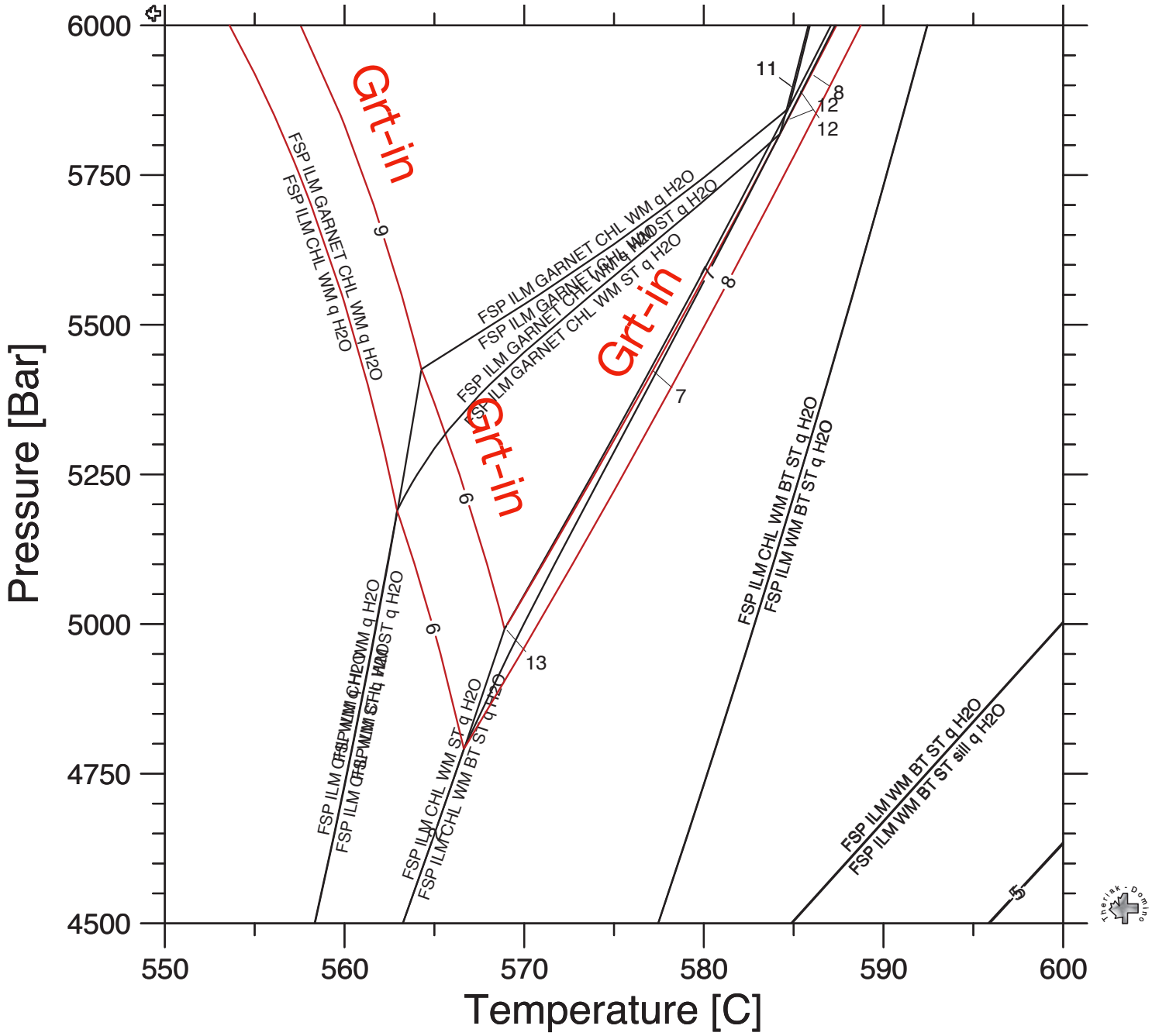




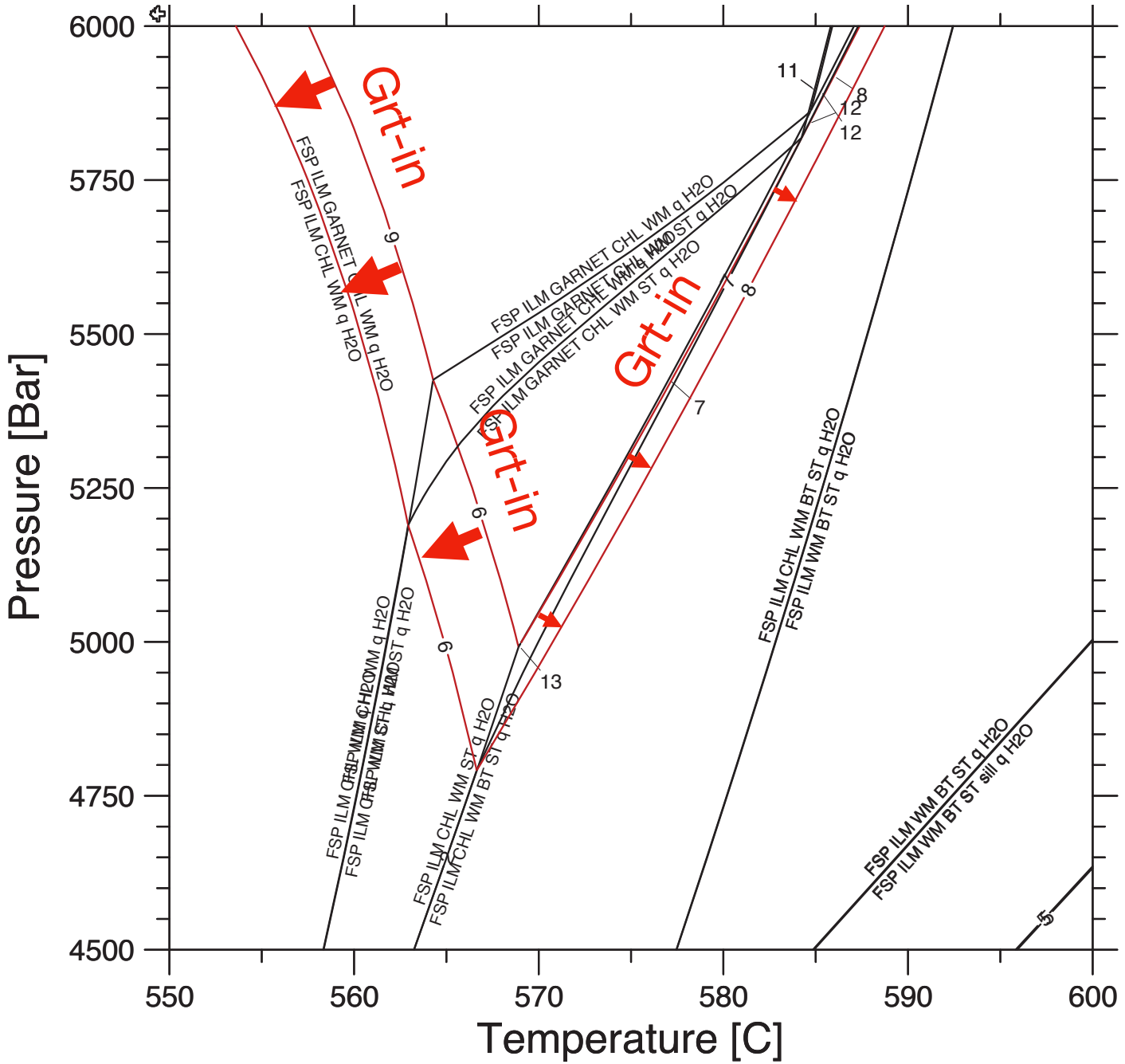
P-T phase relations after garnet growth: 100 C/Ma



P-T phase relations after garnet growth: 100 C/Ma, 0.1 C/Ma



P-T phase relations after garnet growth: 100 C/Ma, 0.1 C/Ma



Internal Metasomatism

geochemical society

The P-T-t Trajectory of Metamorphic Processes

Garnet crystallization simulations with Theria_G to estimate P-T-t trajectories of metamorphism

Fred Gaidies, Carleton U. (fred.gaidies@carleton.ca)

Thank you!
(Questions? Please send me an email)