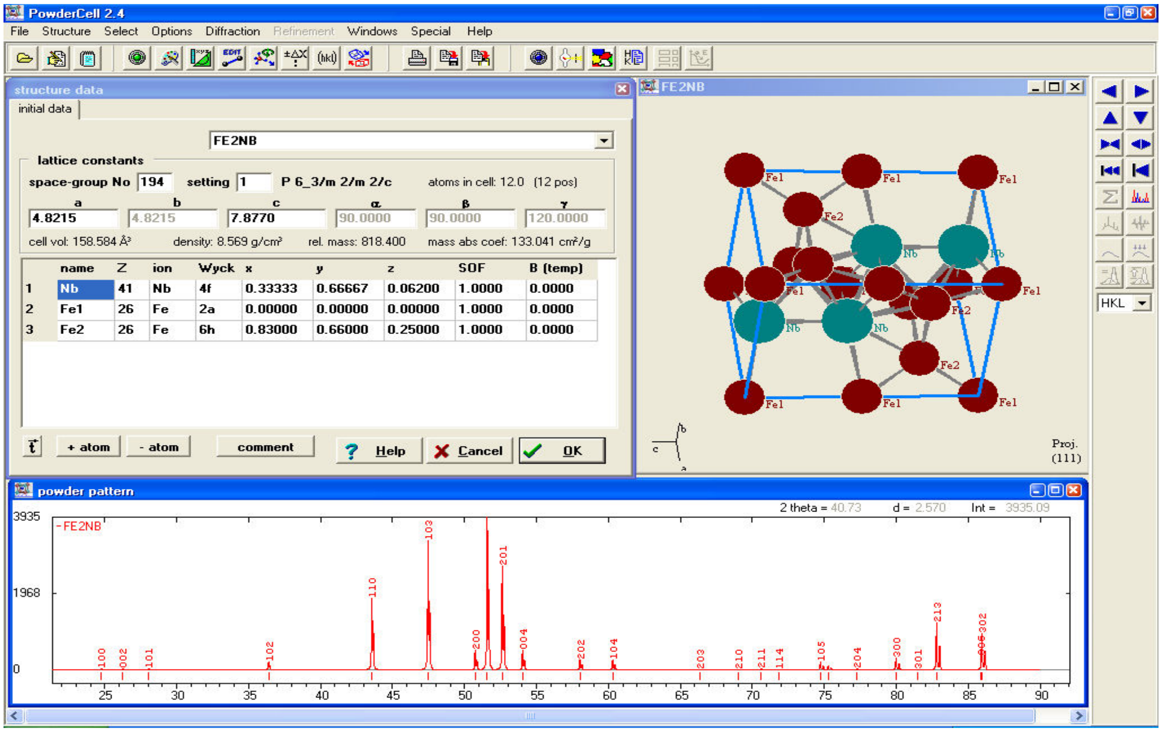
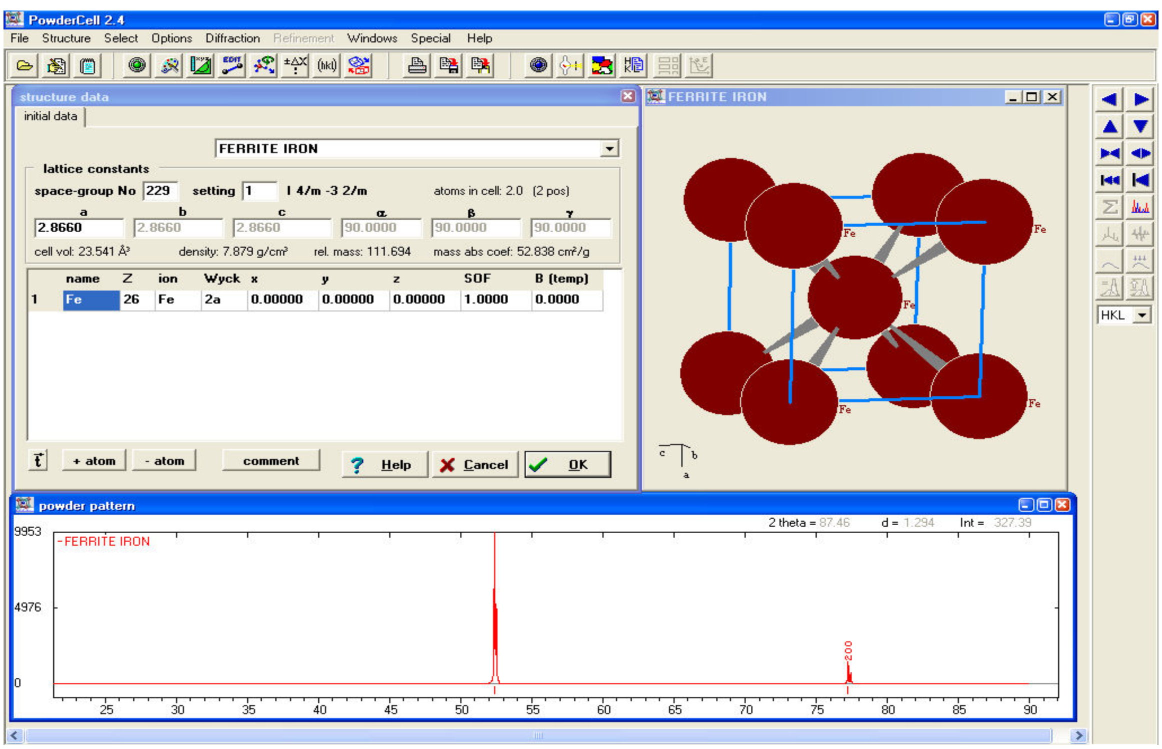
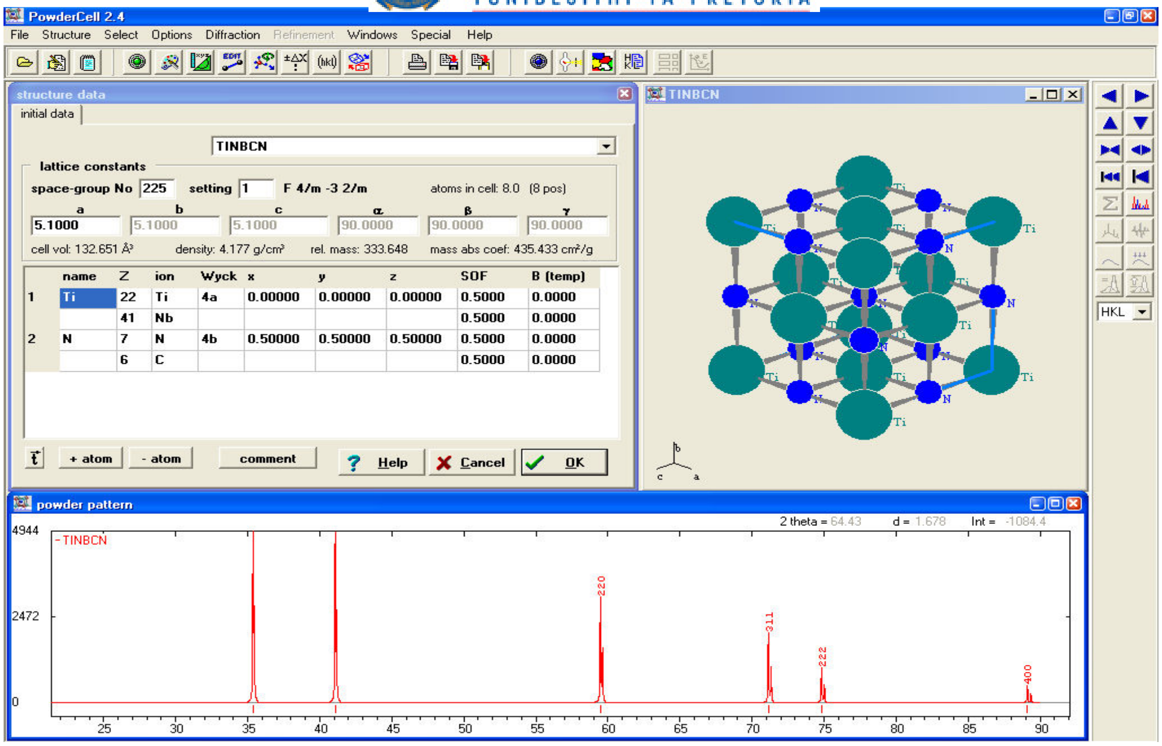
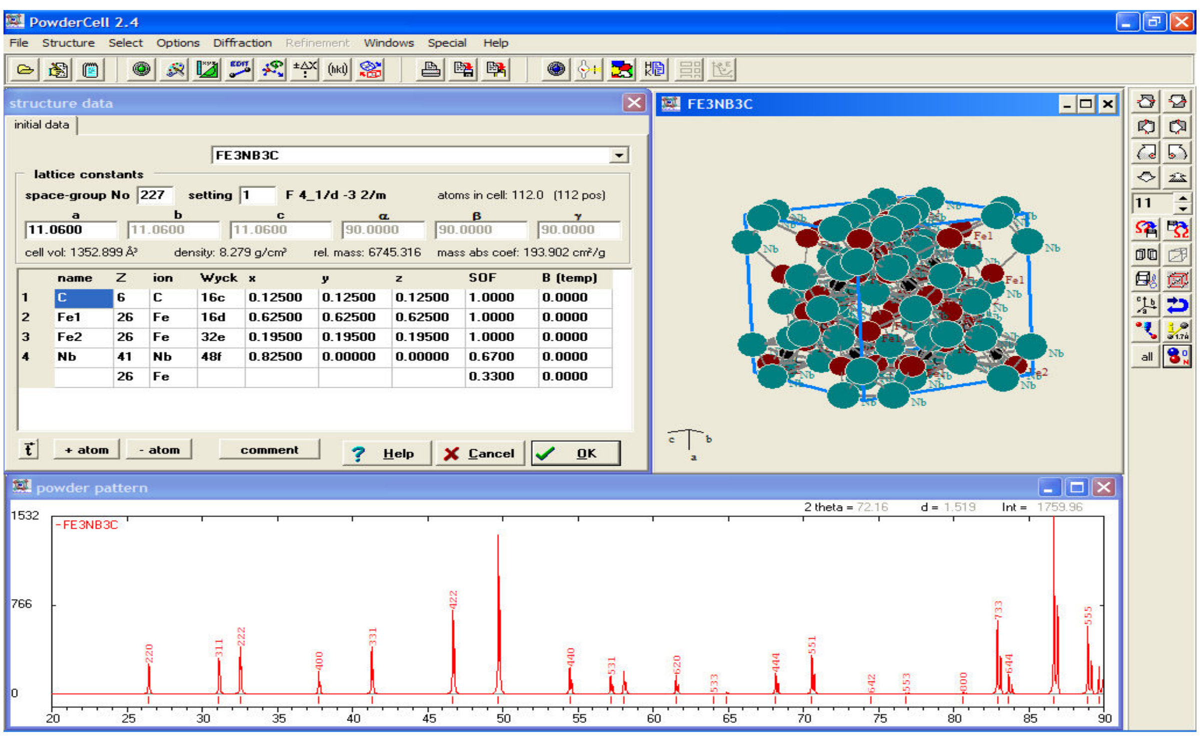
APPENDIX A

SYMMETRY (TRANSLATIONAL AND SPACE GROUP), UNIT CELL DATA AND ATOMIC POSITION PARAMETERS






PowderCell 2.4
File Structure Select Options Diffraction Refinement Windows Special Help
structure data
initial data
TINBCN
lattice constants
space-group No 225 setting 1 F 4/m -3 2/m atoms in cell: 8.0 (8 pos)
a 5.1000 b 5.1000 c 5.1000 α 90.0000 β 90.0000 γ 90.0000
cell vol: 132.651 Å³ density: 4.177 g/cm³ rel. mass: 333.648 mass abs coef: 435.433 cm²/g
name Z ion Wyck x y z SOF B (temp)
1 Ti 22 Ti 4a 0.00000 0.00000 0.00000 0.5000 0.0000
41 Nb 0.5000 0.0000
2 N 7 N 4b 0.50000 0.50000 0.50000 0.5000 0.0000
6 C 0.5000 0.0000
+ atom - atom comment Help Cancel OK
TINBCN
powder pattern
2 theta = 64.43 d = 1.678 Int = -1084.4
TINBCN
220
311
222
400


PowderCell 2.4
File Structure Select Options Diffraction Refinement Windows Special Help
structure data
initial data
FE3NB3C
lattice constants
space-group No 227 setting 1 F 4_1/d -3 2/m atoms in cell: 112.0 (112 pos)
a 11.0600 b 11.0600 c 11.0600 α 90.0000 β 90.0000 γ 90.0000
cell vol: 1352.899 Å³ density: 8.279 g/cm³ rel. mass: 6745.316 mass abs coef: 193.902 cm²/g
name Z ion Wyck x y z SOF B (temp)
1 C 6 C 16c 0.12500 0.12500 0.12500 1.0000 0.0000
2 Fe1 26 Fe 16d 0.62500 0.62500 0.62500 1.0000 0.0000
3 Fe2 26 Fe 32e 0.19500 0.19500 0.19500 1.0000 0.0000
4 Nb 41 Nb 48f 0.82500 0.00000 0.00000 0.6700 0.0000
26 Fe 0.3300 0.0000
+ atom - atom comment Help Cancel OK
FE3NB3C
powder pattern
2 theta = 72.16 d = 1.519 Int = 1759.96
FE3NB3C
220
311
222
400
331
422
440
531
620
533
444
551
642
553
800
733
644
555

APPENDIX B

THERMODYNAMIC MODELLING USING THERMO-CALC® SOFTWARE

Definitions of the Abbreviated Parameters Used In the Calculations

go data – go to thermodynamic database module
sw-dat – switch database
tcfe3 – Thermo-Calc® Steels/Fe-alloys database
def-sys – define system
l-s – list system
get – get data from the database
go p-3 – go to module Poly 3
s-c – set conditions
l-c – list condition
c-e – compute equilibrium
s-a-v – set axis variable
t – temperature
s-d-a – set diagram axis
set – lab – set label
def-mat – define materials

TEMPLATE USED TO CALCULATE EQUILIBRIUM THERMODYNAMIC PARAMETER OF TYPE 441

go data
sw-dat
tcfe3
def-sys
fe c mn co cr b v s si ti ni n al p cu nb o
l-s
CONSTITUENT
*reject phase**
restore phase liquid, fcc, bcc, hcp, laves_phase, m6c, m23c6

get
go p-3
s-c n=1, p=101325, t=1773
s-c w(c)=0.00012
s-c w(mn)=0.0051
s-c w(co)=0.0003
s-c w(cr)=0.1789
s-c w(b)=0.000004
s-c w(v)=0.0012
s-c w(s)=0.00001
s-c w(si)=0.005
s-c w(ti)=0.00153
s-c w(ni)=0.0019
s-c w(n)=0.000085
s-c w(al)=0.00009
s-c w(p)=0.00025
s-c w(cu)=0.0008

```
s-c w(nb)=0.00444
s-c w(o)=0.000076
l-c
@&
c-e
s-a-v
1
t
473
2000
3
save MPO_3533603
step
normal
post
s-d-a x t-c
s-d-a y np(*)
*
plot SCREEN
set-tit
Intermetallic phases
set-lab
d
s-t-m-s
x
s-s x n 450 1800
plot
SCREEN


set-inter
```

TEMPLATE USED TO CALCULATE THE ISOPLETHS OF TYPE 441

```
go p-3
def-mat
tcfe3
fe
Y
c
.012
mn .51
co .03
cr 17.89
v .12
si .5
ti .153
n .0085
nb .444
ni .19
mo .5
s .001
b .0004
al .009
p .0025
cu .08
o .0076

1000
*
liquid, bcc_a2, fcc_a1, laves_phase_c14, m23c6, m3c2, m6c, sigma,
NONE
Y
N
l-e
SCREEN
VWCS
s-a-v 1 w(c)
0
.03
2.5e-4
s-a-v 2 t
200
1800
40
save
map
post
s-p-f
1
plot
SCREEN
s-d-a w-p c
s-d-a x w-p c
s-d-a y t-c
plot
```

```
SCREEN
s-s x n 0 1
s-s y n 200 1600
plot
SCREEN
s-lab n
plot
SCREEN
s-lab b
plot
SCREEN
PLOT,,,,,;
```

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