CompuTherm
FOR MATERIALS DESIGN

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Pandat 软件
第一期优化培训教程

第七讲

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特殊性质数据库

- 摩尔体积 (Molar Volume)
  - 密度
  - 线膨胀系数
- 粘度 (Viscosity)
- 表面张力 (Surface tension)

Build-in

- 热导率 (热阻率)
- 电导率(电阻率)

User-Defined

- 迁移率 (Mobility)

Diffusion related application

用户自定义性质(User-defined property)

Pandat 的用户自定义性质

可以描述为以下形式的任何性质:

$$U = \sum_{i=1}^{c} x_i U_i^o + \sum_{i=1}^{c-1} \sum_{j=i+1}^{c} x_i x_j \sum_k (x_i - x_j)^k L_{ij}^k$$

x_i -- 组元 i 的摩尔分数

U_i^o-- 纯组元 i 的性质 U的值

L_{ij}^k -- 组元 i 和 j 第 k 阶的相互作用参数。

用户定义性质(User-defined property)

多相系统的系统性质: 各相的**加权平均**

❖ “Pandat软件中预定义的各种平均方法

$$Z^{(p)}(z_1, z_2, \cdots, z_\phi) = \left(\sum_{i=1}^{\phi} f_i z_i^p\right)^{\frac{1}{p}} \begin{cases} \min(z_1, z_2, \cdots, z_\phi) & \text{minimum} \\ \dfrac{1}{\dfrac{f_1}{z_1} + \dfrac{f_2}{z_2} + \cdots + \dfrac{f_\phi}{z_\phi}} & \text{harmonic mean} \\ {z_1}^{f_1} {z_2}^{f_2} \cdots {z_\phi}^{f_\phi} & \text{geometric mean} \\ f_1 z_1 + f_2 z_2 + \cdots + f_\phi z_\phi & \text{arithmetic mean} \\ \max(z_1, z_2, \cdots, z_\phi) & \text{maximum} \end{cases}$$

❖ 用户也可以自己定义多相的系统性质计算方法

摩尔体积(Molar Volume)

$$V_i^{\varphi}(T) = V_0\, exp(\int_{T_0}^{T} 3\alpha dT)$$

i: 体系的组元

V_0: φ 相的摩尔体积 (P=1 bar, T=T_0), 常数

α : 线性热膨胀系数

$$\int_{T_0}^{T} 3\alpha dT = a + bT + cT^{-1} + \cdots$$

$$V^{\varphi}(T) = \sum_i x_i V_i^{\varphi} + V_m^{ex}$$

$$V_m^{ex} = \sum_{i=1}^{c-1} \sum_{j=i+1}^{c} x_i x_j \sum_k (x_i - x_j)^k L_{ij}^k + x_i x_j x_p L_{i,j,p}$$

Pandat2020 manual: page 222

摩尔体积(Molar Volume)

```
Phase L12_FCC %v 2 0.75 0.25 !

Constituent L12_FCC: Al,Ni:Al,Ni:!

        Parameter Vm(L12_FCC,Al;0)    298.15 +V_Al_fcc; 3000 N !

        Parameter Vm(L12_FCC,Ni;0)    298.15 +V_Ni_fcc; 3000 N !

        Parameter Vm(L12_FCC,Al,Ni;0) 298.15 -3.2e-6; 3000 N !
```

$$V_m^{L12} = x_{Al} \times V_{Al_{fcc}} + x_{Ni} \times V_{Ni_{fcc}} - 3.2 \times 10^{-6} x_{Al} x_{Ni}$$

```
Type_Definition v GES AMEND_PHASE_DESCRIPTION * VARIABLE_X Vm !
```

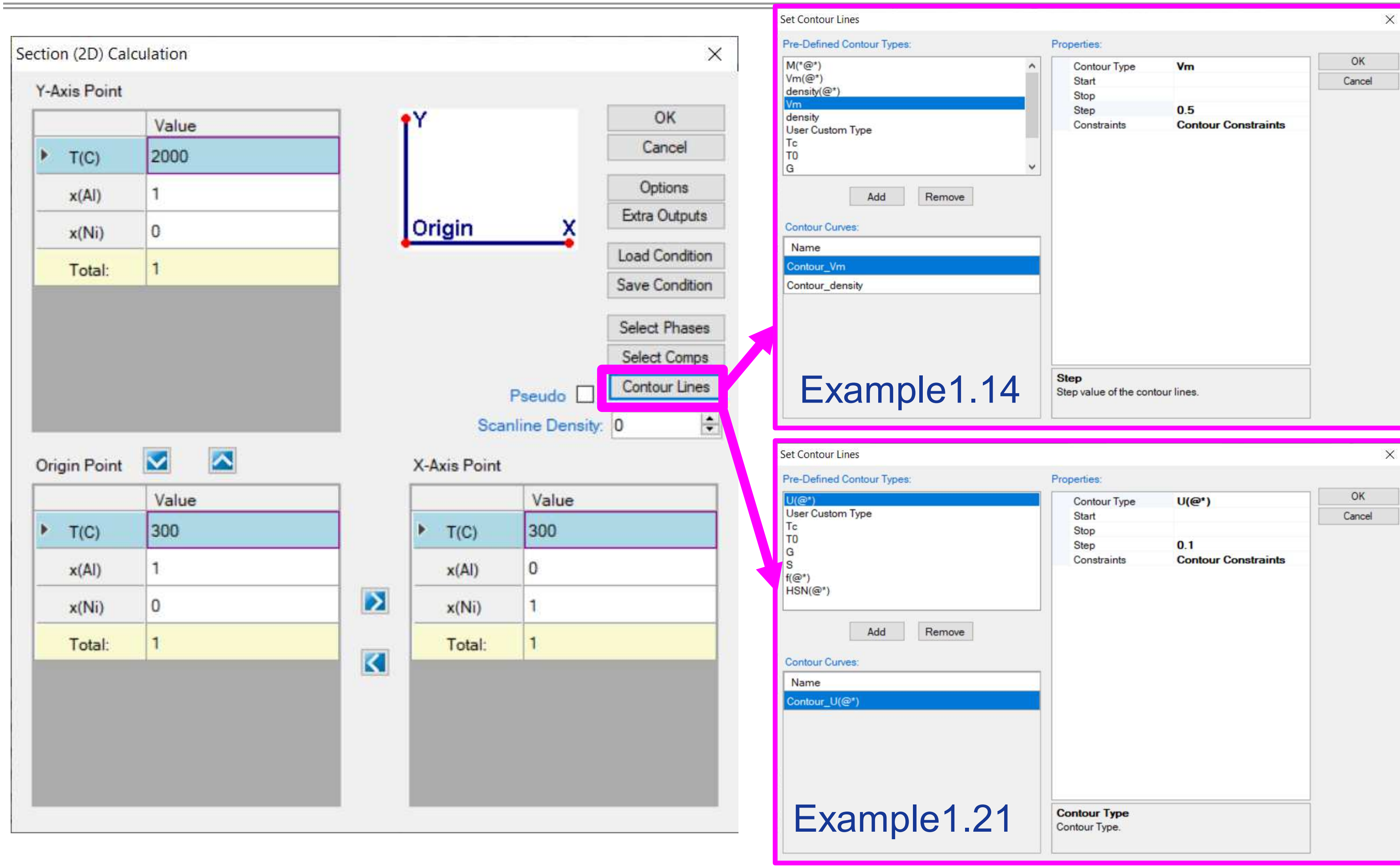
密度(Density)

$$d^{\varphi} = \frac{W_m^{\varphi}}{V_m^{\varphi}}$$

$W_m^{\varphi} = \sum_i x_i W_i$ ： φ相的摩尔质量

V_m^{φ}： φ相的摩尔体积

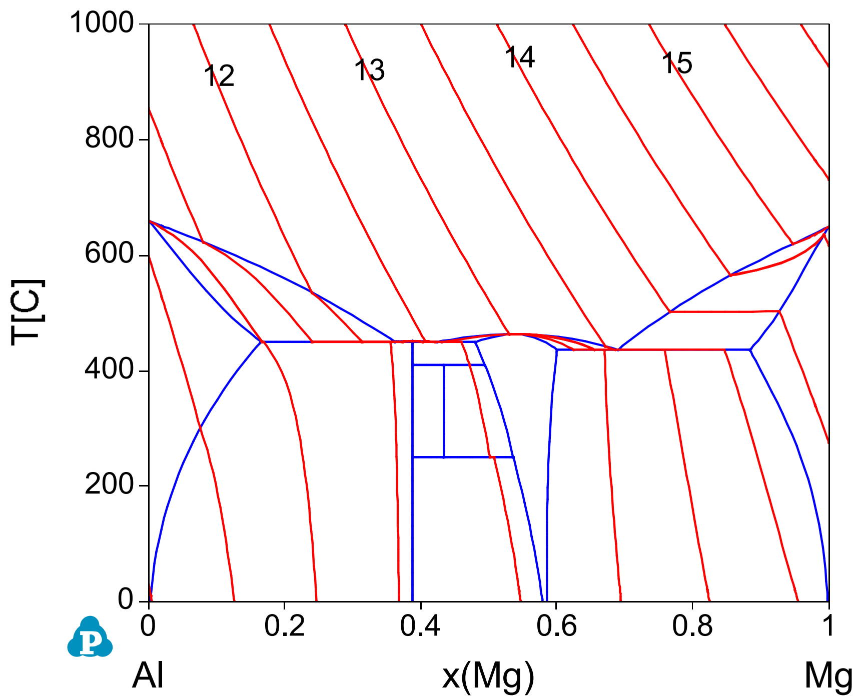
绘制等值线图(摩尔体积与密度)



C:\Program Files (x86)\CompuTherm LLC\Pandat 2020\Pandat 2020 Example book

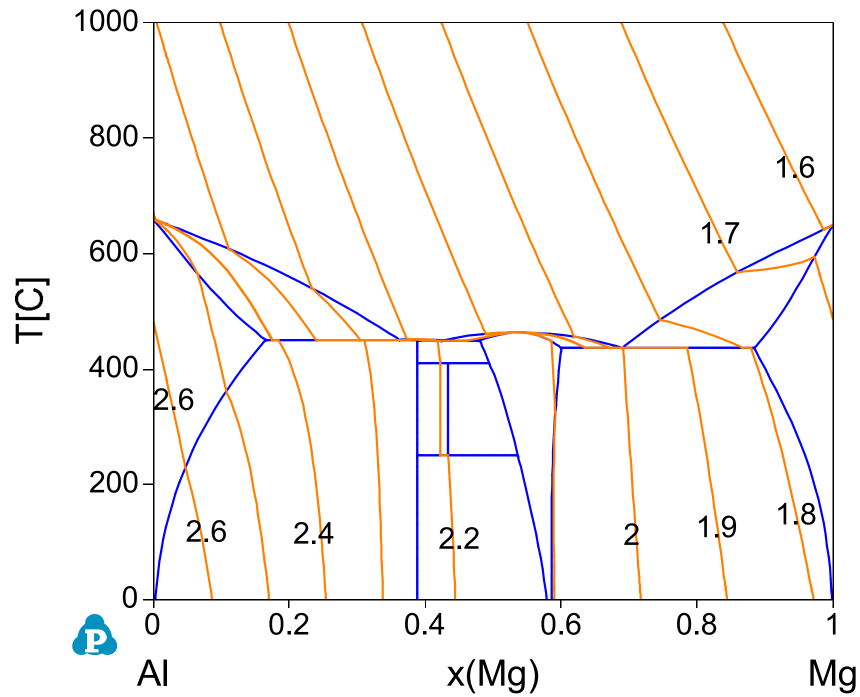
等值线图(摩尔体积与密度)

摩尔体积(Vm)， unit: cm^3/mol



Al-Mg相图与**摩尔体积**等值线图

密度 (density)， unit: g/cm^3



Al-Mg相图与**密度**等值线图

粘度(Viscosity)

$$\eta = A\,exp\left(\frac{\Delta G^*}{RT}\right)$$

$$A = \frac{hN}{V}$$

h: Plank's constant;
N: Avogadro's number
***V*:** molar volume

$$\Delta G^* = \sum x_i \Delta G_i^o + \Delta^m G_{mix} + 3RT \sum\sum x_i x_j$$

ΔG_i^o Gibbs energy of activation of component *i*,

$\Delta^m G_{mix}$ Gibbs energy of mixing

```
Parameter ActivationEnergy(Liquid,Al;0) 298.15 15051+13.519*T; 2000 N !

Parameter ActivationEnergy(Liquid,Si;0) 298.15 6437+25.836*T; 2000 N !
```

表面张力(Surface Tension)

$$\sigma = \sigma_i + \frac{RT}{S_i} ln \frac{a_i'}{a_i}$$

σ_i : surface tension of component i
a_i : activity of component i in the bulk
a_i' : activity of component i at the surface = A*a_i
S_i : surface monolayer area

$$S_i = bN^{1/3}V_i^{2/3}$$

b : geometric factor
N : Avogadro's number
V_i : molar volume of component i.

```
Parameter Beta(Liquid,Al;0) 298.15  0.83;  2000  N !
```

自定义性质：热导率(热阻率)

$$\lambda = \frac{1}{W}$$

W: 热阻率
λ : 热导率

$$W^{\varphi}(T) = \sum_{i} x_i W_i^{\varphi} + W^{ex}$$

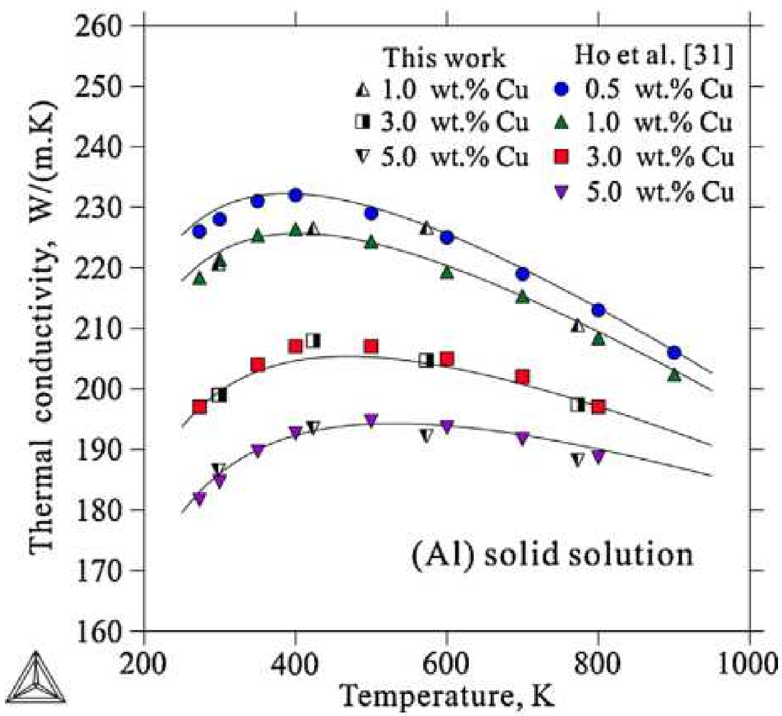
$$W = x_A W_A + x_B W_B + L \cdot x_A \cdot x_B$$

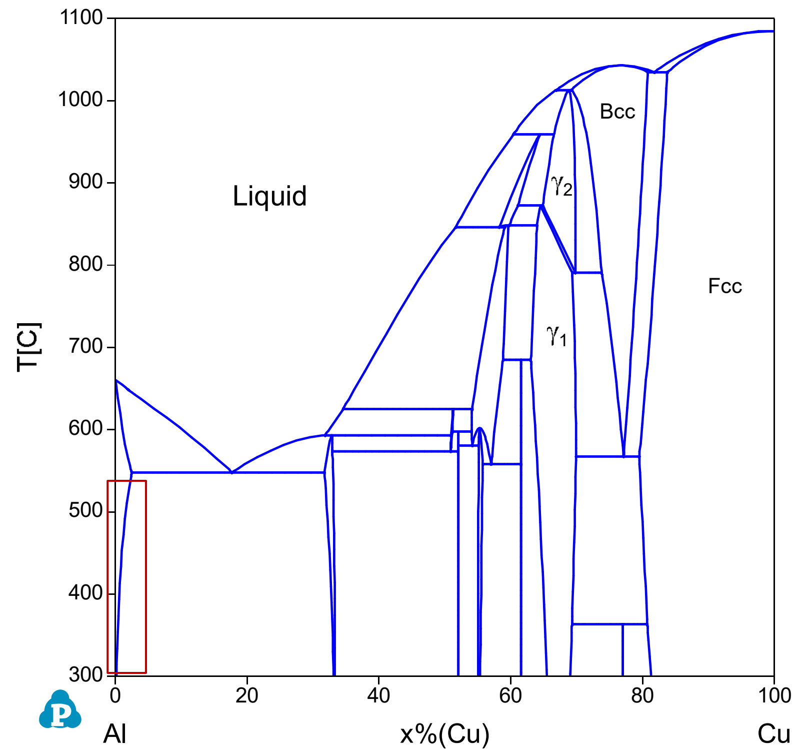
$$\lambda = \frac{1}{W}$$

$$\boxed{\lambda_{AB}^{\alpha} = x_A \cdot \lambda_A + x_B \cdot \lambda_B + x_A \cdot x_B \cdot \sum_{i=0}^{i} LAB_{\alpha} \cdot (x_A - x_B)^{i},}$$

Wrong and misleading

参数的影响





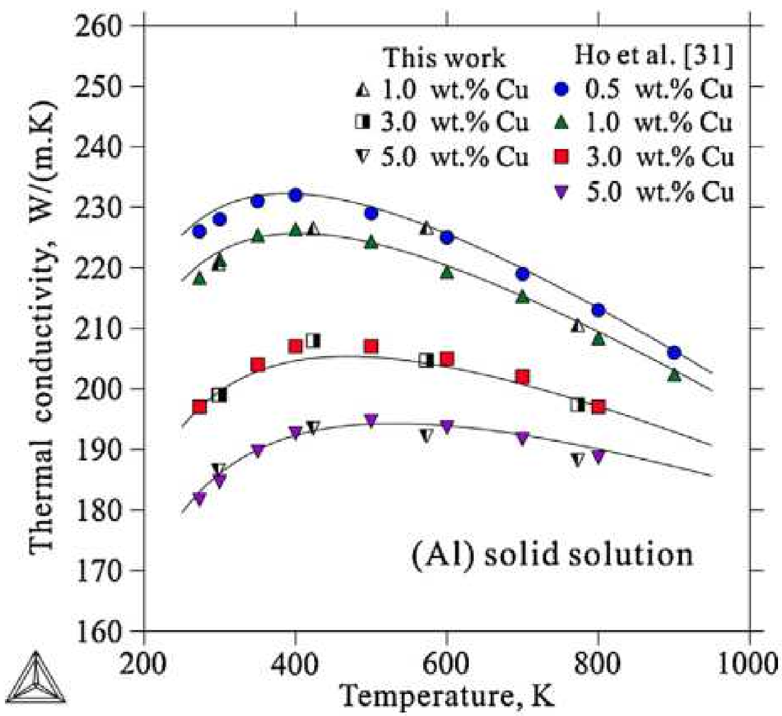
Al-Cu system

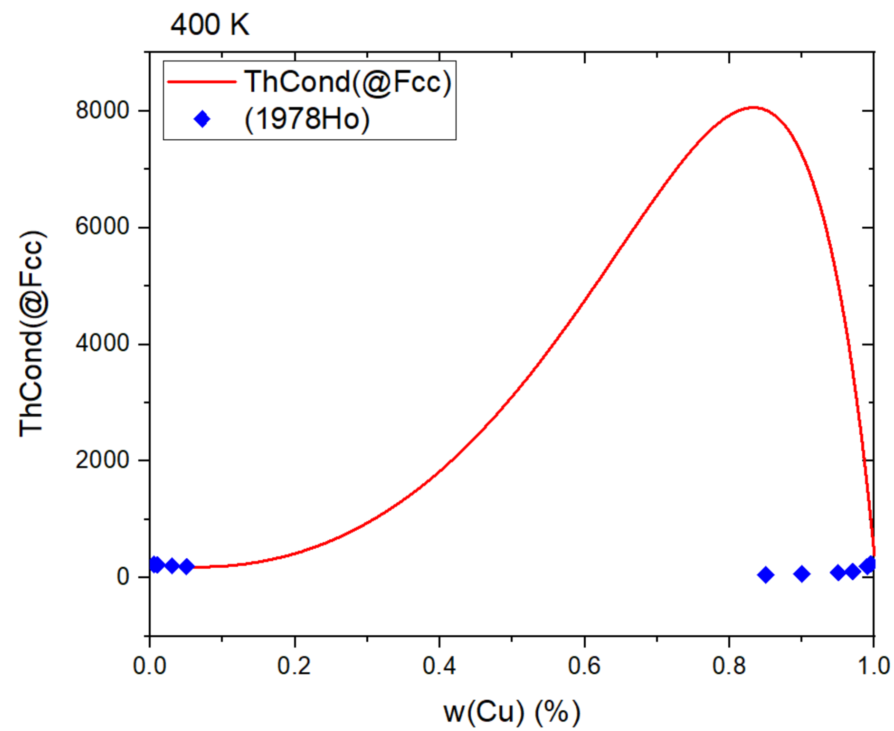
$$\lambda = x_{Al}\lambda_{Al} + x_{Cu}\lambda_{Cu} + L \cdot x_{Al} \cdot x_{Cu}$$

L0 = 34954.92-24.601*T

L1 = -39974.45+28.122*T

参数的影响





Al-Cu system

$$\lambda = x_{Al}\lambda_{Al} + x_{Cu}\lambda_{Cu} + L \cdot x_{Al} \cdot x_{Cu}$$

L0 = 34954.92-24.601*T

L1 = -39974.45+28.122*T

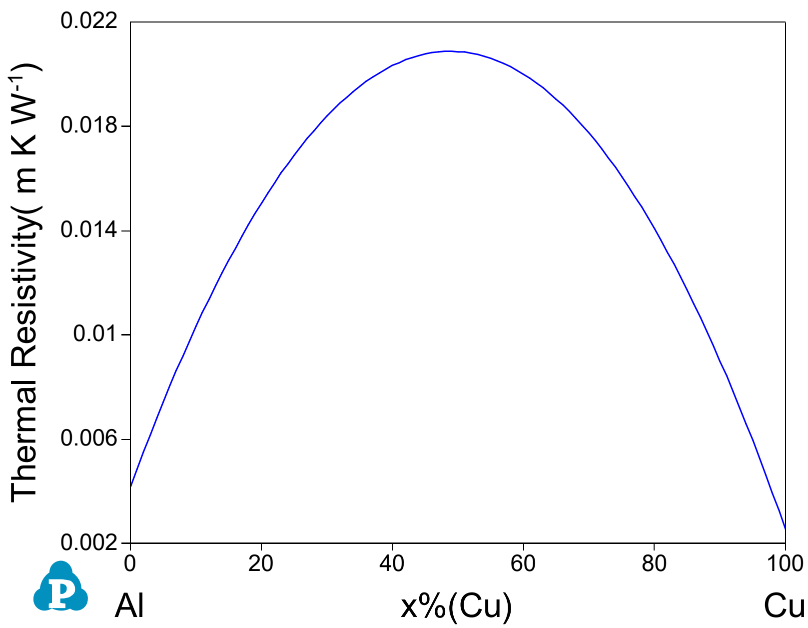
T=400K

= 25114.5

= - 28725.65

参数的影响

电阻率

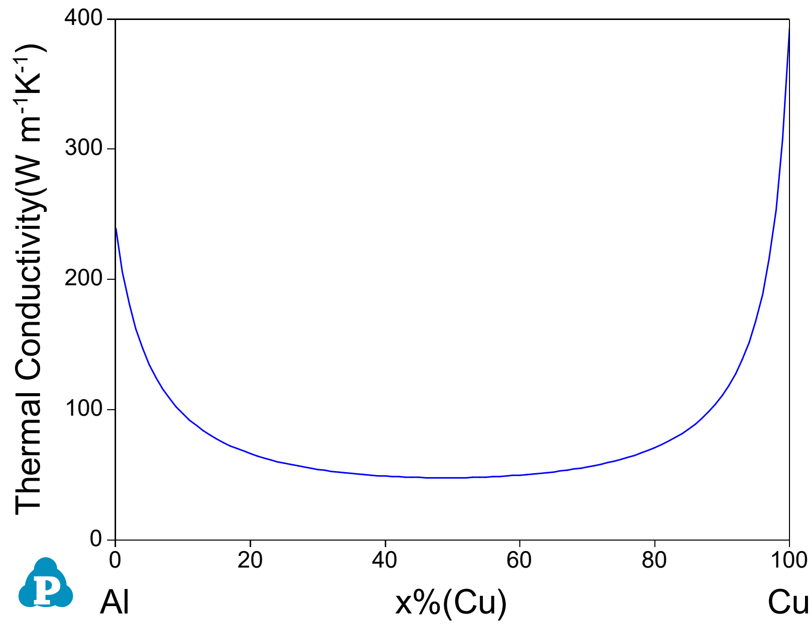


$$W = x_{Al}W_{Al} + x_{Cu}W_{Cu} + L \cdot x_{Al} \cdot x_{Cu}$$

$$= x_{Al}/\lambda_{Al} + x_{Cu}/\lambda_{Cu} + L \cdot x_{Al} \cdot x_{Cu}$$

L = 0.07

电导率



$$\lambda = 1/W$$

TDB 中的描述

```
Type_Definition e GES AMEND_PHASE_DESCRIPTION * VARIABLE_X ThRss !
Type_Definition z PHASE_PROPERTY ThRss 1 !

Parameter ThRss(Fcc,Fe;0) 298.15       1/ThCond_Fe_Fcc; 3000 N !
Parameter ThRss(Fcc,Ni;0) 298.15       1/ThCond_Ni_Fcc; 3000 N !
Parameter ThRss(Fcc,Fe,Ni;0) 298.15
       0.226869-13.0186e-5*T-27.593*T**(-1); 3000 N !

System_Property Sys_ThCond 1 !
 Parameter L(Sys_ThCond,Fcc;0) 298.15   1/ThRss(@Fcc); 3000 N !

System_Property Sys_ThRss 1 !
 Parameter L(Sys_ThRss,Fcc;0) 298.15   ThRss(@Fcc); 3000 N !
```

迁移率 (Mobility) 数据

迁移率数据库(Mobility database)使用：

扩散模拟 (PanDiffusion);

析出模拟 (PanPrecipitation);

凝固模拟 (PanSolidification)

- Atomic Mobility
- Tracer Diffusivity
- Chemical Diffusivity

Atomic Mobility (M)

$$M_k = M_k^{\circ} e^{-Q_k/RT}$$

M_k: 组元 k 的迁移率
M_k°: 指前因子
Q_k: 激活能因子

$$MQ_k = RT\ ln\ M_k = RT\ ln\ M_k^{\circ} - Q_k$$

$$MQ_{Al}^{Al,Fcc},\ MQ_{Al}^{Ni,Fcc}$$

```
Parameter MQ(Fcc&Al,Al;0) 298.15 -126719-92.92*T; 6000 N !

Parameter MQ(Fcc&Al,Ni;0) 298.15 -285517+R*T*Ln(0.0007933); 6000 N !
```

```
M(*@*):  M(Al@Fcc)
```

2017Zhang_JPED_434.pdf

Tracer and chemical Diffusivity

Chemical Diffusivity

Tracer Diffusivity

n: solvent atom

$$D_k^* = RTM_k$$

$$D_{kj}^n = D_{kj} - D_{kn}$$ when j is substitutional

DT(*@*)

$$D_{kj}^n = D_{kj}$$ when j is interstitial

DT(Al@Fcc)

$$D_{kj} = \sum_{i \in S} (\delta_{ik} - u_k) u_i M_i \frac{\partial \mu_i}{\partial u_j} + \sum_{i \notin S} \delta_{ik} u_i y_{Va} M_i \frac{\partial \mu_i}{\partial u_j}$$

logDT(*@*)

S: represents the set of the substitutional species

δ_{ik}: Kronecker delta

μ_i chemical potential of species i

$$u_k = \frac{x_k}{\sum_{i \in S} x_j}$$

DC(k,j@p:n): Chemical diffusivity of species *k* in phase p; j: gradient species; n: reference species.

Questions?