JMatPro钛合金模块介绍

中仿科技
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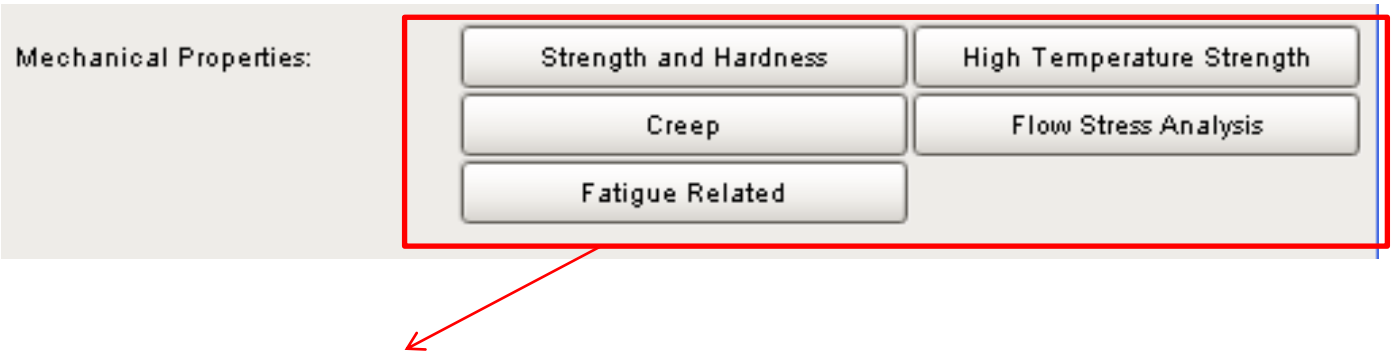
目　　录

- 钛合金背景知识介绍
- 钛合金模块功能介绍、演示
  - ✓ 热力学计算
  - ✓ 凝固计算
  - ✓ 热物性能计算
  - ✓ 机械性能计算
  - ✓ 相转变计算
  - ✓ 数据导出

四.机械性能的计算



① Strength and Hardness: 室温机械性能计算

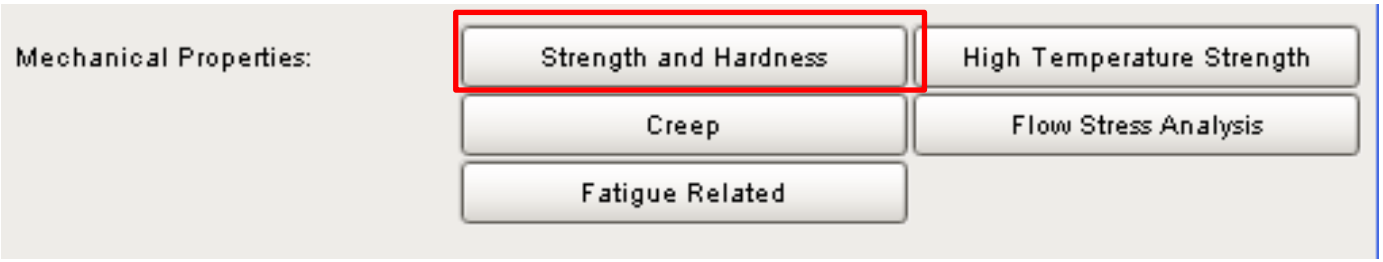
② High Temperature Strength: 高温屈服强度计算

③ Creep：蠕变计算

④ Flow Stress Analysis: 流动应力分析

⑤ Fatigue Related: 疲劳破坏分析

四.机械性能计算—1. Strength and Hardness



屈服强度（σ_s /$\sigma_{0.2}$）：材料开始产生明显塑性变形时的应力

硬度：材料局部抵抗硬物压入其表面的能力

① 维氏硬度（VPN）

② 洛氏硬度（HRC）

③ 布氏硬度（HB）

抗张强度：材料或构件受拉力时抵抗破坏的能力

计算模型

① 计算室温组织

② 计算屈服强度

考虑溶质元素

固溶强化 $\sigma_y = \sigma_0 + k_{den}\lambda^{-0.5}$ （Hall—Petch公式）

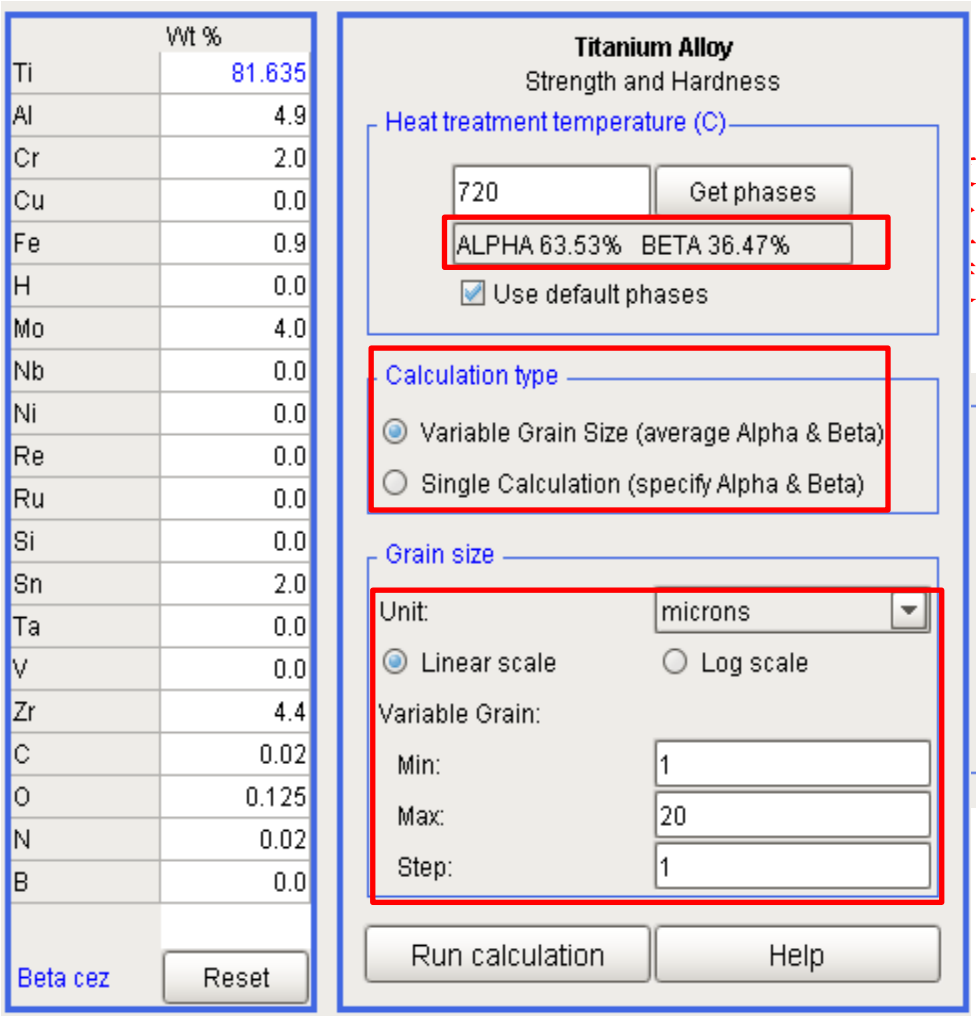
③ 计算硬度和抗张强度

硬度的计算： $Hv = C\sigma_y (40)^m$

抗张强度的计算： $\sigma_t = \sigma_y (40)^m (1-m)(\frac{12.5m}{1-m})^m$

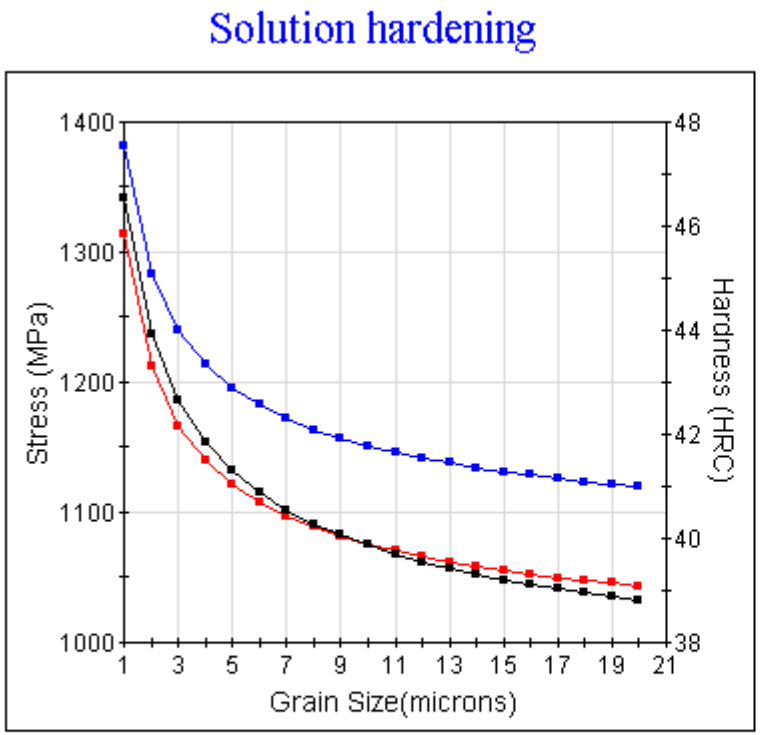
加工硬化数m： $m = a\exp(b\sigma_y)$

参数设置界面



置热处理温度
温组织与该温
下的组织相同

计算结果



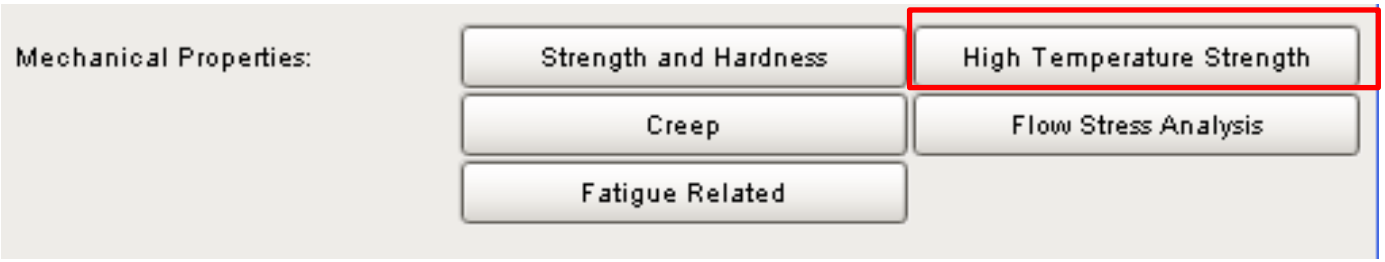
Heat treatment : 720.0 C
ALPHA 63.53% BETA 36.47%
Hall-Petch : 0.36 MN/m^3/2

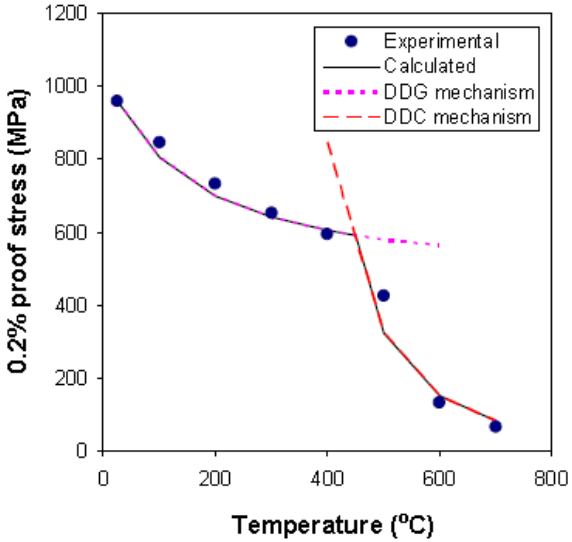
COMPOSITION (Wt%)
Ti: 81.635
Al: 4.9
Cr: 2.0
Fe: 0.9
Mo: 4.0
Sn: 2.0
Zr: 4.4
C: 0.02
O: 0.125
N: 0.02

wt °C MPa HRC µm lin

选择一种晶粒尺寸

四.机械性能计算—2. High Temperature Strength





合金变形的两种机制

DDG（dislocation glide）：位错运动

DDC（ dislocation climb）：位错攀升

计算模型

低温下

考虑内在因素：溶质元素

固溶强化： $\sigma_y = \sigma_0 + k_{den}\lambda^{-0.5}$ （Hall-Petch公式）

考虑外在因素：应变速率$\dot{\varepsilon}$

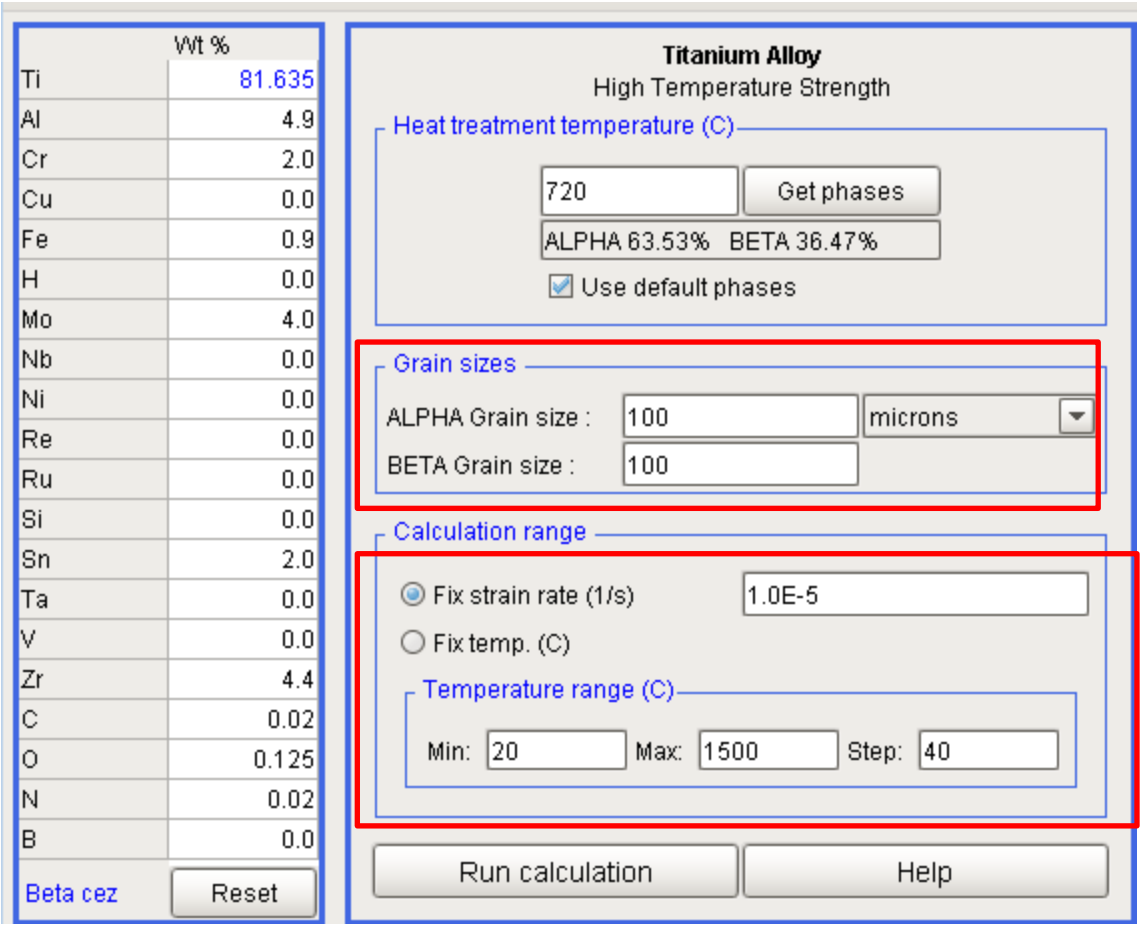
$$\sigma_{(y,\dot{\varepsilon})} = \sigma_{(y,\dot{\varepsilon}_0)}(\dot{\varepsilon}/\dot{\varepsilon}_0)^m$$

高温下

位错可借助于外界提供的热激活能和空位扩散克服某些短程障碍，发生位错攀移，从而导致变形

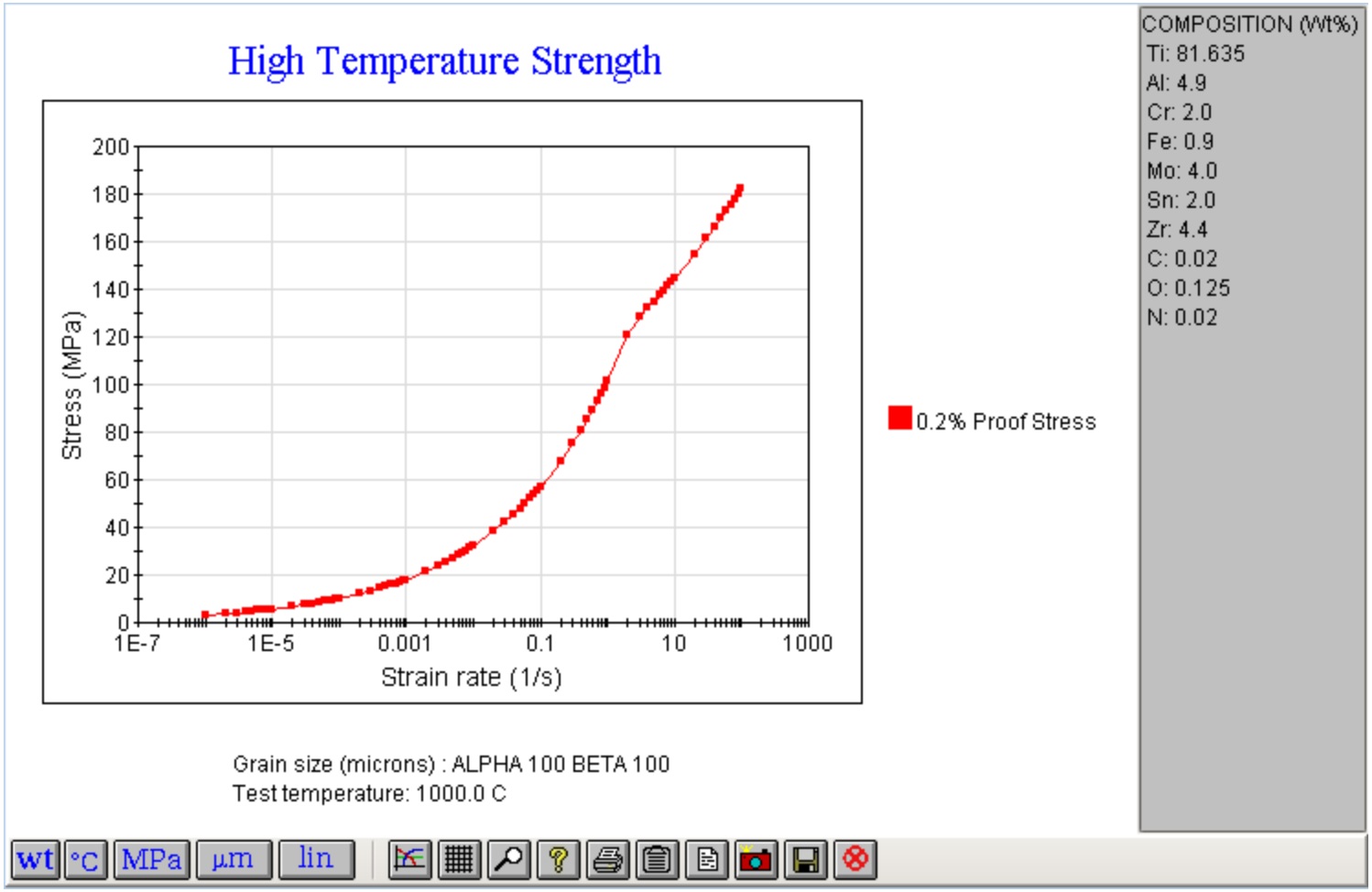
$$\sigma_y(T) = \alpha + \beta exp(\frac{-Q}{RT})$$

参数设置界面

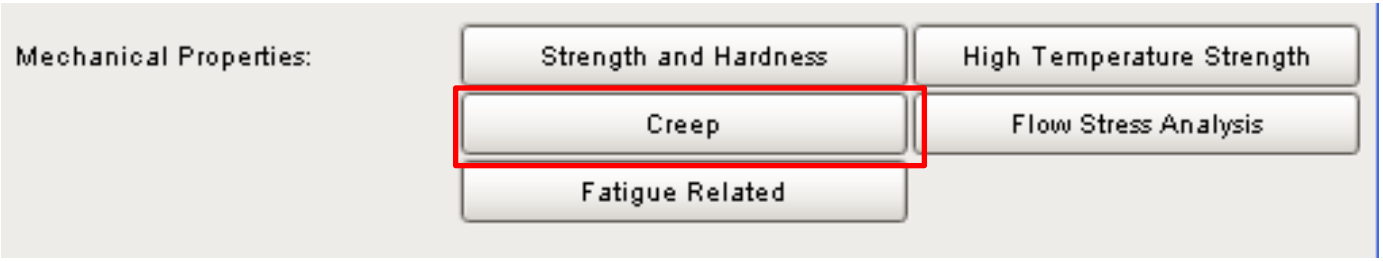


选择计算类型

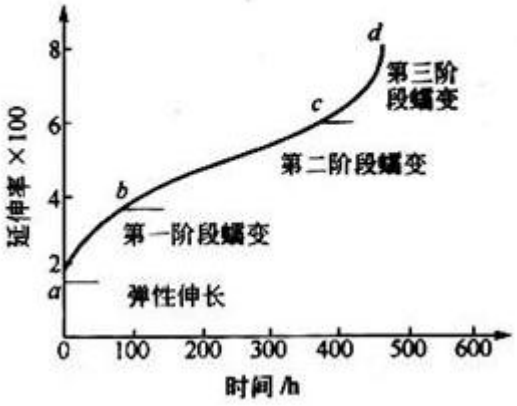
计算结果


High Temperature Strength
Stress (MPa)
200
180
160
140
120
100
80
60
40
20
0
1E-7
1E-5
0.001
0.1
10
1000
Strain rate (1/s)
0.2% Proof Stress
COMPOSITION (Wt%)
Ti: 81.635
Al: 4.9
Cr: 2.0
Fe: 0.9
Mo: 4.0
Sn: 2.0
Zr: 4.4
C: 0.02
O: 0.125
N: 0.02
Grain size (microns) : ALPHA 100 BETA 100
Test temperature: 1000.0 C
wt
°C
MPa
µm
lin

四.机械性能计算—3. Creep



高温蠕变：固体材料在保持应力不变的情况下，应变随时间的延长而增加的现象



① 初始蠕变：应变随时间延续而增加，但增加的速度逐渐减慢

② 稳定蠕变：应变随时间延续而匀速增加，这个阶段较长

③ 加速蠕变：应变随时间延续而加速增加,直达破裂点

计算模型

① 稳态蠕变速率于外加应力关系：

$$\dot{\varepsilon} = AD_{eff}[\frac{r_{SFE}}{Gb}]^n[\frac{\sigma-\sigma_0}{E}]^m$$

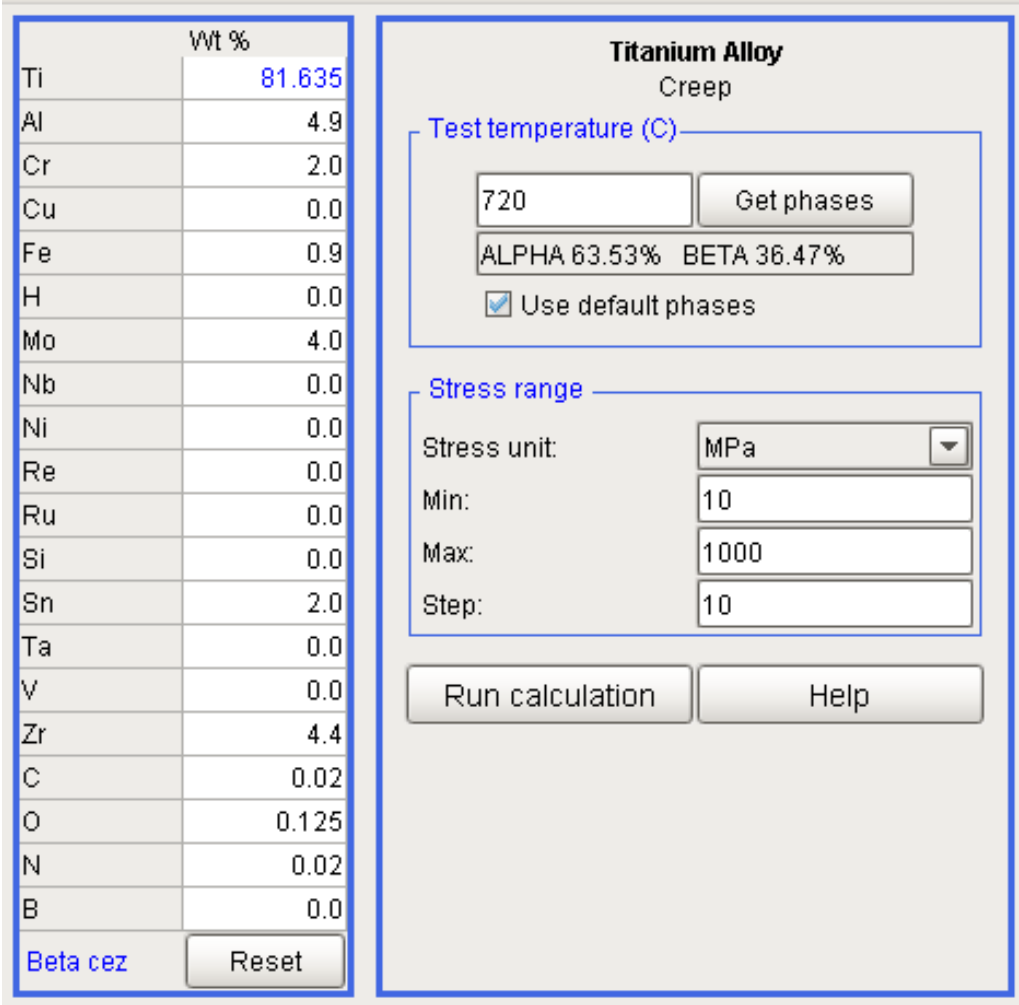
考虑了堆垛层错能（r_{SFE}）和背应力函数（σ_0）

$$\sigma_0 = 0.75\sigma_P, \sigma < 4/3\sigma_P \qquad \sigma_0 = \sigma_P, \sigma > 4/3\sigma_P$$

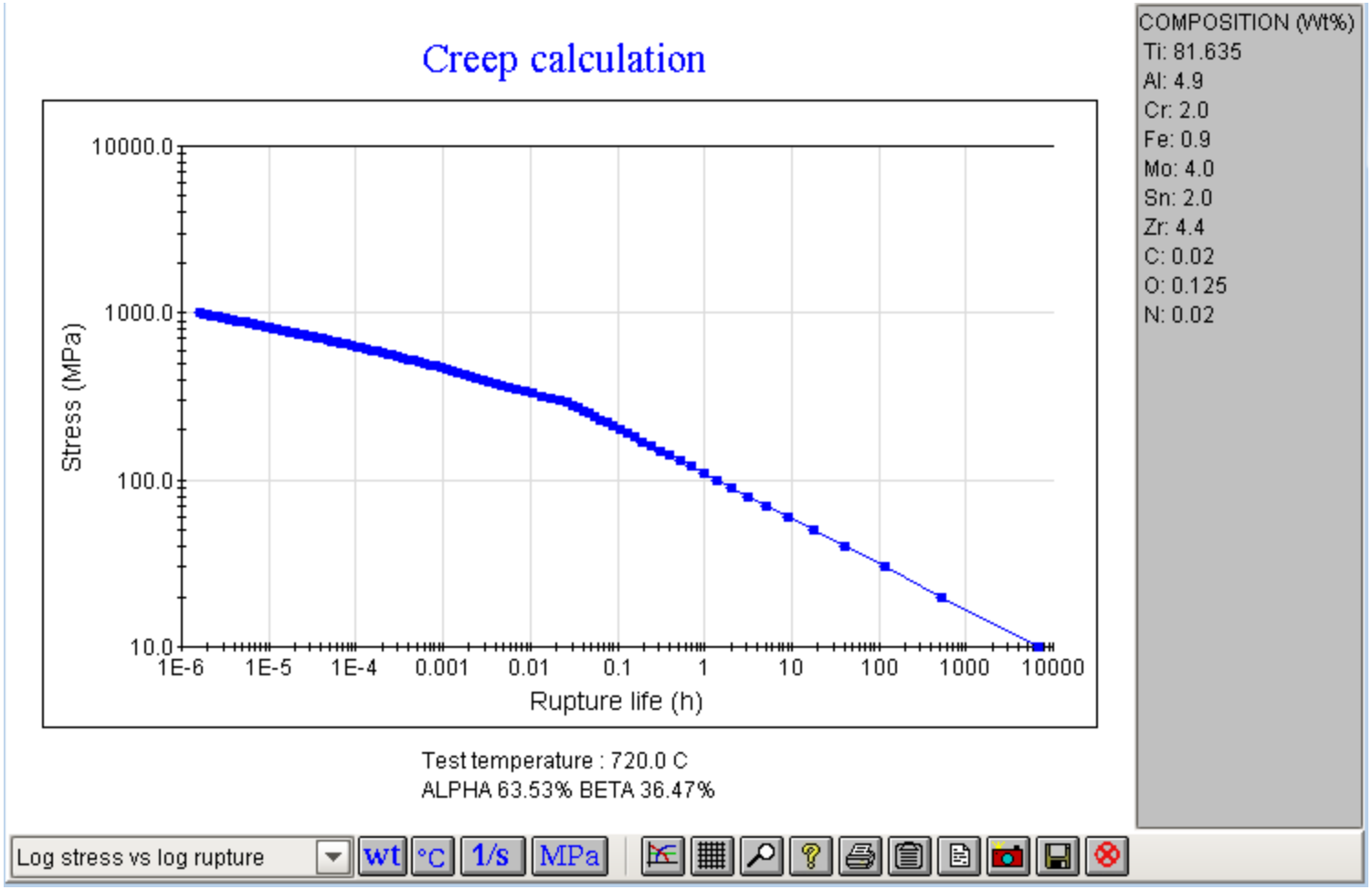
② 蠕变速率与破坏时间关系：

$$t_r = a\dot{\varepsilon}^b$$

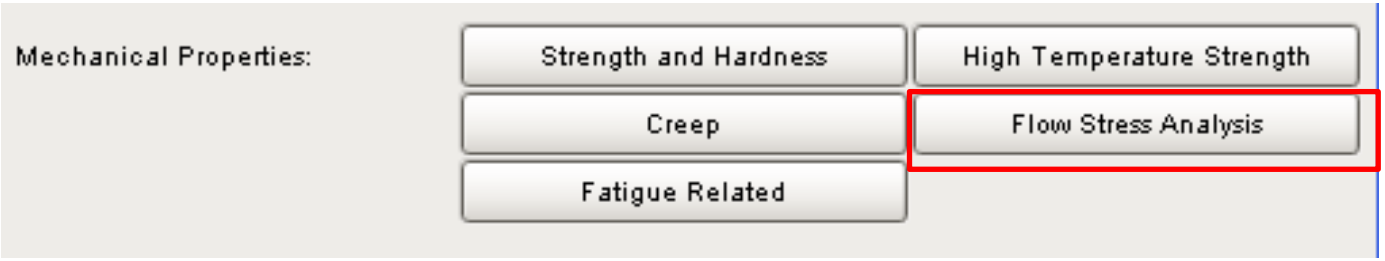
参数设置界面


Wt %
Ti 81.635
Al 4.9
Cr 2.0
Cu 0.0
Fe 0.9
H 0.0
Mo 4.0
Nb 0.0
Ni 0.0
Re 0.0
Ru 0.0
Si 0.0
Sn 2.0
Ta 0.0
V 0.0
Zr 4.4
C 0.02
O 0.125
N 0.02
B 0.0
Beta cez
Reset
Titanium Alloy
Creep
Test temperature (C)
720
Get phases
ALPHA 63.53% BETA 36.47%
Use default phases
Stress range
Stress unit:
MPa
Min:
10
Max:
1000
Step:
10
Run calculation
Help

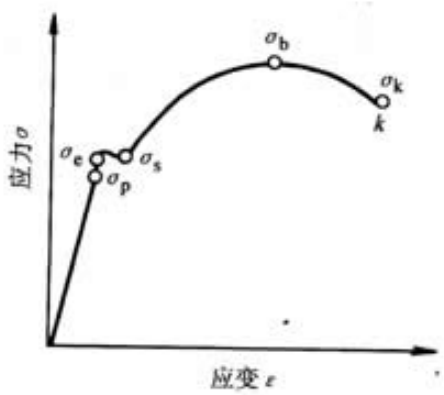
计算结果


Creep calculation
10000.0
1000.0
100.0
10.0
Stress (MPa)
1E-6
1E-5
1E-4
0.001
0.01
0.1
1
10
100
1000
10000
Rupture life (h)
Test temperature : 720.0 C
ALPHA 63.53% BETA 36.47%
COMPOSITION (Wt%)
Ti: 81.635
Al: 4.9
Cr: 2.0
Fe: 0.9
Mo: 4.0
Sn: 2.0
Zr: 4.4
C: 0.02
O: 0.125
N: 0.02
Log stress vs log rupture
wt
°C
1/s
MPa

四.机械性能计算—4. Flow Stress Analysis



流动应力：对应于变形过程某一瞬时进行塑性流动所需的真实应力叫做该瞬时的屈服应力（Y），亦称流动应力



计算模型

① 低温DDG机制

a) 只考虑应变对流动应力的影响

$$\sigma = K\varepsilon^n$$

加工硬化数 $n = a\exp(b\sigma_{0.2})$ $K = \sigma_{0.2}/\varepsilon_0^n$

b) 同时考虑应变速率对流动应力的影响

$$\sigma = K\varepsilon^n\dot{\varepsilon}^m$$

计算模型

② 高温DDC机制

初期蠕变： $\dot{\varepsilon}_p = \frac{\dot{\varepsilon}_s}{K_0}\ln[1 + \frac{\dot{\varepsilon}_i - \dot{\varepsilon}_s}{\dot{\varepsilon}_s}(1 - e^{-k_0 t})]$ $\dot{\varepsilon}_p$：初期蠕变速率

稳定蠕变： $\dot{\varepsilon}_s = AD(\frac{Gb}{RT})\left(\frac{\sigma}{E}\right)^{n'}$ $\dot{\varepsilon}_s$：稳定蠕变速率

加速蠕变： $\dot{\varepsilon}_t = [2C_d + \left(\frac{t}{R_l}\right)^4]\dot{\varepsilon}_s$ $\dot{\varepsilon}_t$：加速蠕变速率

应变—应变速率关系： $\varepsilon = (\dot{\varepsilon}_p + \dot{\varepsilon}_s + \dot{\varepsilon}_t)t$

参数设置界面

	Wt %
Ti	81.635
Al	4.9
Cr	2.0
Cu	0.0
Fe	0.9
H	0.0
Mo	4.0
Nb	0.0
Ni	0.0
Re	0.0
Ru	0.0
Si	0.0
Sn	2.0
Ta	0.0
V	0.0
Zr	4.4
C	0.02
O	0.125
N	0.02
B	0.0
Beta cez	Reset

Titanium Alloy

Flow Stress Analysis

Heat treatment temperature (C)

720 | Get phases

ALPHA 63.53% BETA 36.47%

☑ Use default phases

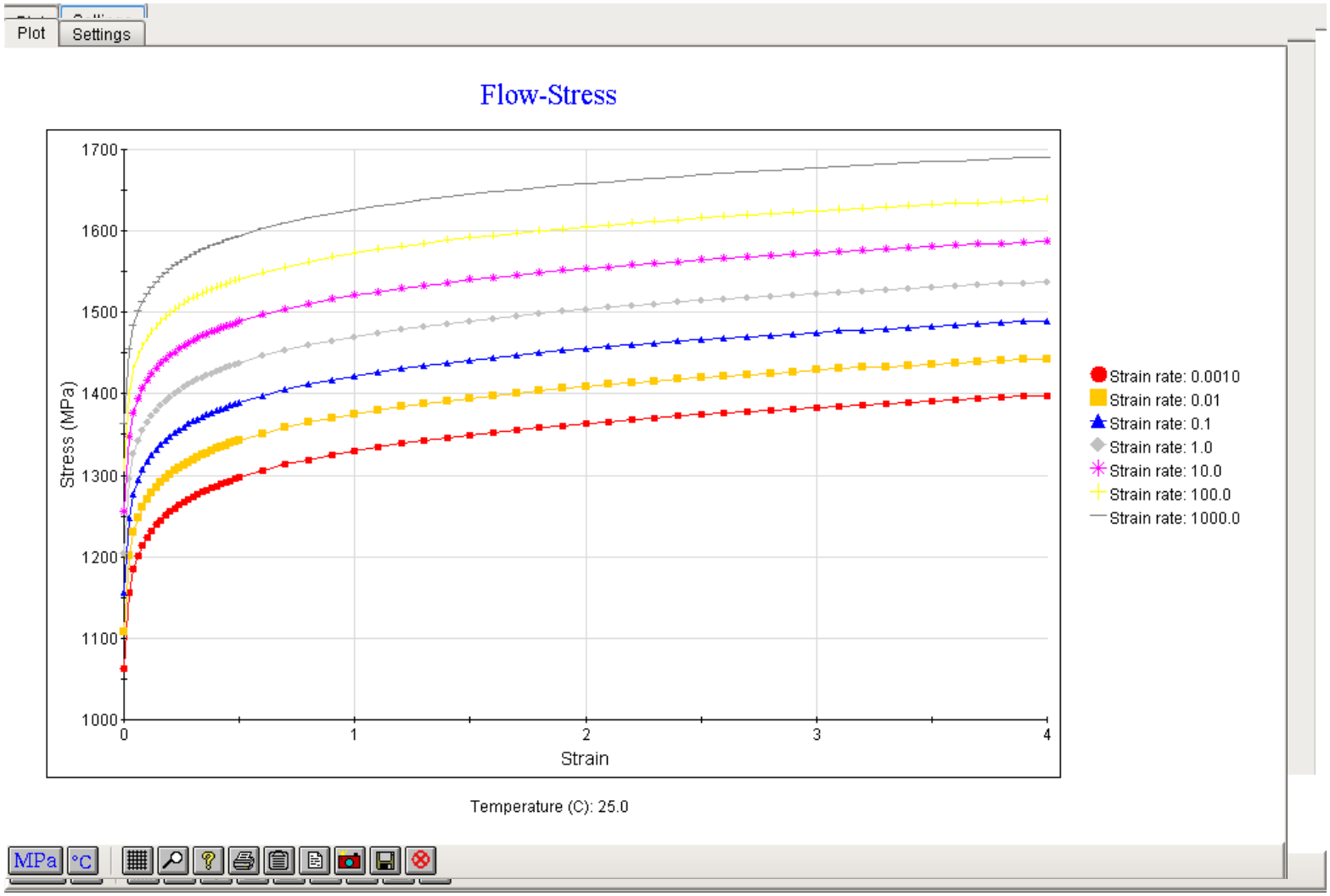
Grain sizes

ALPHA Grain size : 100 | microns

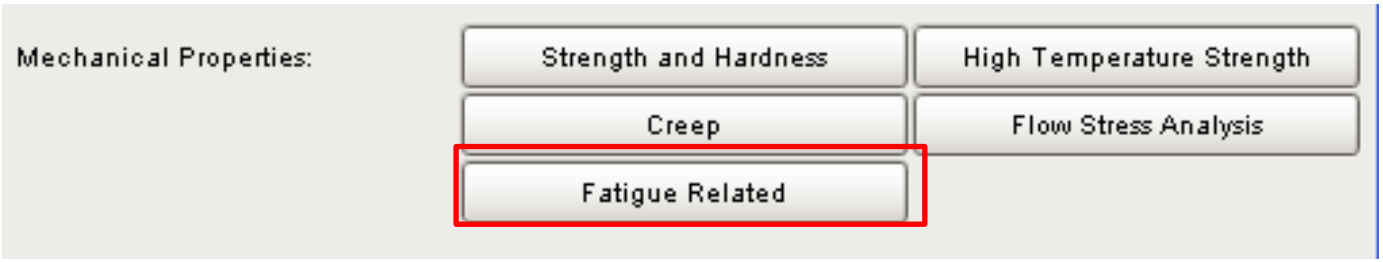
BETA Grain size : 100

Run calculation | Help

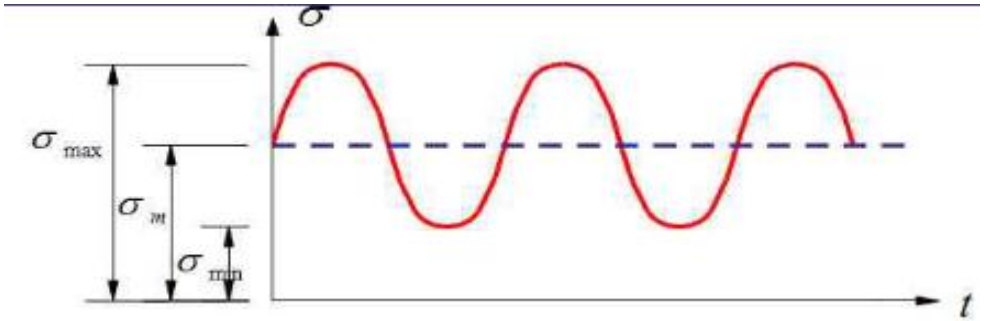
计算结果


Plot
Settings
Flow-Stress
Stress (MPa)
1700
1600
1500
1400
1300
1200
1100
1000
0
1
2
3
4
Strain
Strain rate: 0.0010
Strain rate: 0.01
Strain rate: 0.1
Strain rate: 1.0
Strain rate: 10.0
Strain rate: 100.0
Strain rate: 1000.0
Temperature (C): 25.0
MPa
°C

四.机械性能计算—5. Fatigue Related



疲劳破坏：材料在低于静态极限强度载荷的循环载荷作用下，出现断裂破坏的现象.



载荷的大小甚至方向呈周期变化

$\Delta\sigma=\sigma_{max}-\sigma_{min}$ 应力范围（应力幅度）

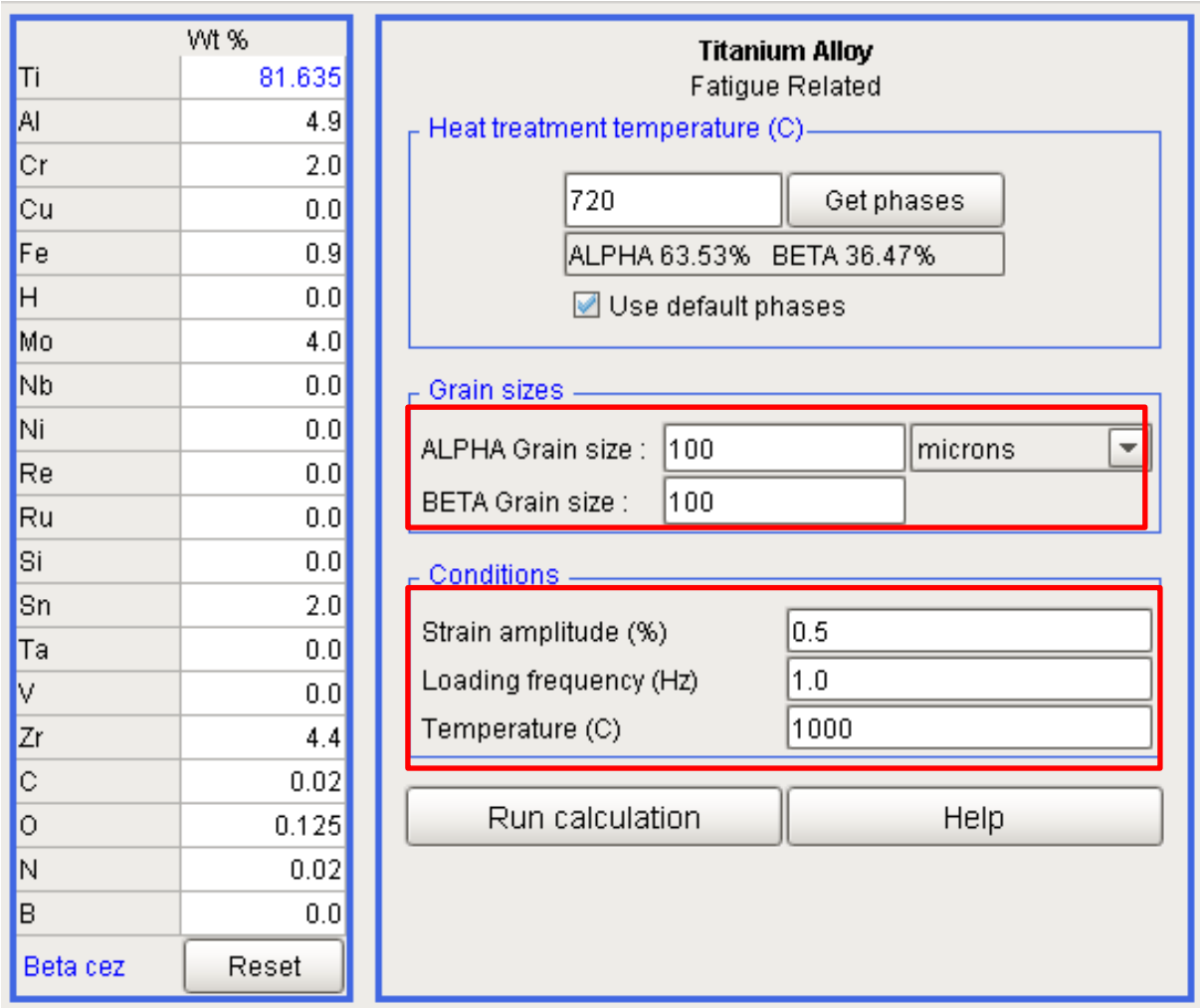
$\Delta\varepsilon=\varepsilon_{max}-\varepsilon_{min}$ 应变范围（应变幅度）

计算模型

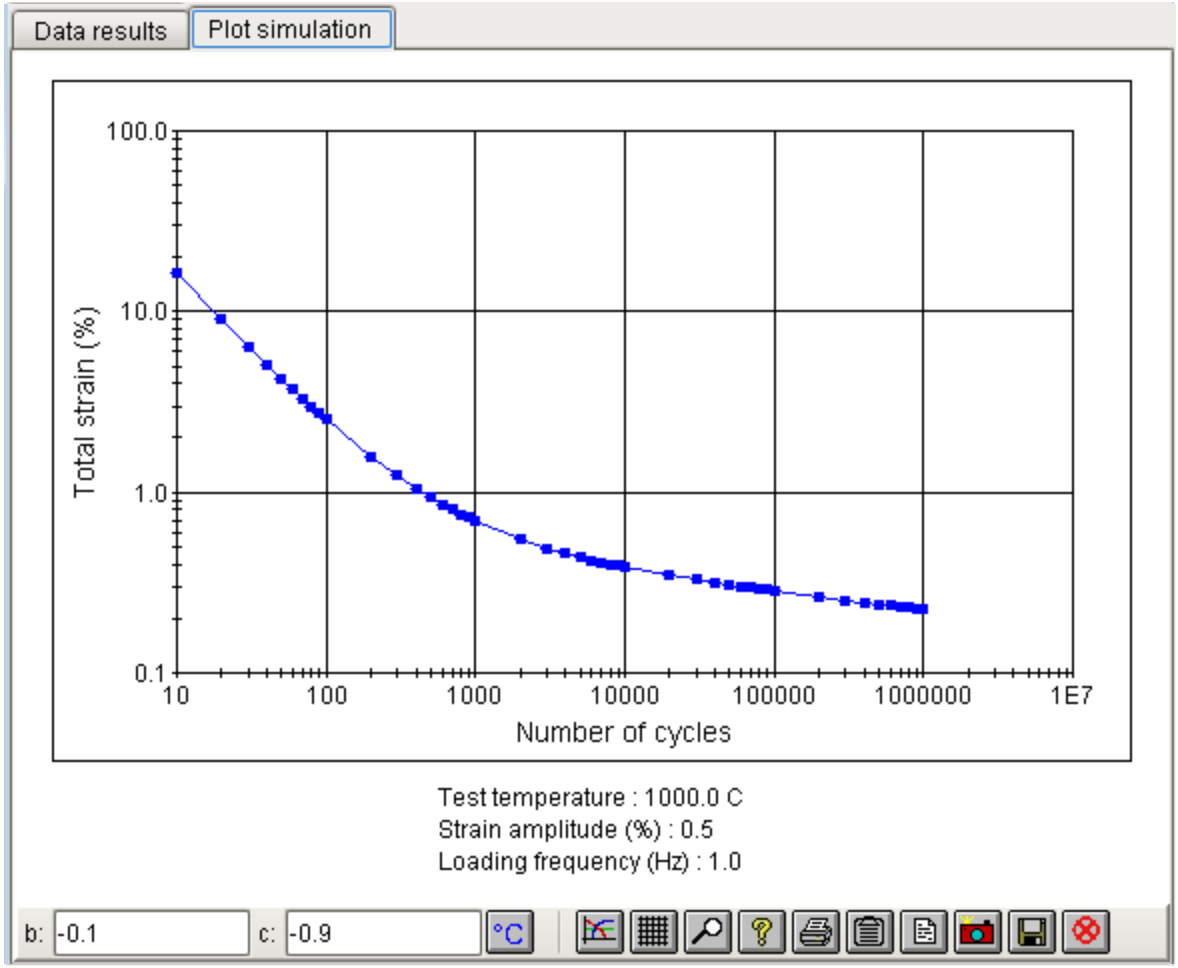
对于疲劳分析采用$\Delta\varepsilon$-N曲线

Coffin-Manson方程 $$\frac{\Delta\varepsilon}{2}=\frac{\Delta\varepsilon_e}{2}+\frac{\Delta\varepsilon_P}{2}=\frac{\sigma_f^{'}}{E}(2N)^b+\varepsilon_f^{'}(2N)^c$$

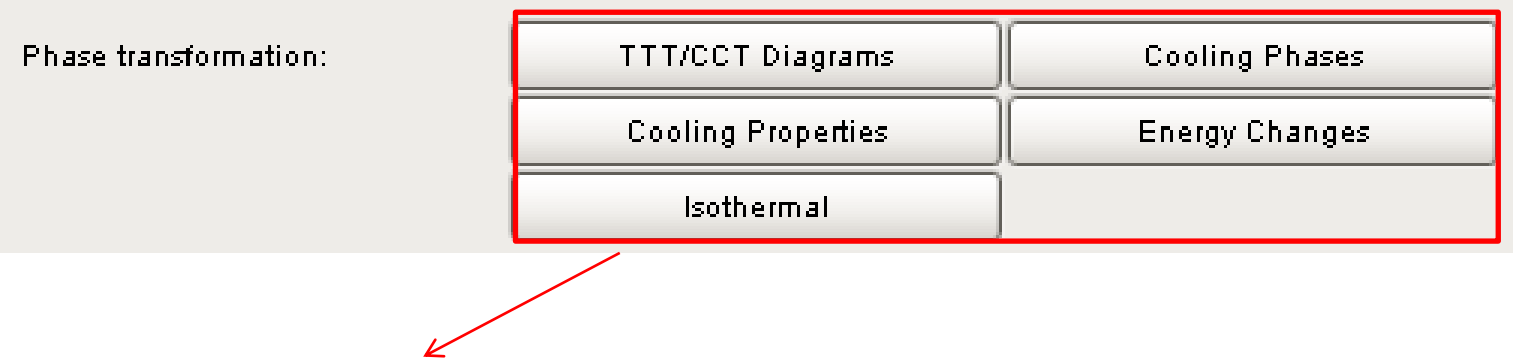
参数设置界面


Wt %
Ti 81.635
Al 4.9
Cr 2.0
Cu 0.0
Fe 0.9
H 0.0
Mo 4.0
Nb 0.0
Ni 0.0
Re 0.0
Ru 0.0
Si 0.0
Sn 2.0
Ta 0.0
V 0.0
Zr 4.4
C 0.02
O 0.125
N 0.02
B 0.0
Beta cez
Reset
Titanium Alloy
Fatigue Related
Heat treatment temperature (C)
720
Get phases
ALPHA 63.53% BETA 36.47%
Use default phases
Grain sizes
ALPHA Grain size : 100
microns
BETA Grain size : 100
Conditions
Strain amplitude (%) 0.5
Loading frequency (Hz) 1.0
Temperature (C) 1000
Run calculation
Help

计算结果


Data results
Plot simulation
100.0
10.0
1.0
0.1
Total strain (%)
10
100
1000
10000
100000
1000000
1E7
Number of cycles
Test temperature : 1000.0 C
Strain amplitude (%) : 0.5
Loading frequency (Hz) : 1.0
b: -0.1
c: -0.9
°C

五.相转变计算



① TTT/CCT Diagrams：绘制TTT/CCT图

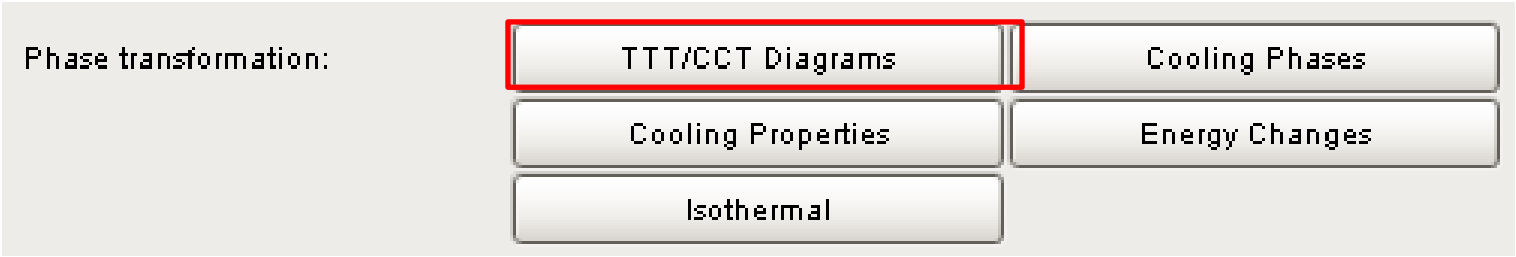
② Isothermal：等温时效

③ Cooling Phases：计算不同冷速下的相转变

④ Cooling Properties：计算不同冷速下的性能

⑤ Energy Changes：不同温度下两相的吉布斯自由能之差

五.相转变计算——1.TTT/CCT图绘制



TTT图：反映合金在进行热处理时按照等温冷却的方式冷却，转变产物类型以及转变量与时间，温度之间的关系曲线

CCT图：反映合金在进行热处理时按照连续冷却的方式冷却，转变产物类型以及转变量与冷却速度的关系曲线

TTT/CCT图计算模型

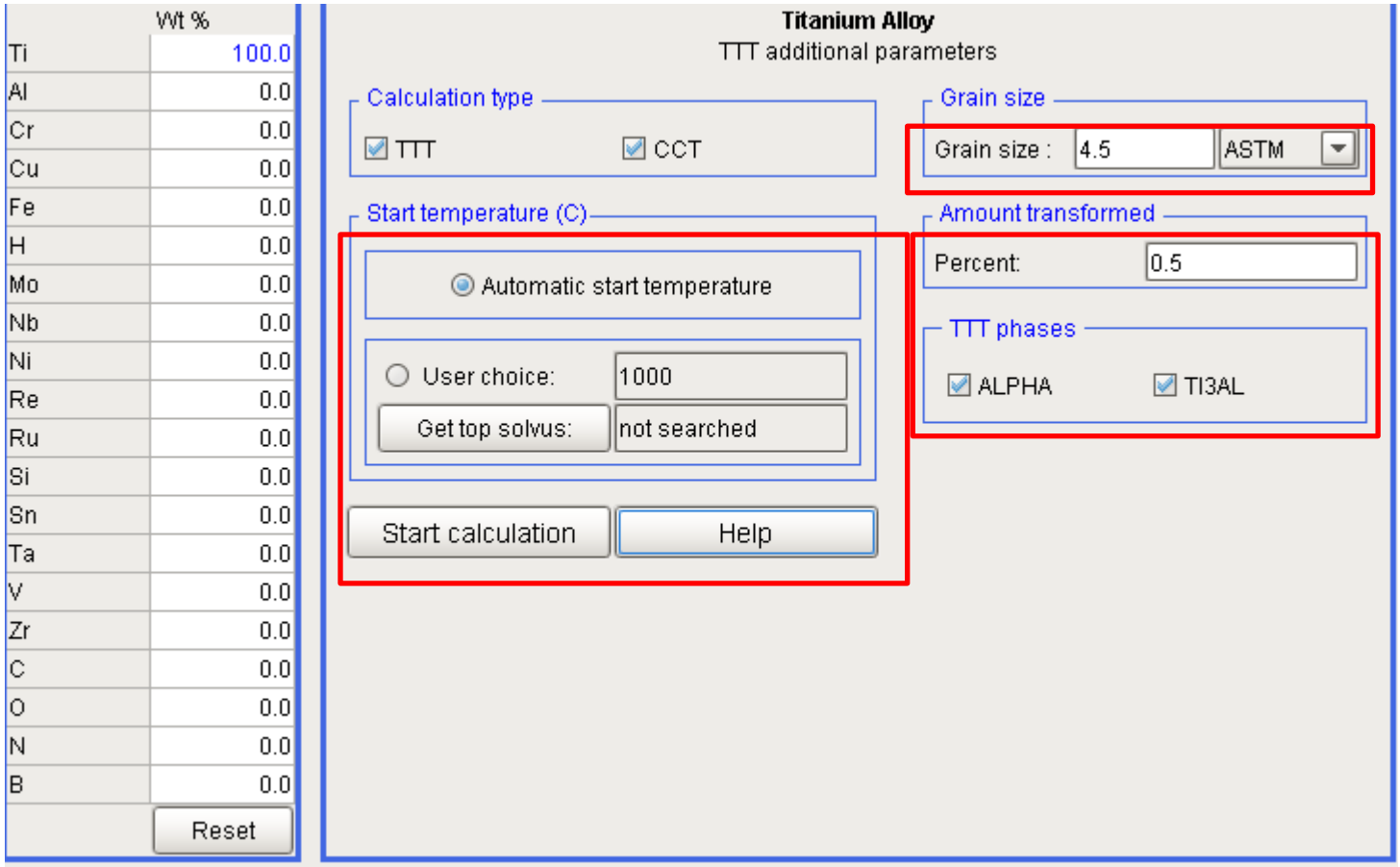
采用经典的Johnson—Mehl—Avrami方程

$$x（T，t）=\frac{V（T）}{Veq(T)}=1-\exp(-\frac{\pi}{3}NrG_r^3t^4)$$

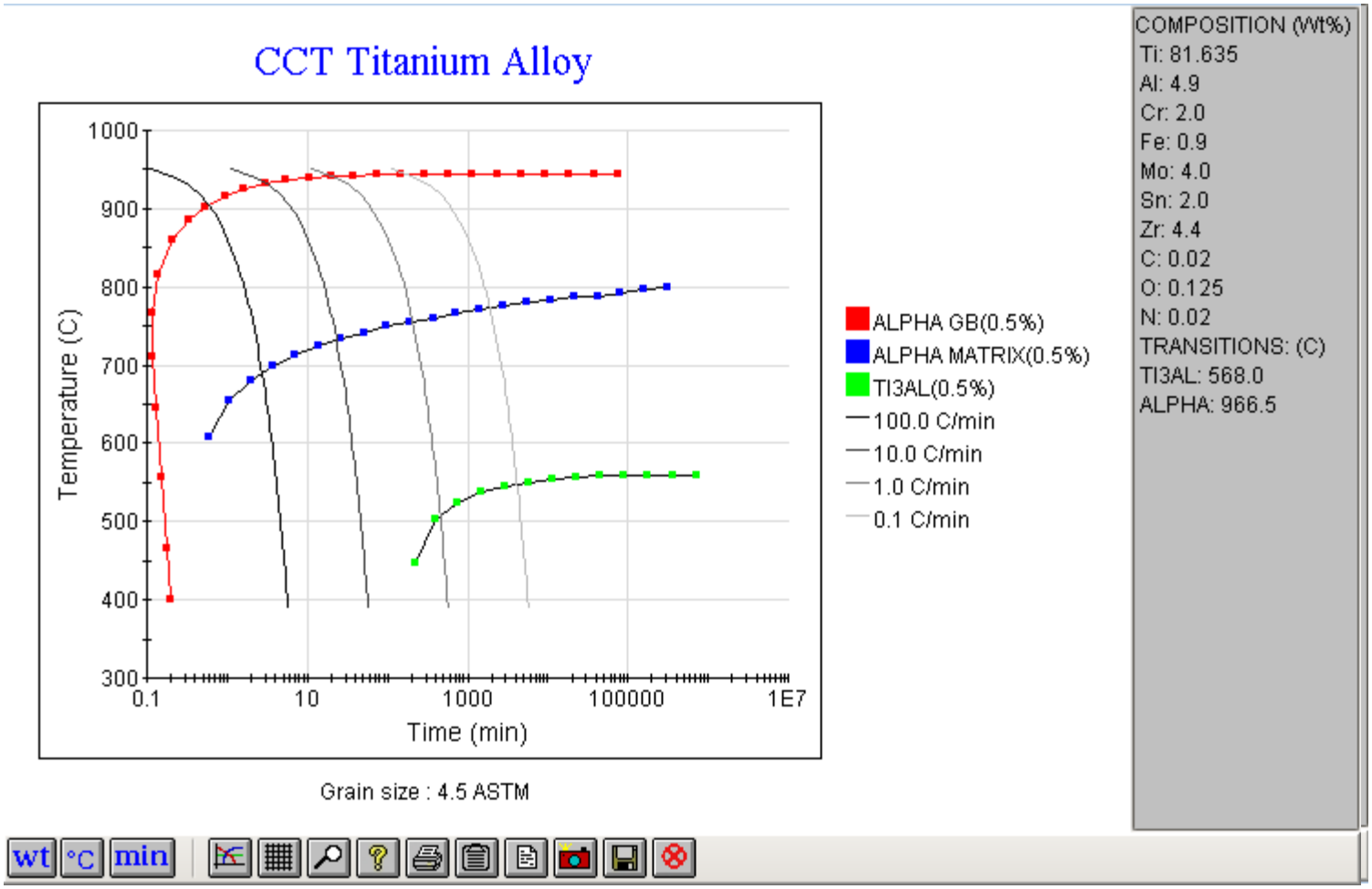
形核速率：$Nr=\frac{N_0D_{eff}}{a_0^2}\exp(-\frac{G^*}{kT})$

生长速率：$Gr=bD_{eff}(\frac{\Delta G_m}{RT})$

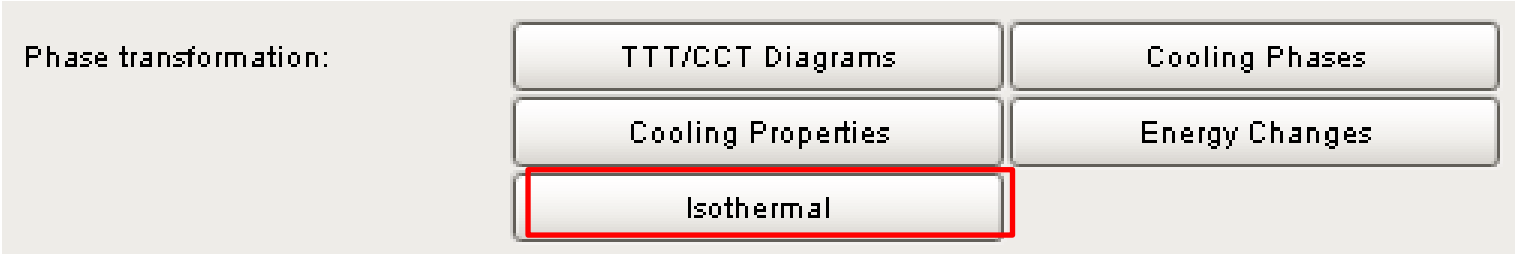
参数设置界面


Wt %
Ti 100.0
Al 0.0
Cr 0.0
Cu 0.0
Fe 0.0
H 0.0
Mo 0.0
Nb 0.0
Ni 0.0
Re 0.0
Ru 0.0
Si 0.0
Sn 0.0
Ta 0.0
V 0.0
Zr 0.0
C 0.0
O 0.0
N 0.0
B 0.0
Reset
Titanium Alloy
TTT additional parameters
Calculation type
TTT
CCT
Grain size
Grain size : 4.5
ASTM
Start temperature (C)
Automatic start temperature
User choice: 1000
Get top solvus: not searched
Amount transformed
Percent: 0.5
TTT phases
ALPHA
TI3AL
Start calculation
Help

计算结果


CCT Titanium Alloy
Temperature (C)
1000
900
800
700
600
500
400
300
0.1
10
1000
100000
1E7
Time (min)
ALPHA GB(0.5%)
ALPHA MATRIX(0.5%)
TI3AL(0.5%)
100.0 C/min
10.0 C/min
1.0 C/min
0.1 C/min
COMPOSITION (Wt%)
Ti: 81.635
Al: 4.9
Cr: 2.0
Fe: 0.9
Mo: 4.0
Sn: 2.0
Zr: 4.4
C: 0.02
O: 0.125
N: 0.02
TRANSITIONS: (C)
TI3AL: 568.0
ALPHA: 966.5
Grain size : 4.5 ASTM
wt
°C
min

五.相转变计算——2.Isothermal

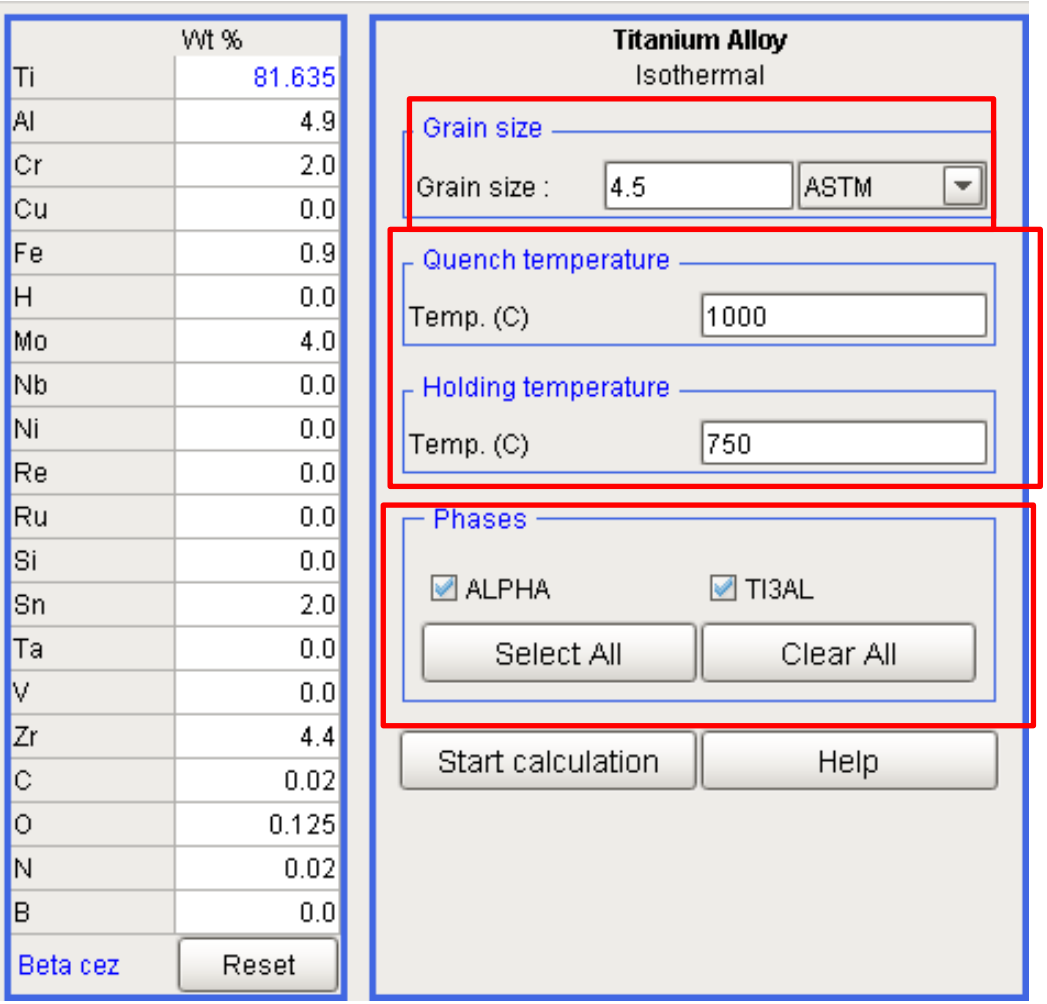


脱溶：从过饱和固溶体中析出第二相（沉淀相）或形成溶质原子偏聚区及亚稳定过渡相的过程

时效：在脱溶过程中，合金机械性能，物理性能，化学性能等随之变化的现象

回火：将淬火组织加热到某一温度，保温一定时间，使淬火组织转变为稳定的回火组织，然后以适当方式冷却到室温

参数设置界面



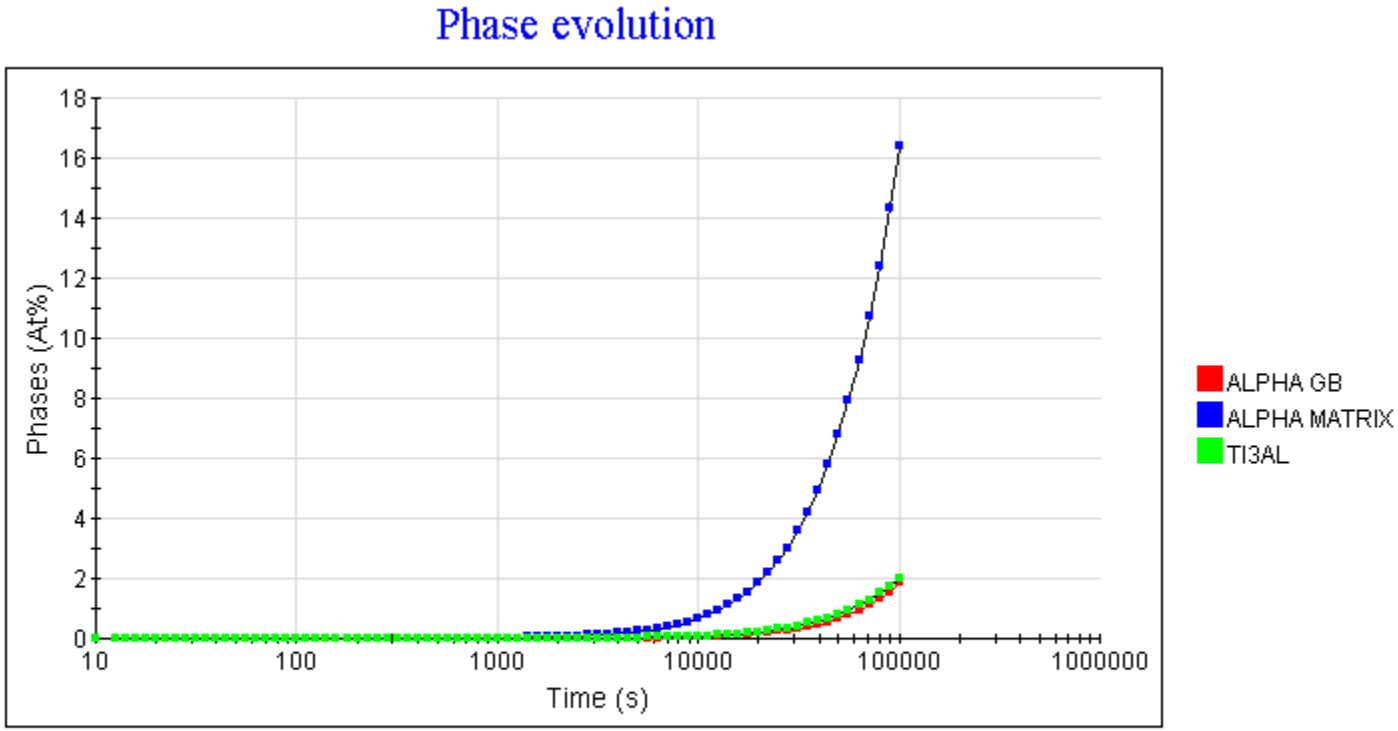
设置晶粒尺寸

设置淬火温度

以及回火温度

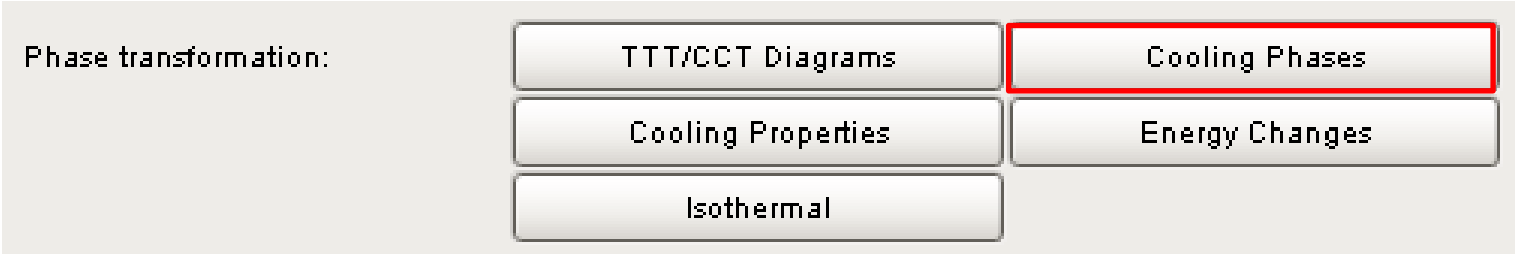
选择计算的相

计算结果



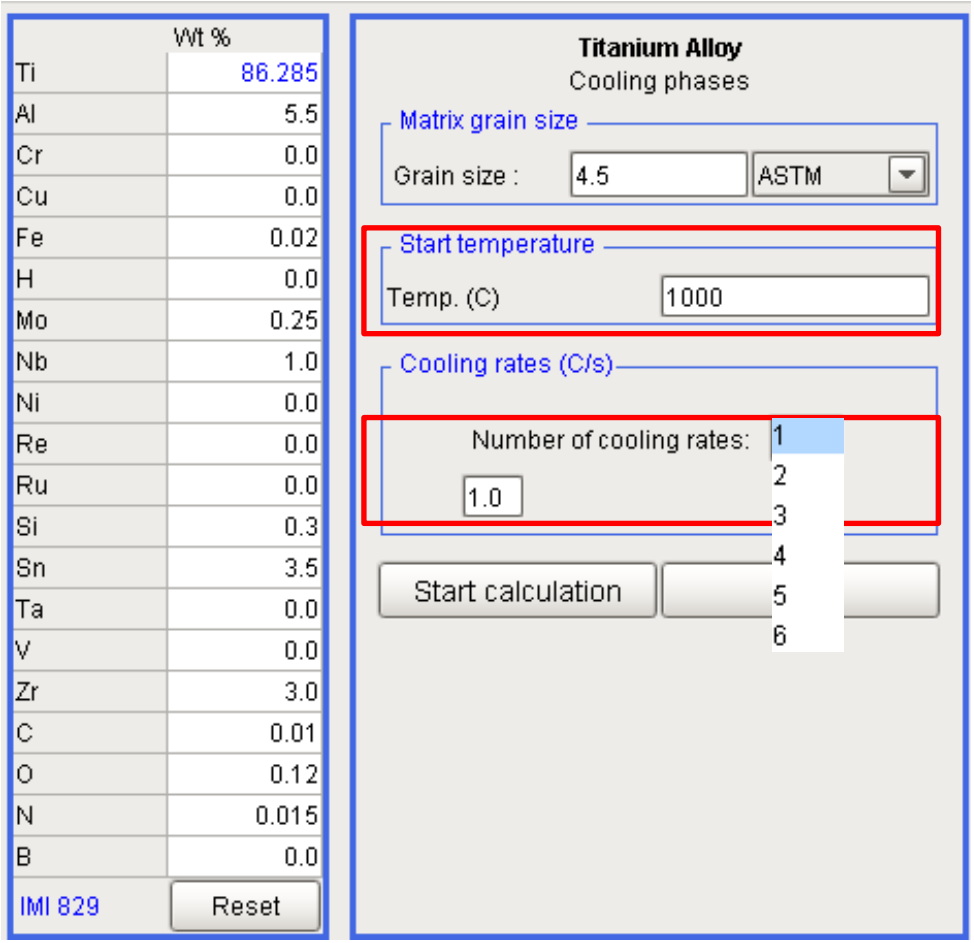
Holding temperature (C) : 400.0
Quench temperature (C) : 1000.0
Grain size : 4.5 ASTM

五.相转变计算——3.Cooling Phsaes

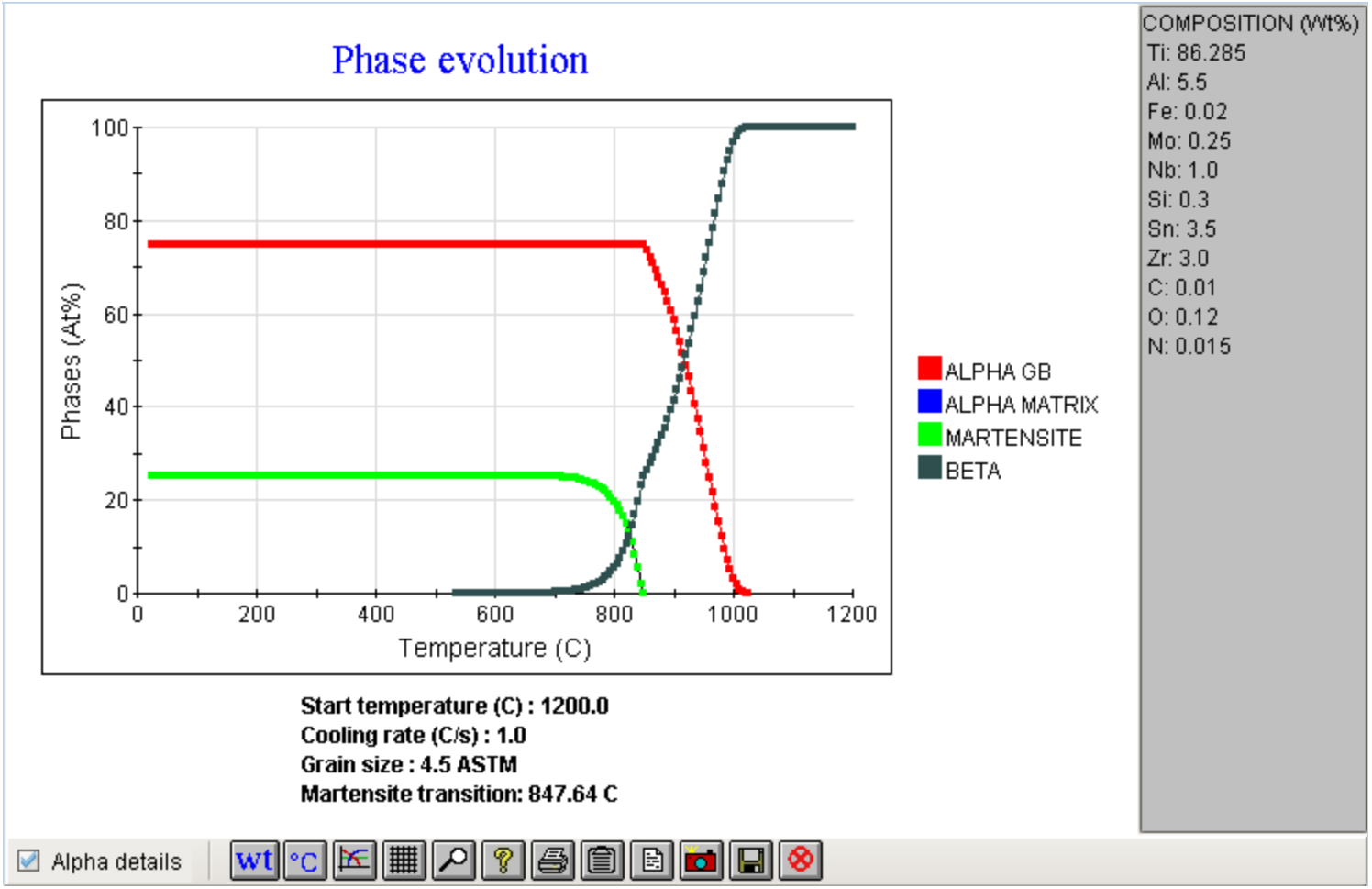


定量计算，在一定的冷速下，β相转变为α相的转变过程以及β相发生马氏体转变的温度

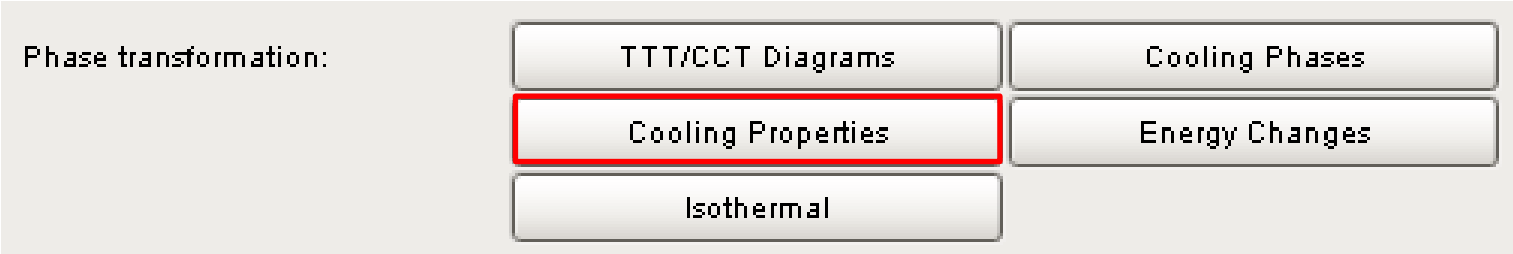
参数设置界面


Wt %
Ti 86.285
Al 5.5
Cr 0.0
Cu 0.0
Fe 0.02
H 0.0
Mo 0.25
Nb 1.0
Ni 0.0
Re 0.0
Ru 0.0
Si 0.3
Sn 3.5
Ta 0.0
V 0.0
Zr 3.0
C 0.01
O 0.12
N 0.015
B 0.0
IMI 829
Reset
Titanium Alloy
Cooling phases
Matrix grain size
Grain size :
4.5
ASTM
Start temperature
Temp. (C)
1000
Cooling rates (C/s)
Number of cooling rates:
1
2
3
4
5
6
1.0
Start calculation

计算结果

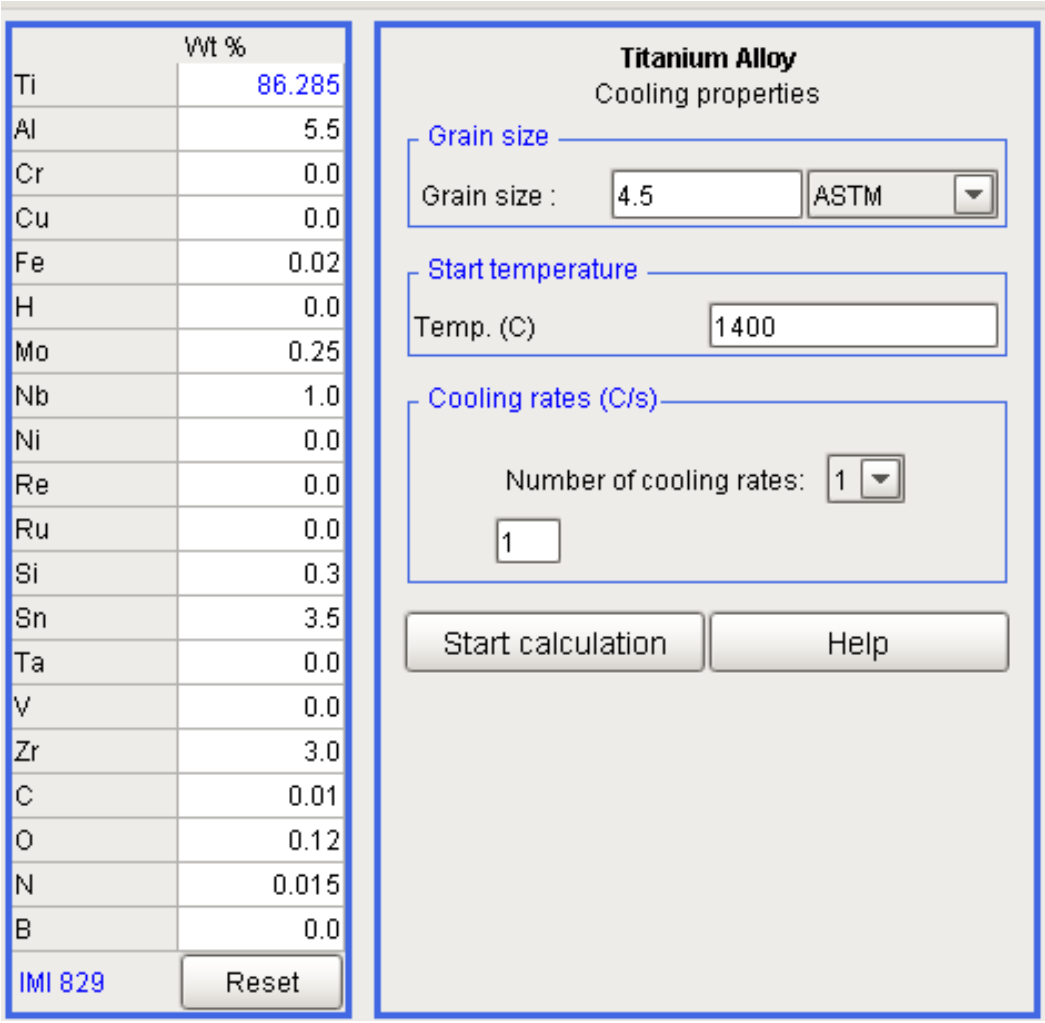

Phase evolution
Phases (At%)
100
80
60
40
20
0
0
200
400
600
800
1000
1200
Temperature (C)
ALPHA GB
ALPHA MATRIX
MARTENSITE
BETA
COMPOSITION (Wt%)
Ti: 86.285
Al: 5.5
Fe: 0.02
Mo: 0.25
Nb: 1.0
Si: 0.3
Sn: 3.5
Zr: 3.0
C: 0.01
O: 0.12
N: 0.015
Start temperature (C) : 1200.0
Cooling rate (C/s) : 1.0
Grain size : 4.5 ASTM
Martensite transition: 847.64 C
Alpha details
wt
°C

五.相转变计算——4.Cooling Properties

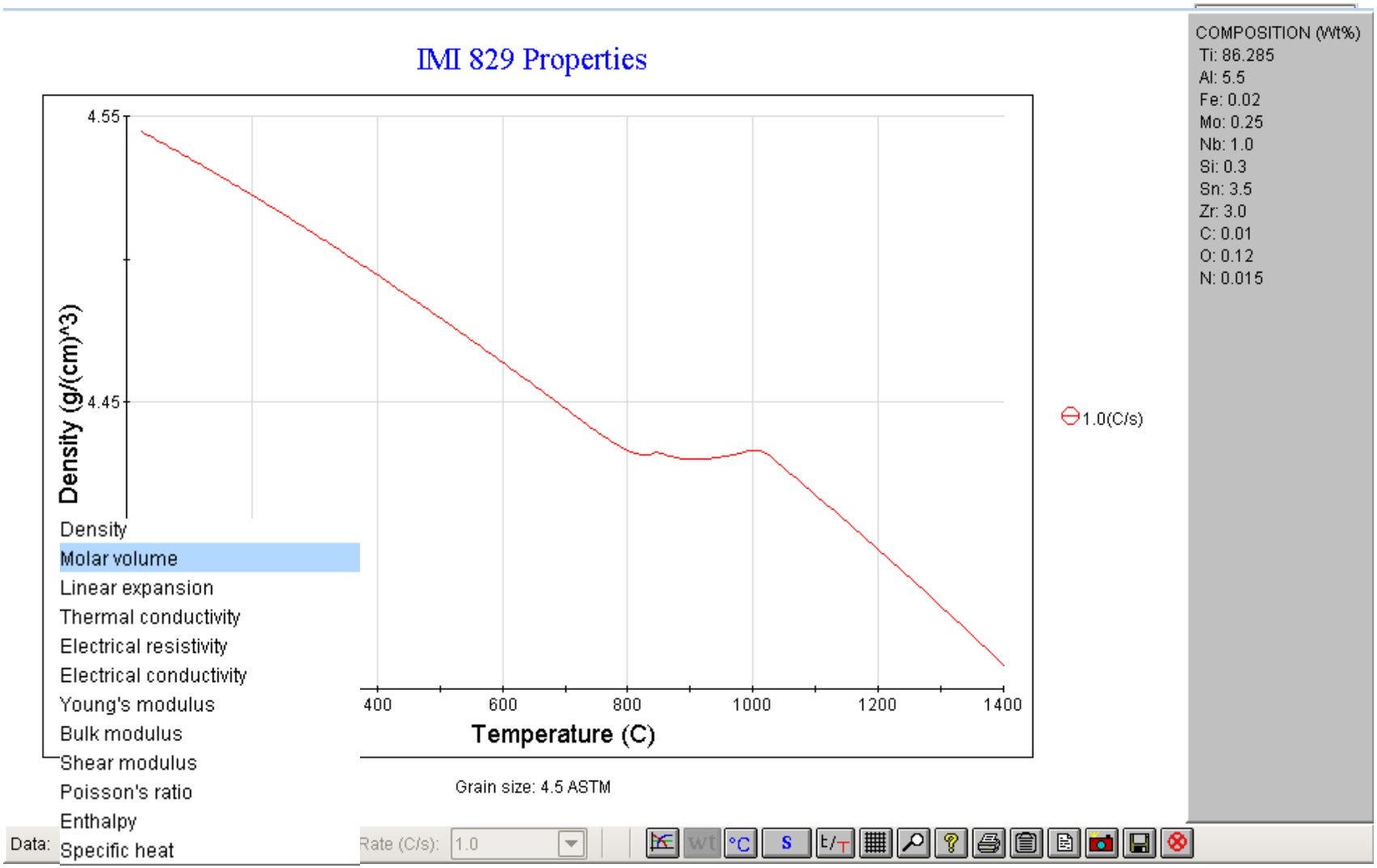


根据Cooling Phases计算得到的在各个冷速下的相组织，计算材料的相关性能

参数设置界面


Wt %
Ti 86.285
Al 5.5
Cr 0.0
Cu 0.0
Fe 0.02
H 0.0
Mo 0.25
Nb 1.0
Ni 0.0
Re 0.0
Ru 0.0
Si 0.3
Sn 3.5
Ta 0.0
V 0.0
Zr 3.0
C 0.01
O 0.12
N 0.015
B 0.0
IMI 829
Reset
Titanium Alloy
Cooling properties
Grain size
Grain size :
4.5
ASTM
Start temperature
Temp. (C)
1400
Cooling rates (C/s)
Number of cooling rates:
1
1
Start calculation
Help

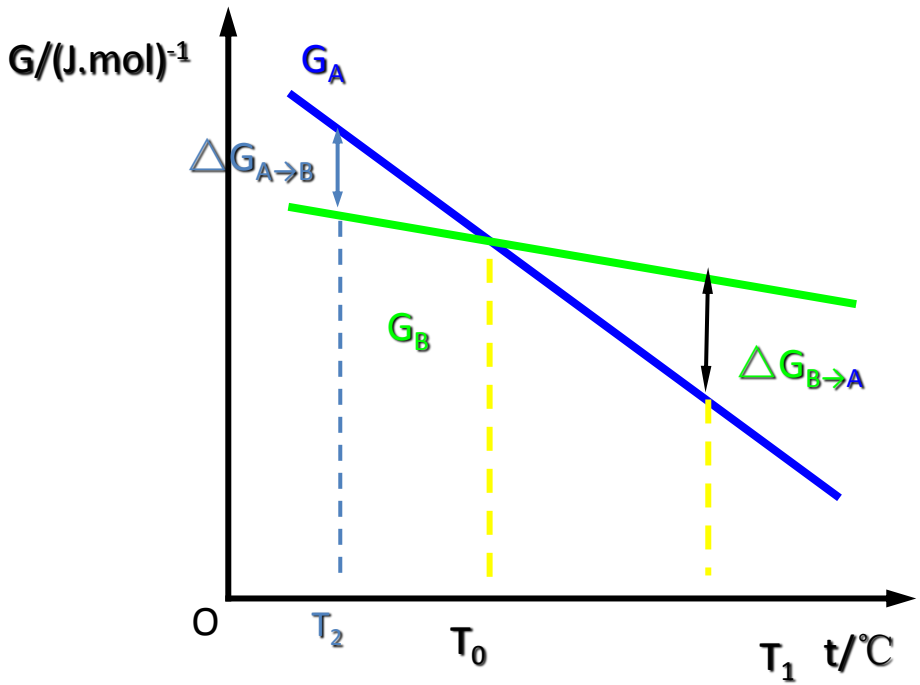
计算结果


IMI 829 Properties
COMPOSITION (Wt%)
Ti: 86.285
Al: 5.5
Fe: 0.02
Mo: 0.25
Nb: 1.0
Si: 0.3
Sn: 3.5
Zr: 3.0
C: 0.01
O: 0.12
N: 0.015
4.55
4.45
Density (g/(cm)^3)
400
600
800
1000
1200
1400
Temperature (C)
1.0(C/s)
Grain size: 4.5 ASTM
Density
Molar volume
Linear expansion
Thermal conductivity
Electrical resistivity
Electrical conductivity
Young's modulus
Bulk modulus
Shear modulus
Poisson's ratio
Enthalpy
Specific heat
Data:
Rate (C/s):
1.0
wt
°C
S

五.相转变计算——5.Energy Changes

Energy Changes：计算新相与母相之间的自由能之差

新相形成时系统总的自由能变化 $\Delta G = \Delta G_V + \Delta G_s + \Delta G_e$



◆当T=T0(A1)时， △GB→A=0

◆当T＞T0（T=T1）时，GB＞ GA。

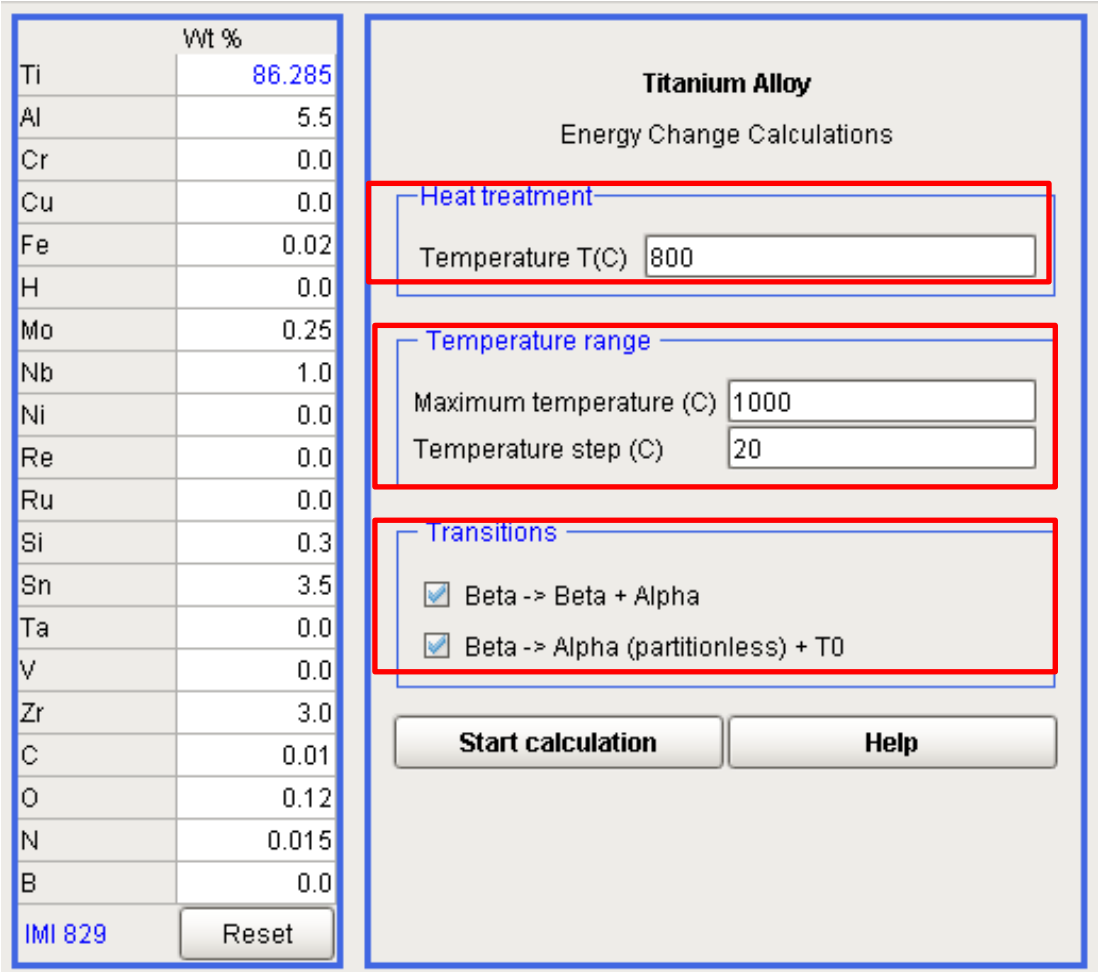
△GB→A＜0

即GA－GB ＜0，驱动力能够克服相变阻力，A相自发形成。

◆当T＜T0（T=T2）时， GB＜ GA。

△GB→A＞0

参数设置界面

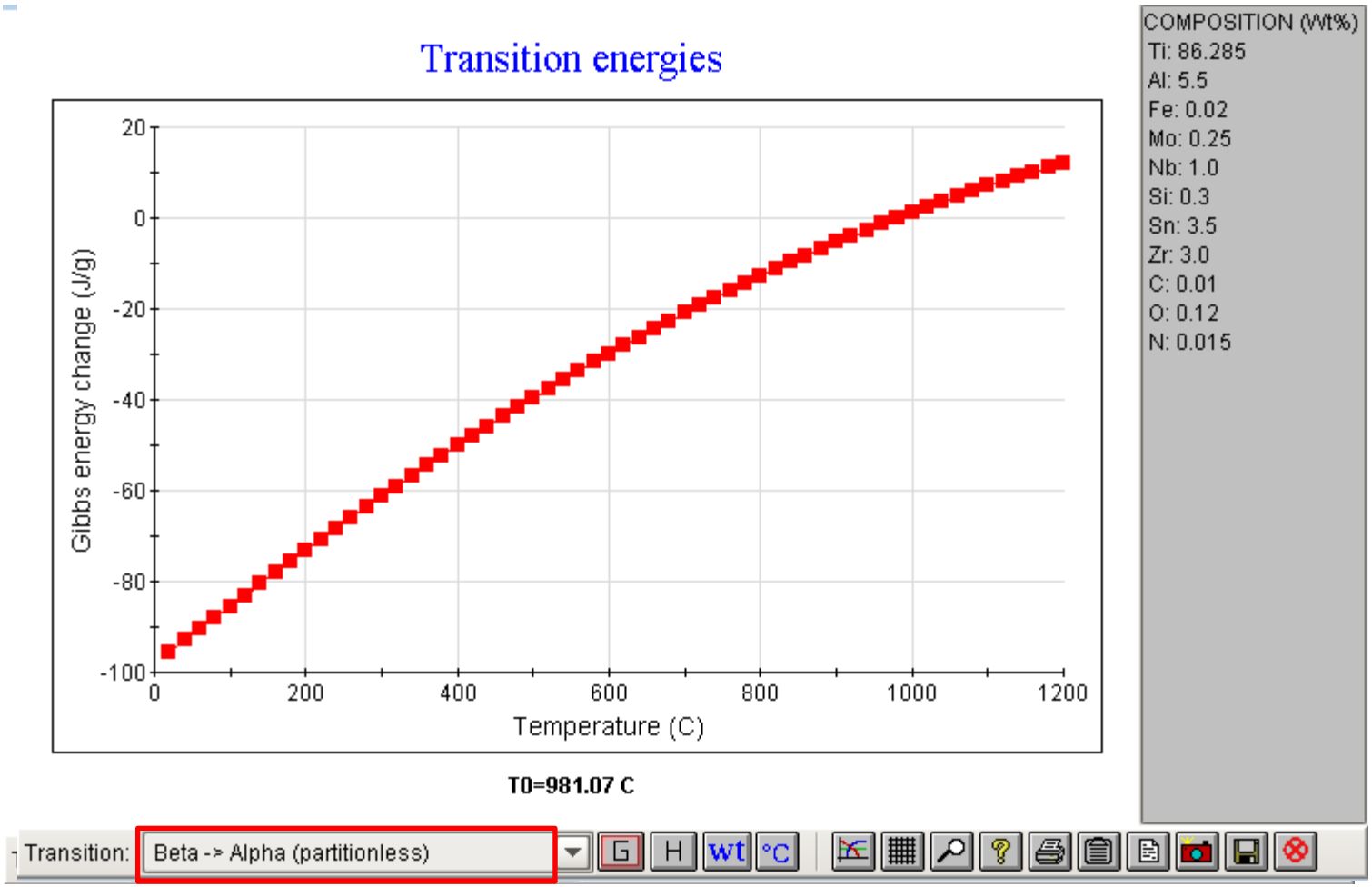


设定热处理温度
确定组织结构

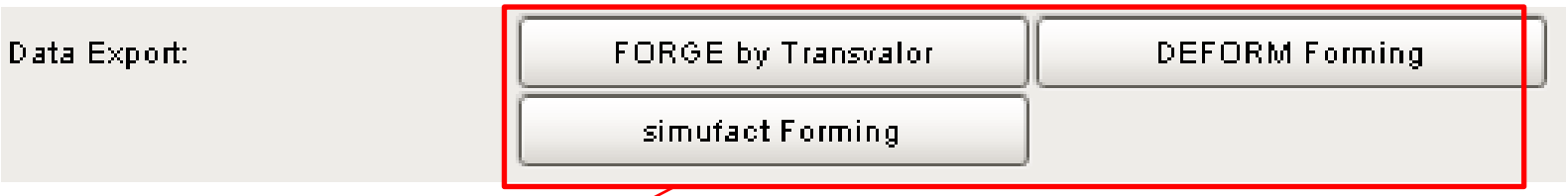
设定温度范围

选择不同相转变
的能量变化计算

计算结果


Transition energies
Gibbs energy change (J/g)
20
0
-20
-40
-60
-80
-100
0
200
400
600
800
1000
1200
Temperature (C)
T0=981.07 C
COMPOSITION (Wt%)
Ti: 86.285
Al: 5.5
Fe: 0.02
Mo: 0.25
Nb: 1.0
Si: 0.3
Sn: 3.5
Zr: 3.0
C: 0.01
O: 0.12
N: 0.015
Transition:
Beta -> Alpha (partitionless)
G
H
wt
°C

六.数据导出



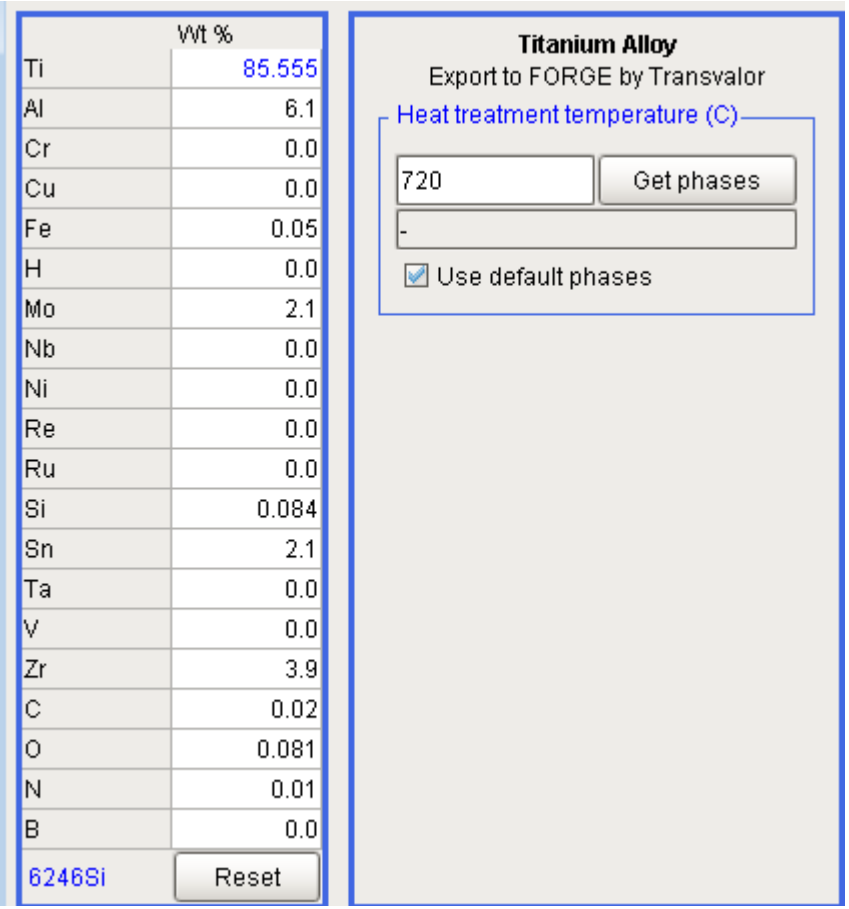
FORGE by Transvalor

DEFORM Forming

Simufact Forming

计算流动应力曲线以及的热物性能等数据

设置界面



JMatPro安装文件夹-〉export -〉

- Simufact
- DEFORM
- FORGE

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