



上海思响信息科技有限公司

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# Pandat 软件

## 第一期优化培训教程

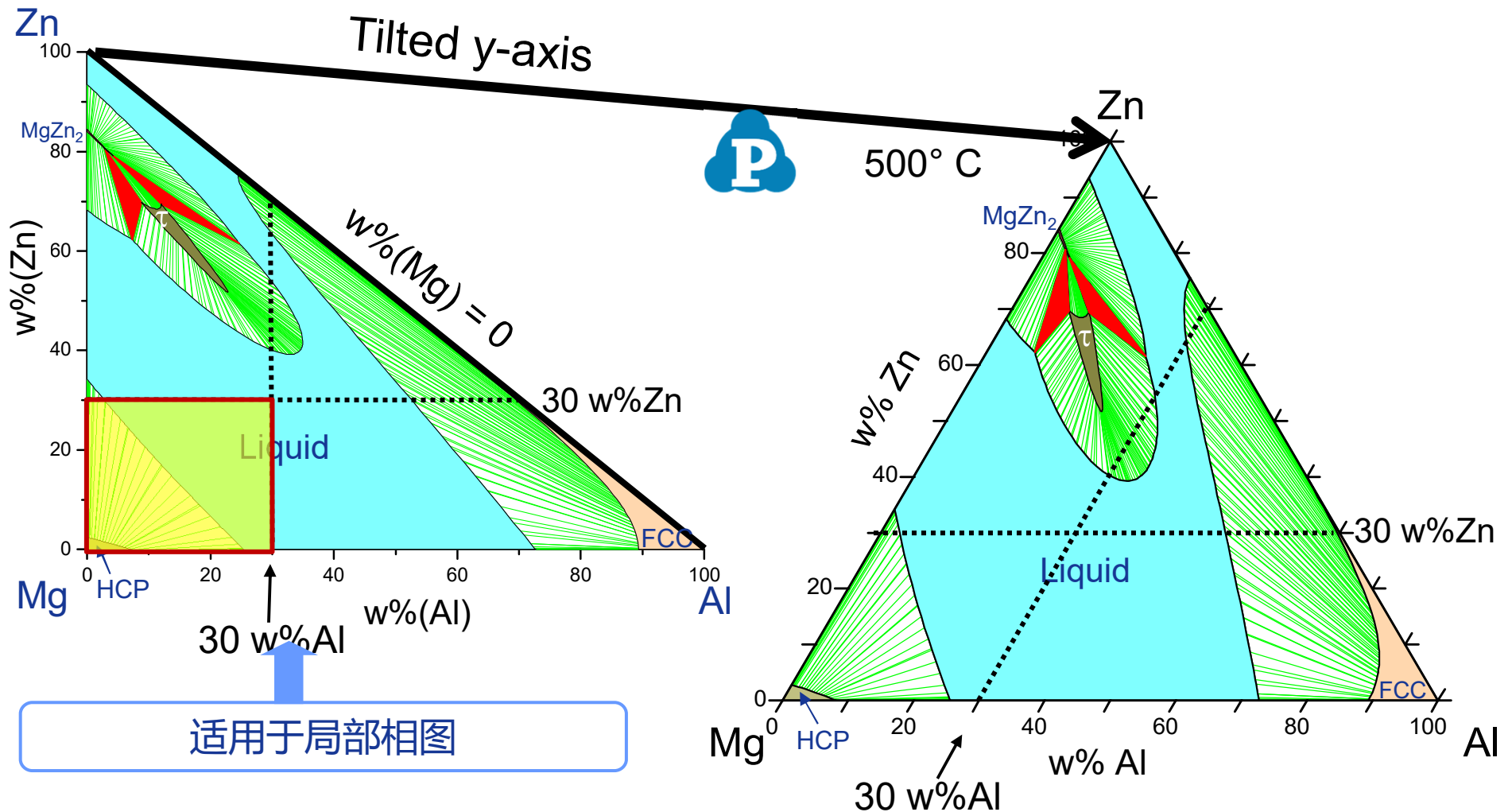
### 第六讲

2020年7月12日

CompuTherm, LLC  
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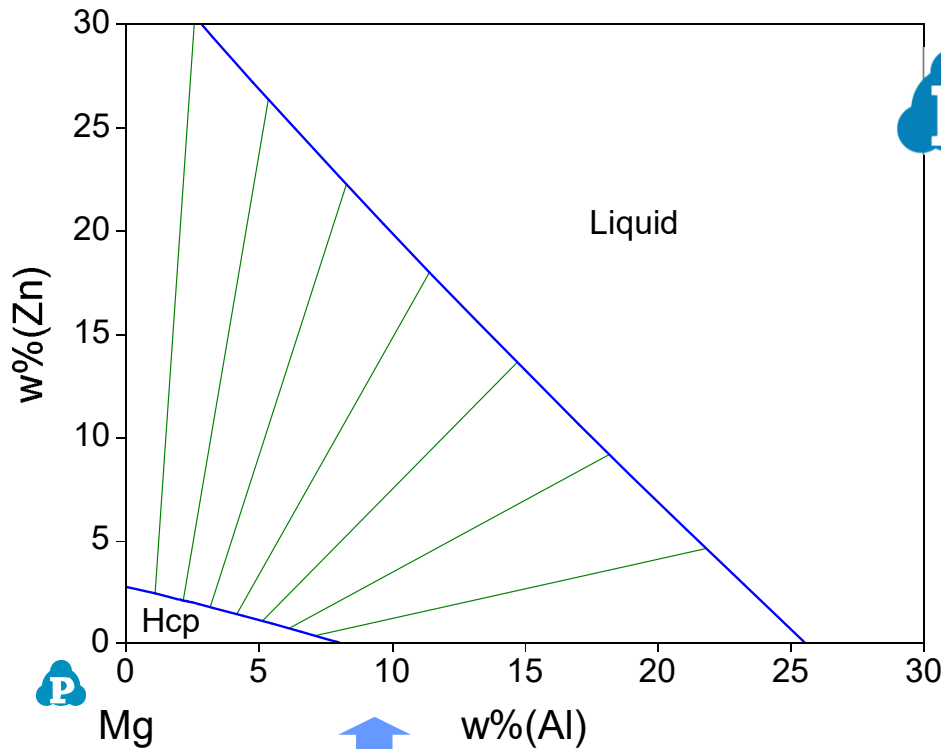
# 三元相图: Mg-Al-Zn, 500°C, 1bar

$$w\%(Mg) = 100 - w\%(Al) - w\%(Zn)$$

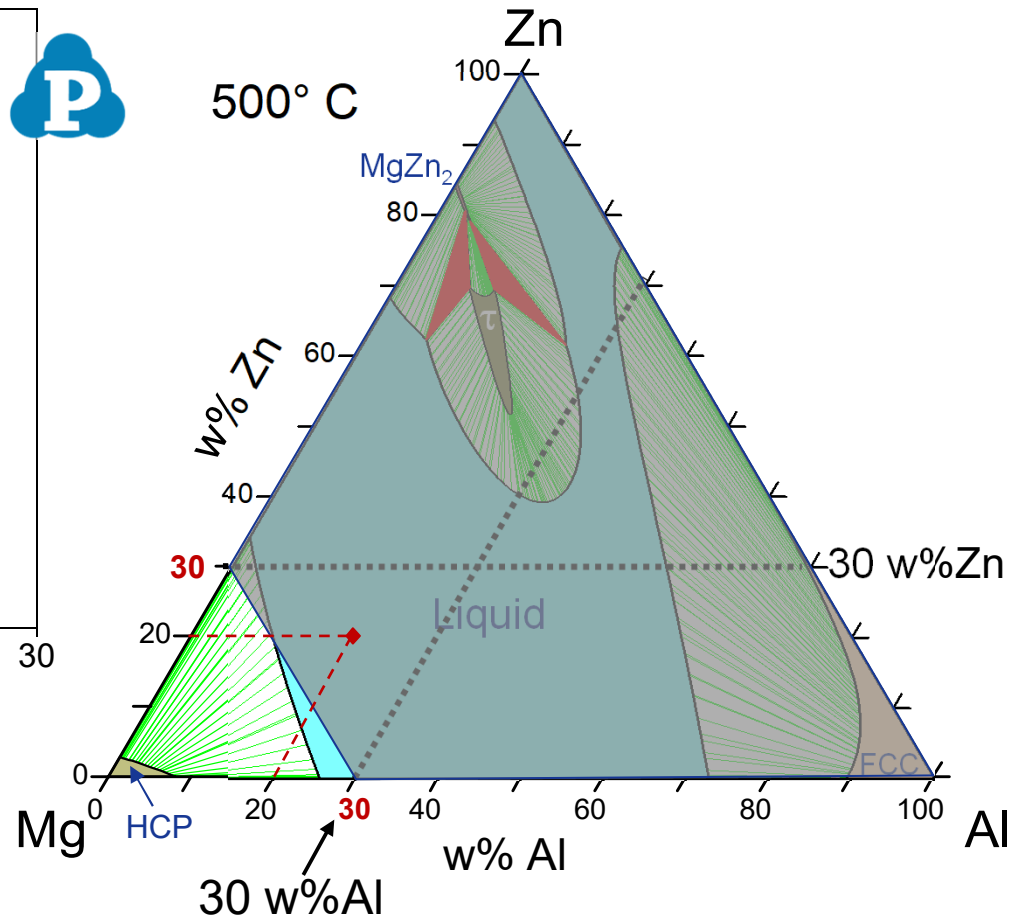


# 三元相图: Mg-Al-Zn, 500°C, 1bar

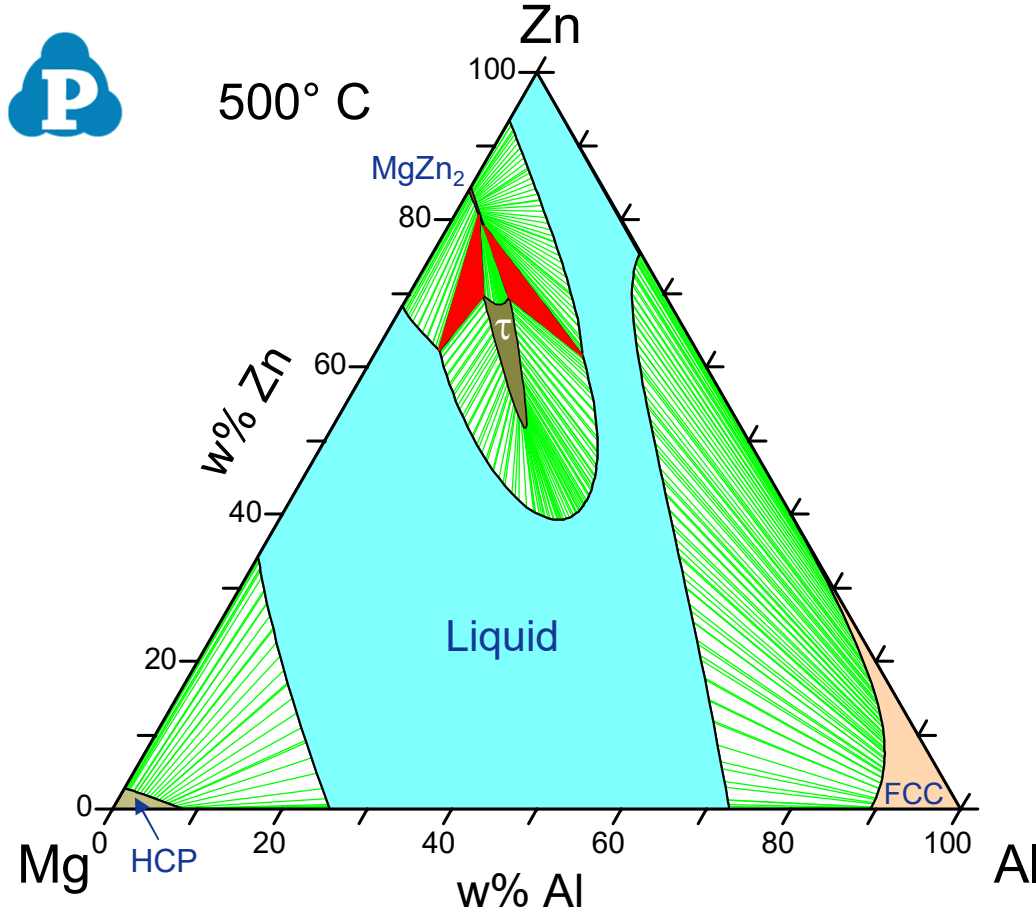
$$w\%(Mg) = 100 - w\%(Al) - w\%(Zn)$$



适用于局部相图



# 三元相图: Mg-Al-Zn, 500°C, 1bar



单相区:

Liquid, HCP, FCC,  $\text{MgZn}_2$ ,  $\tau$

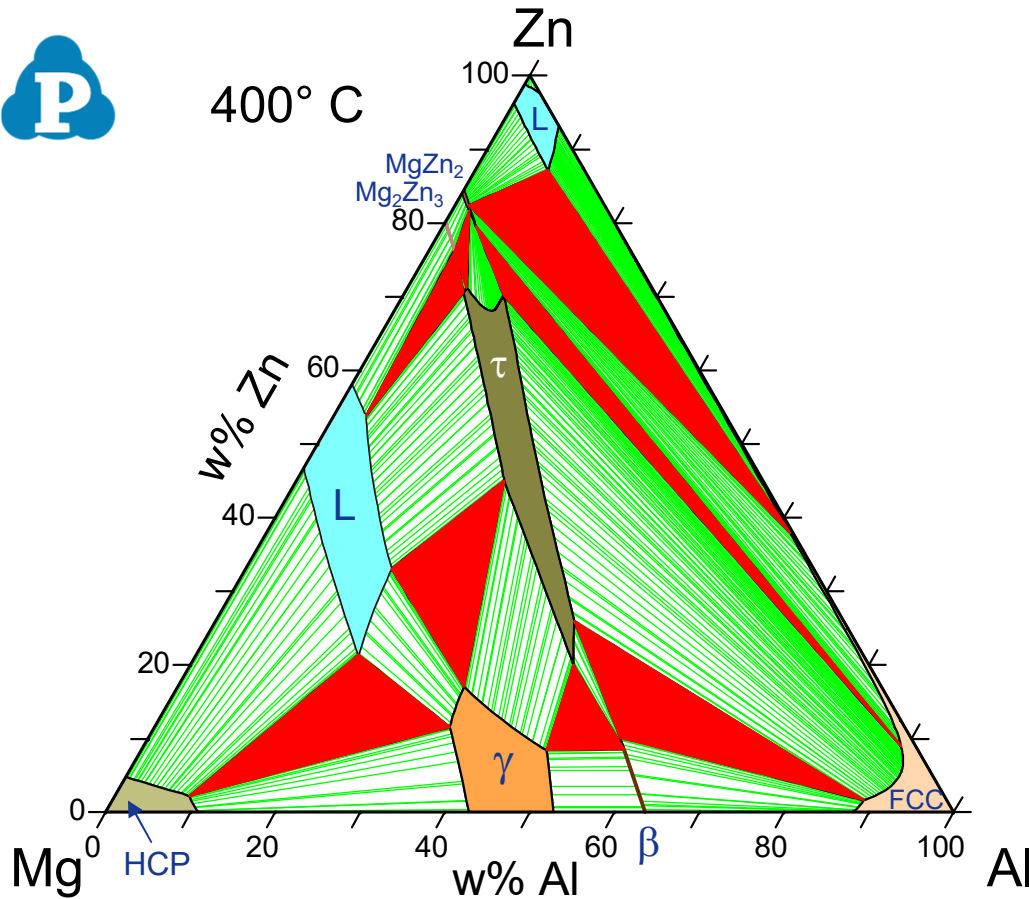
两相区:

 tie lines

三相区:

 tie triangles

# 三元相图: Mg-Al-Zn, 400°C, 1bar



## 单相区:

Liquid, HCP, FCC,  $\text{MgZn}_2$ ,  $\text{Mg}_2\text{Zn}_3$ ,  $\gamma$ ,  $\beta$ ,  $\tau$

## 两相区:

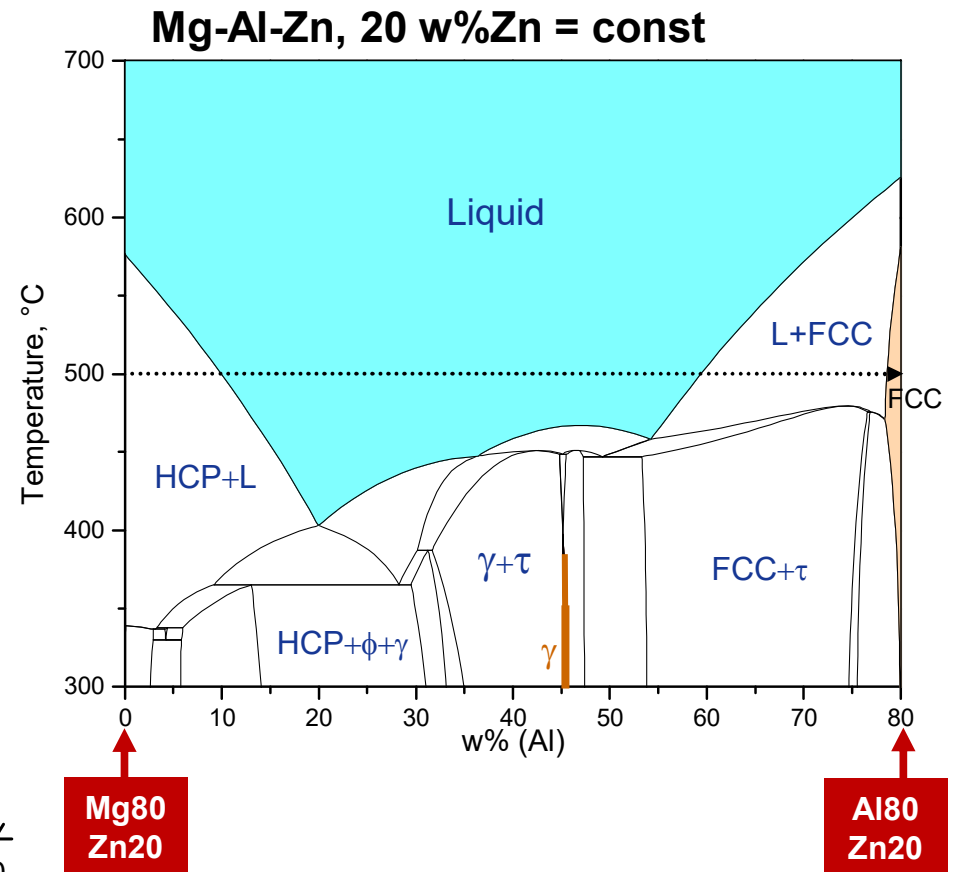
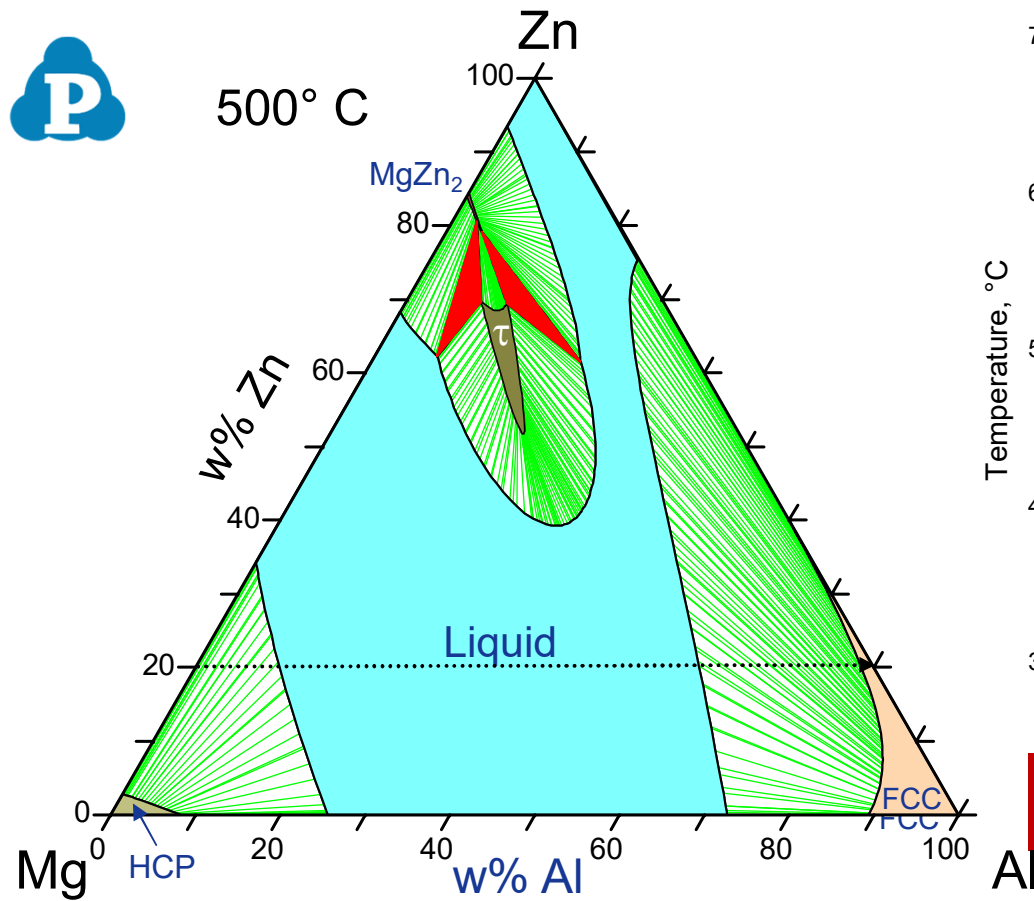
 tie lines

## 三相区:

 tie triangles



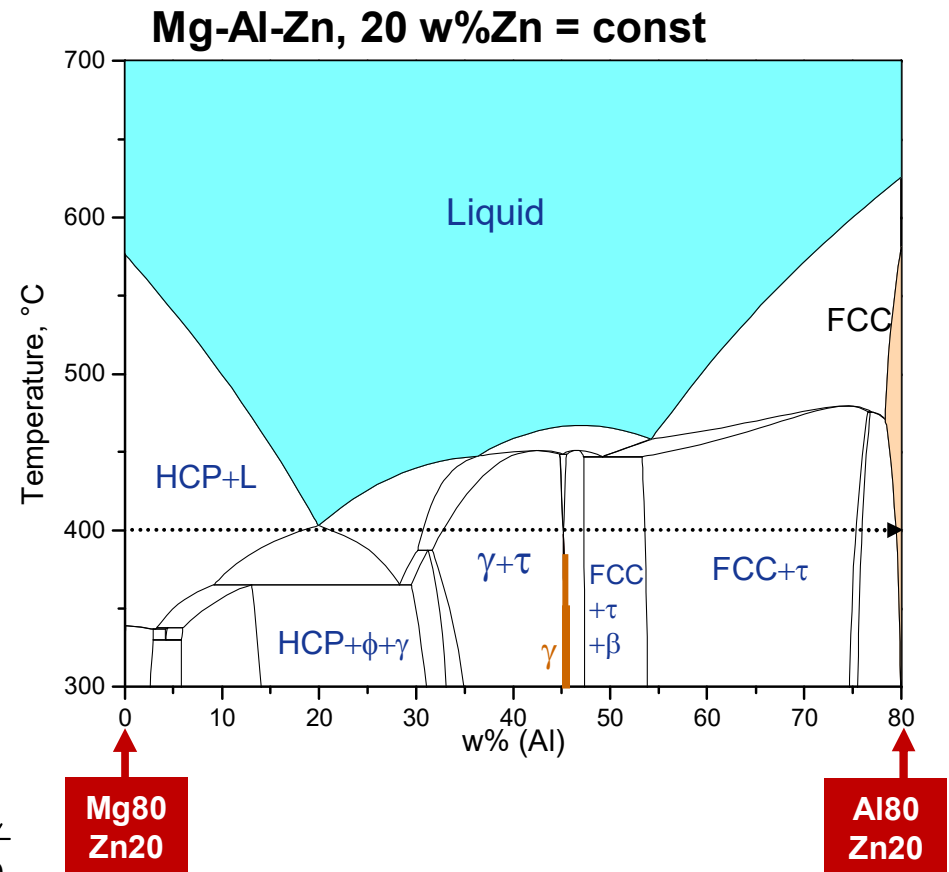
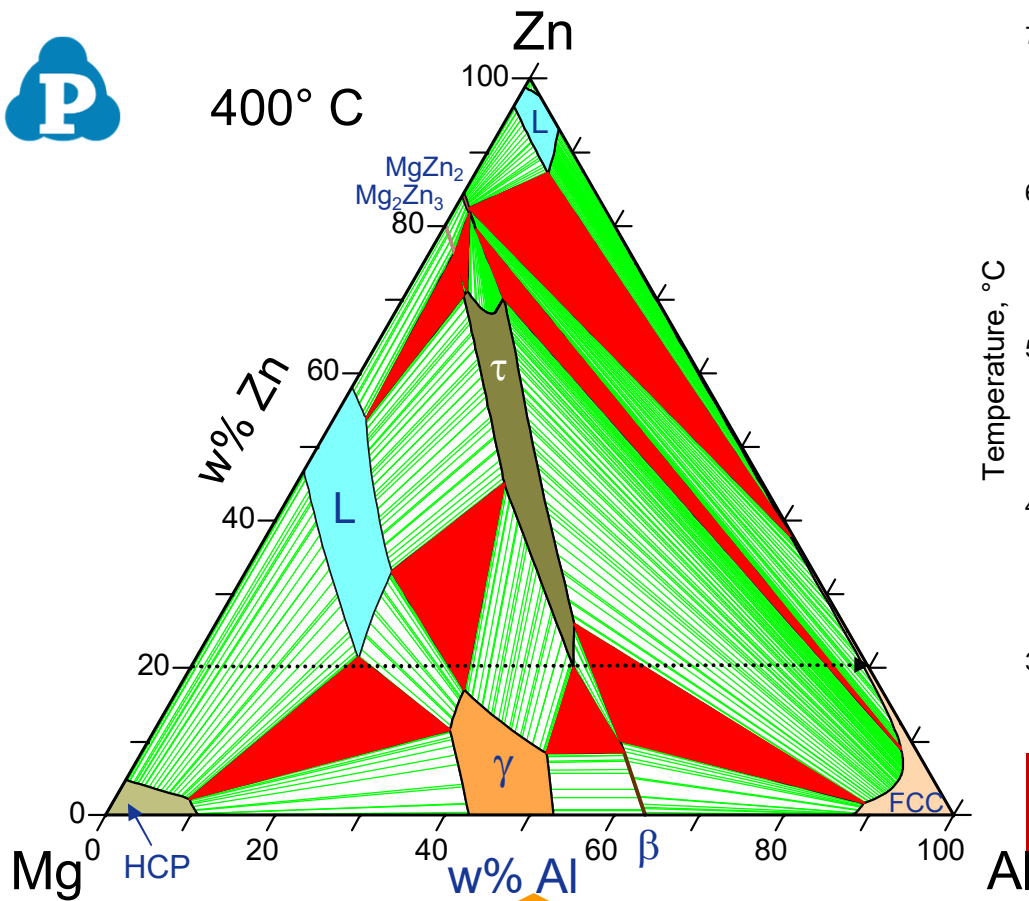
# 三元相图：垂直截面



ALL tie lines in this plane  
→ Read Type & Composition & Fraction of phase(s)

Tie lines **not** in plane: "Isopleth"  
→ Read Type of phase(s) only !

# 三元相图: 垂直截面



ALL tie lines in this plane  
→ Read Type & Composition & Fraction of phase(s)

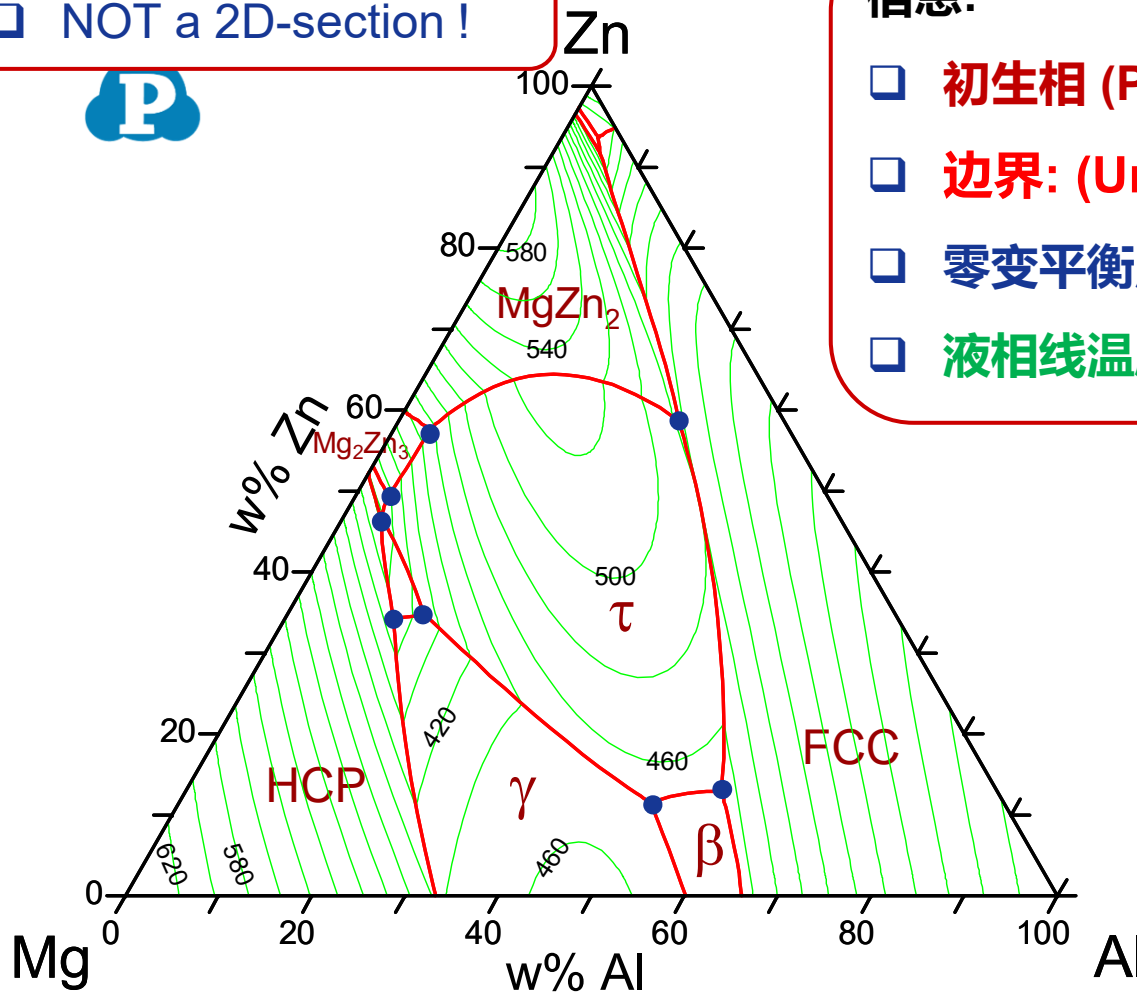
Tie lines **not** in plane: "Isopleth"  
→ Read Type of phase(s) only !





# 三元相图：液相面投影图

- Polythermal projection
- NOT a 2D-section !



信息:

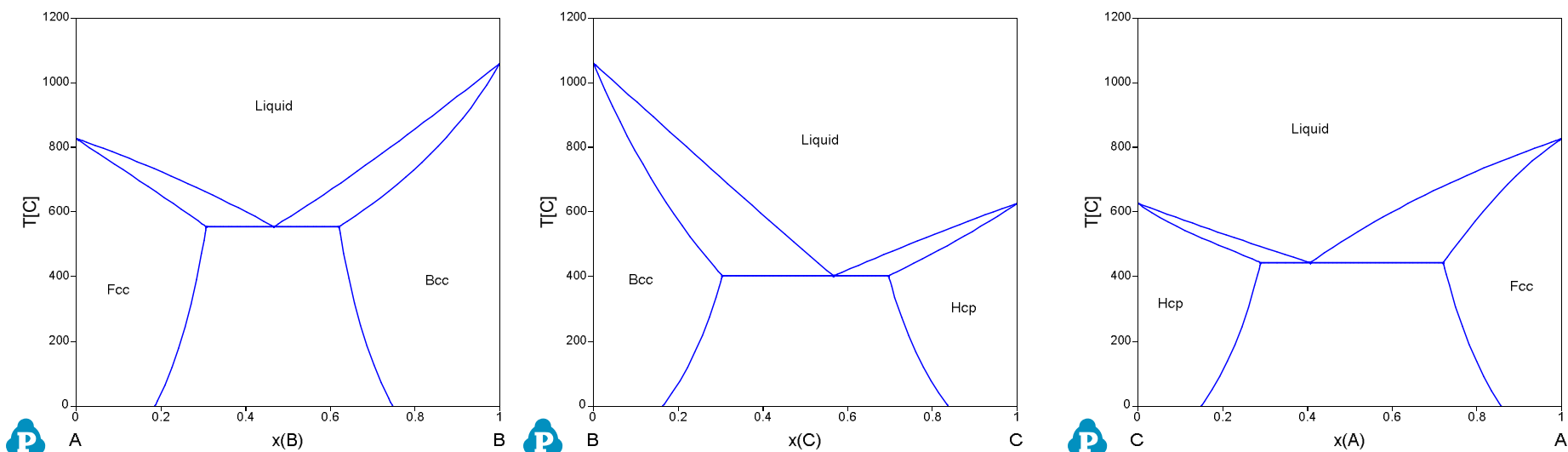
- 初生相 (Primary phase)
- 边界: (Univariant reaction line)
- 零变平衡点 (invariant reaction)
- 液相线温度 (等温线, isotherms)



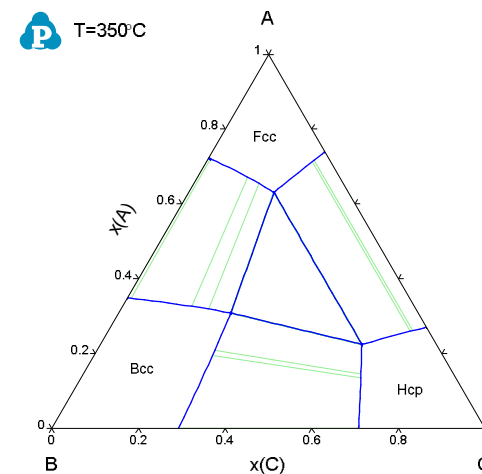
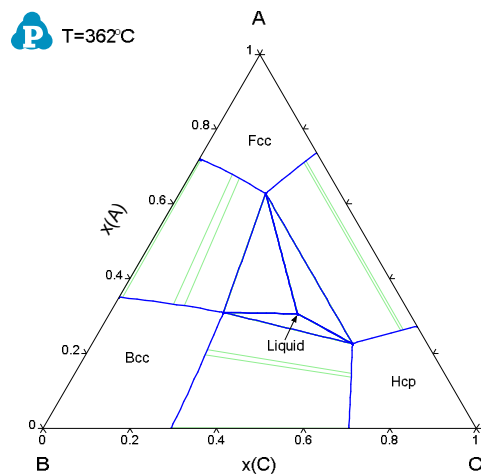
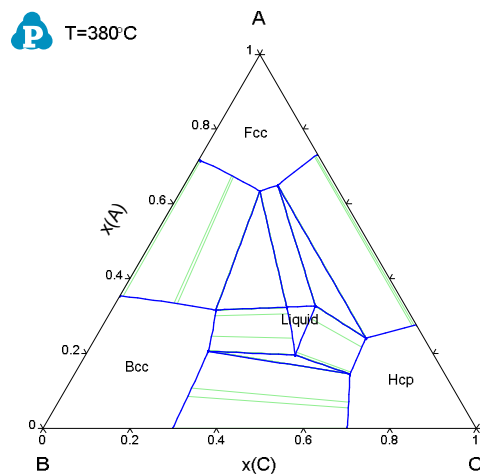
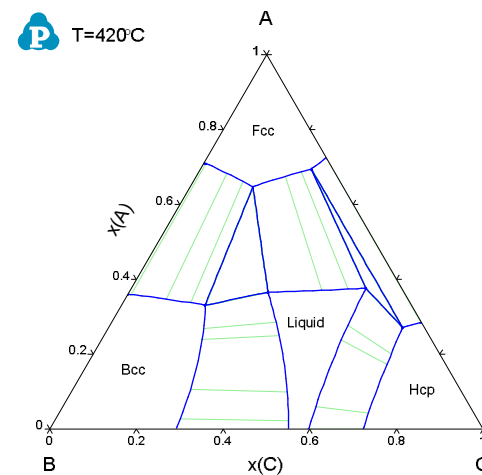
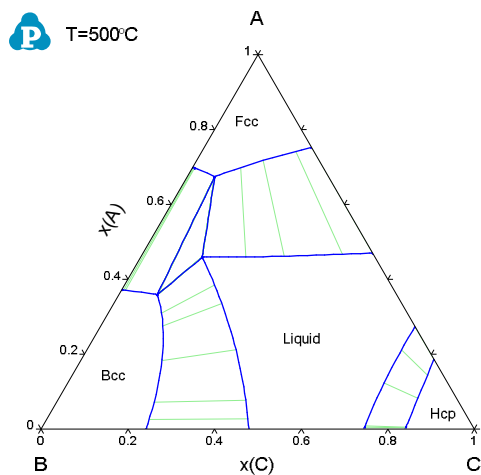
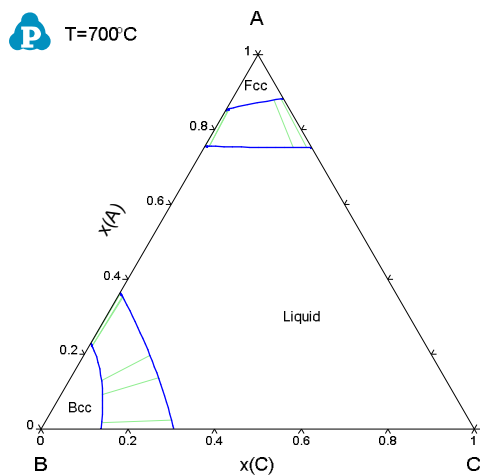


# 三元共晶体系

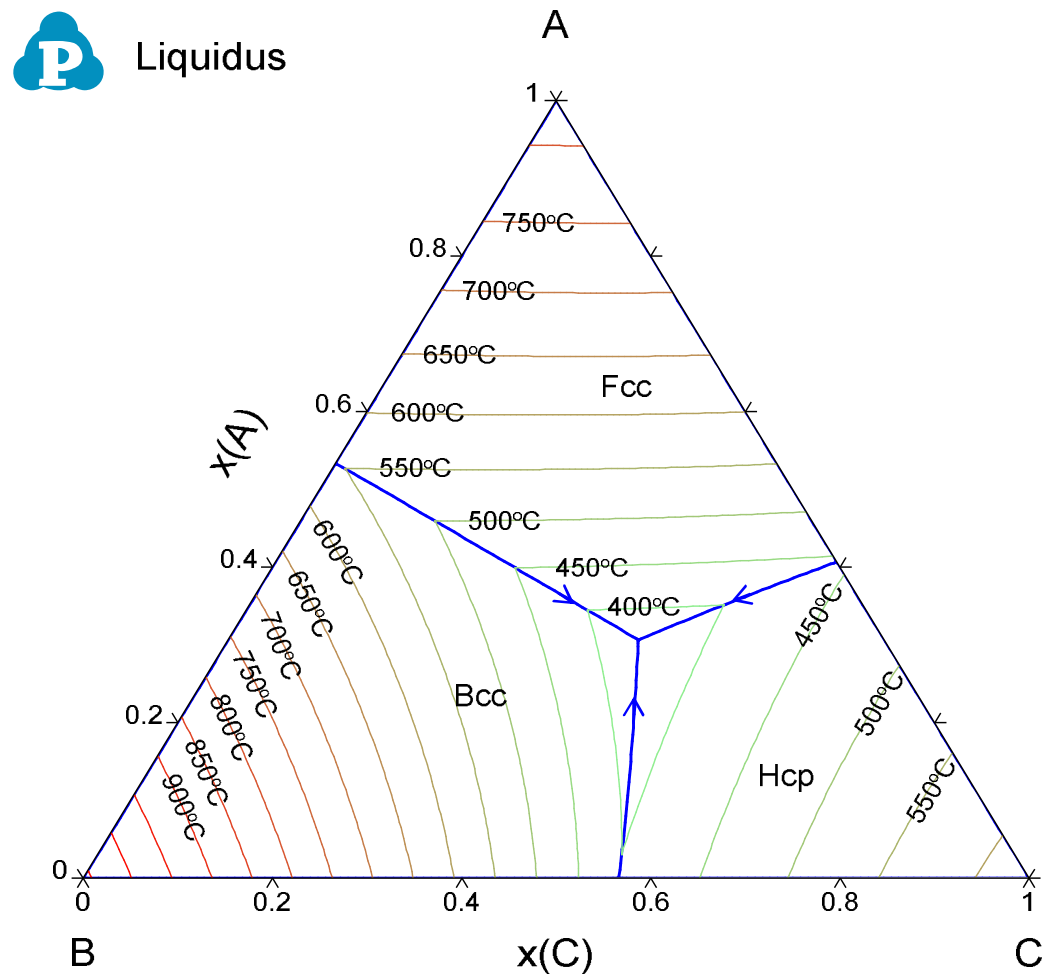
三个二元体系均为共晶体系



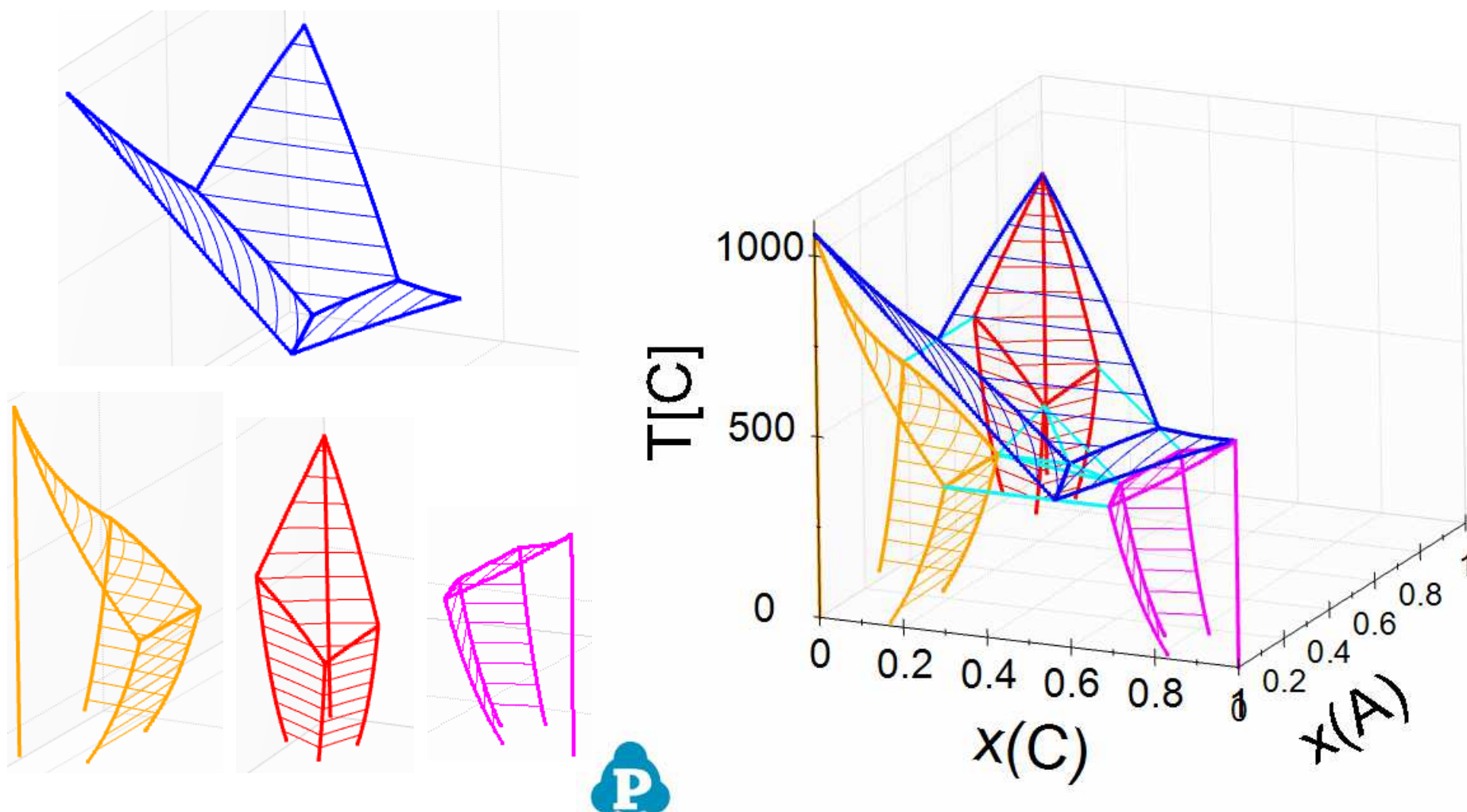
# 等温截面



# 液相面投影图



# 3D相图



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# Questions



# 三元体系溶液相模型

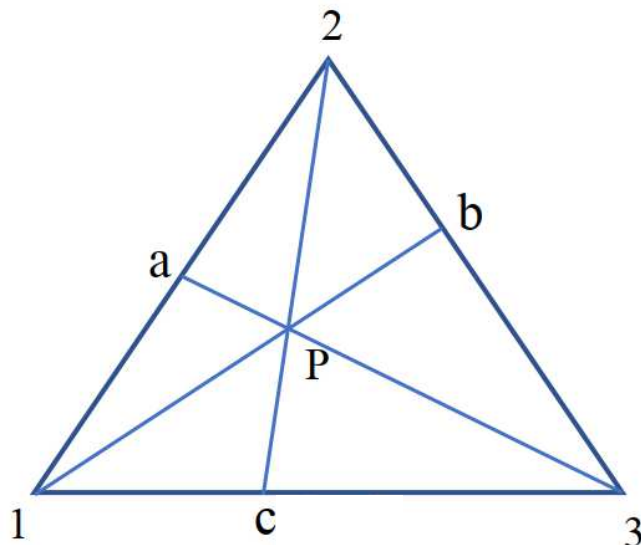
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$$G^\varphi = \sum_{i=1}^3 x_i \cdot G_i^{0,\varphi} + RT \sum_{i=1}^3 x_i \cdot \ln x_i + {}^{ex}G^{bin,\varphi} + {}^{ex}G^{tern,\varphi}$$

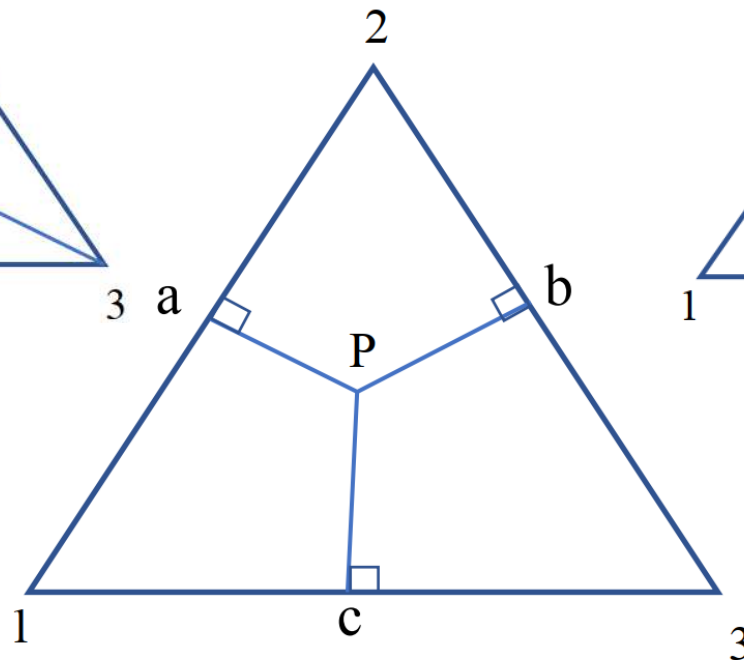
$${}^{ex}G^{bin,\varphi} = \sum_{i,j>i} x_i \cdot x_j \cdot \sum_v L_{i,j}^{v,\varphi} \cdot (x_i - x_j)^v$$

$${}^{ex}G^{tern,\varphi} = x_1 x_2 x_3 \{ L_{123}^{0,\varphi} x_1 + L_{123}^{1,\varphi} x_2 + L_{123}^{2,\varphi} x_3 \}$$

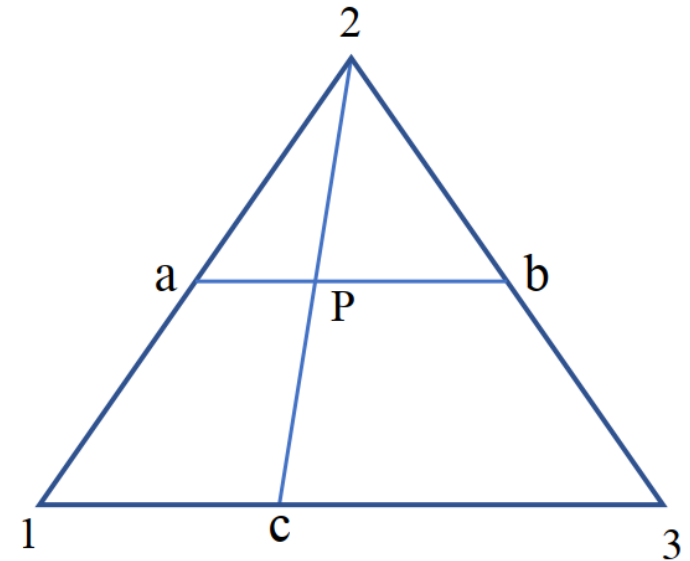
# 三元体系外推方法



Kohler Model



Muggianu Model



Toop-Kohler Model

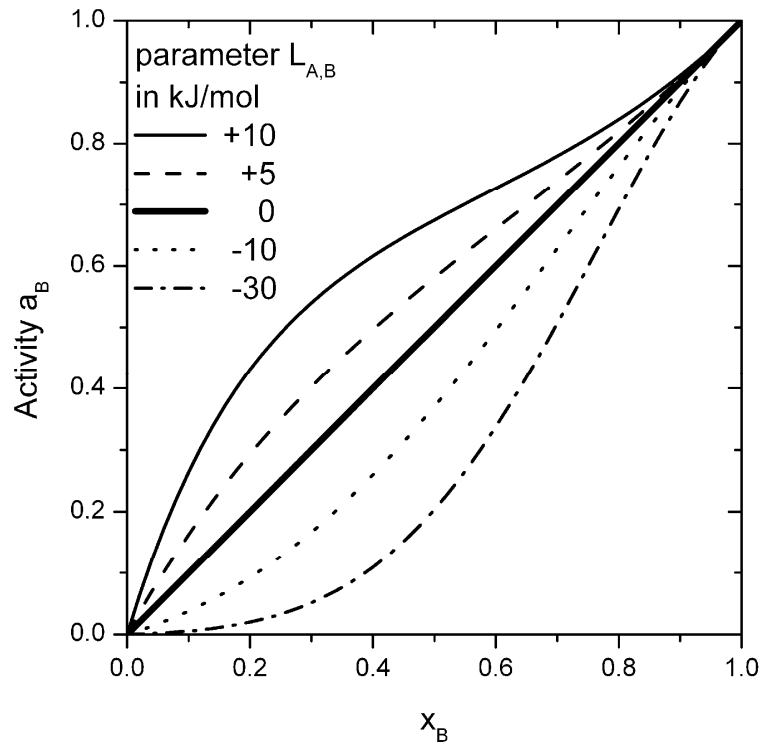
**Pandat 采用Muggianu Model.**





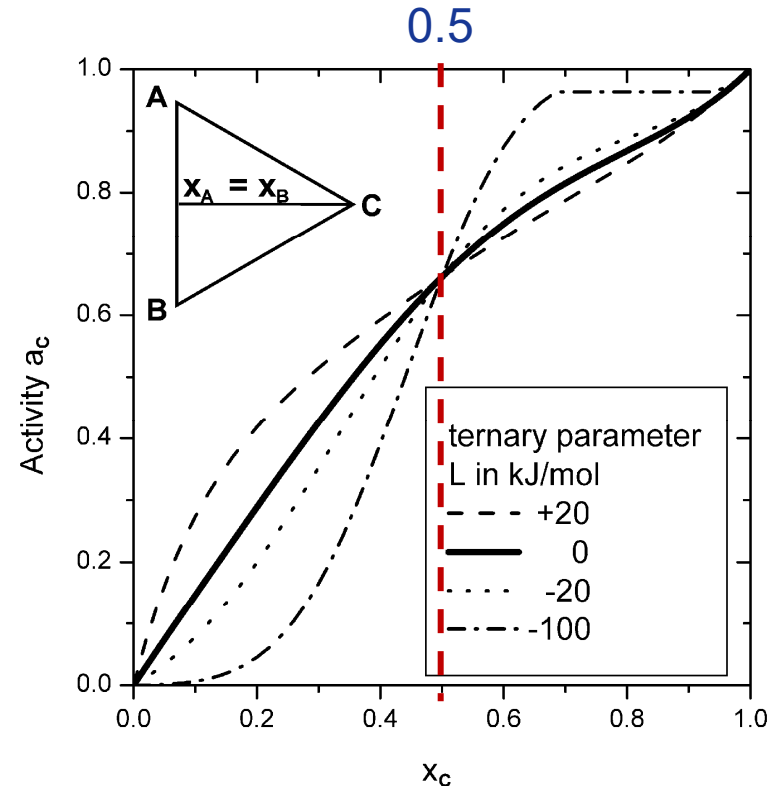
# 三元交互作用参数

$${}^{ex}G^{tern,\varphi} = x_1 x_2 x_3 \{L_{123}^{0,\varphi} x_1 + L_{123}^{1,\varphi} x_2 + L_{123}^{2,\varphi} x_3\} \quad L = L_{123}^{0,\varphi} = L_{123}^{1,\varphi} = L_{123}^{2,\varphi}$$



二元交互作用参数对活度的影响

**直觉的 (intuitive)**

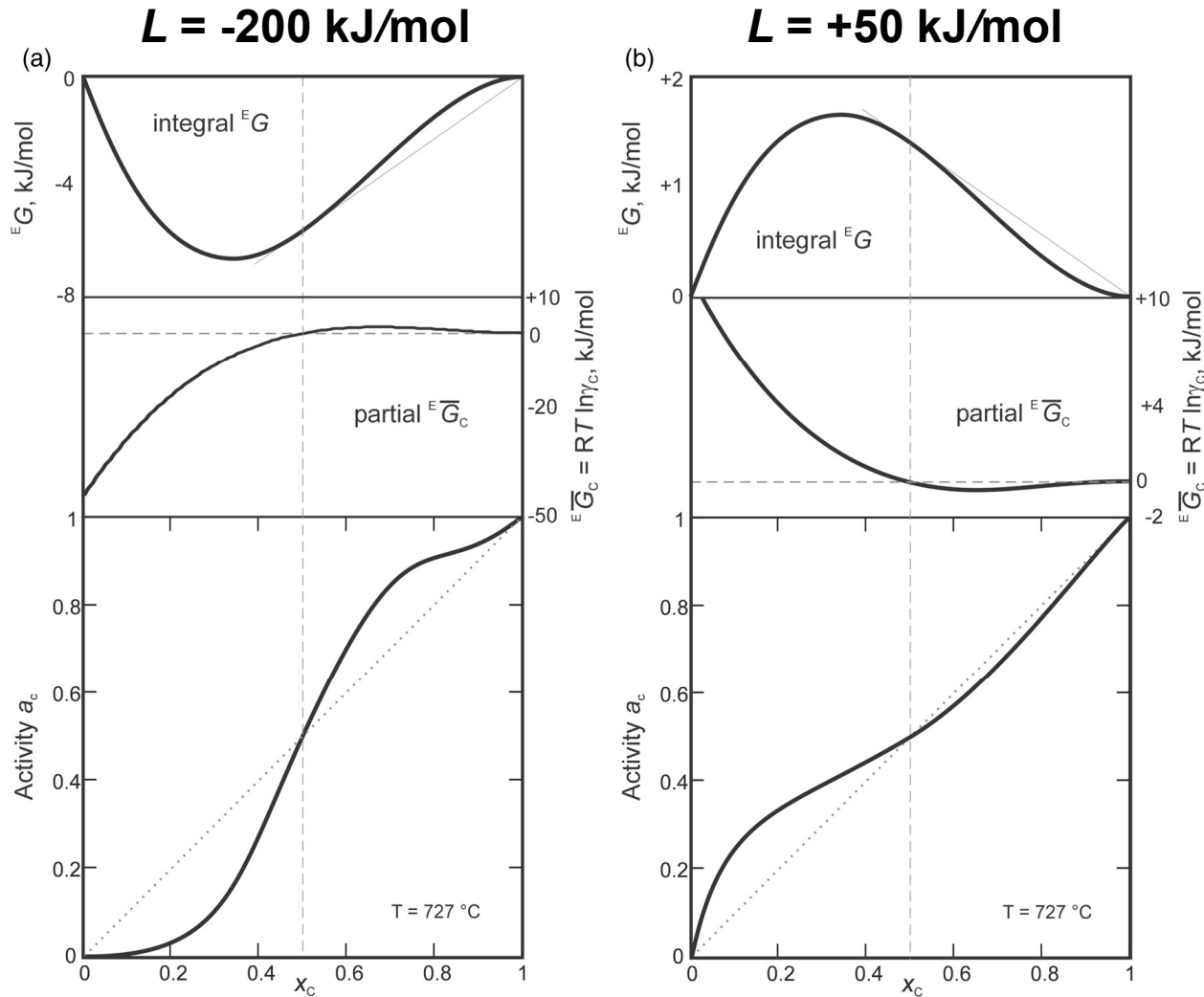


三元交互作用参数对活度的影响

**反直觉的 (counter-intuitive)**

2005Janz\_Calphad\_37.pdf

# 三元交互作用参数



Integral 量:  
公切线在  $x_c = 0.5$

Partial 量:  
 $x_c = 0.5$  为 **0**。



谨慎使用三元  
交互作用参数

2005Janz\_Calphad\_37.pdf

## 多亚点阵固溶体相

$\sigma$  相:  $(\text{Fe}, \text{Ni})_8(\text{Cr})_4(\text{Cr}, \text{Fe}, \text{Ni})_{18}$

$$G^\sigma = \sum_{i,j} y_i^I \cdot y_j^{III} \cdot G_{i:\text{Cr}:j}^{0,\sigma} + 8RT \sum_i y_i^I \ln y_i^I + 18RT \sum_j y_j^{III} \ln y_j^{III} + G^{ex,\varphi}$$

$i = \text{Fe}, \text{Ni}; j = \text{Cr}, \text{Fe}, \text{Ni}$

$$G_{\text{Fe:Cr:Cr}}^{0,\sigma} \quad G(\text{Sigma}, \text{Fe:Cr:Cr}; 0)$$

$$G_{\text{Fe:Cr:Fe}}^{0,\sigma} \quad G(\text{Sigma}, \text{Fe:Cr:Fe}; 0)$$

$$G_{\text{Fe:Cr:Ni}}^{0,\sigma} \quad G(\text{Sigma}, \text{Fe:Cr:Ni}; 0)$$

$$G_{\text{Ni:Cr:Cr}}^{0,\sigma} \quad G(\text{Sigma}, \text{Ni:Cr:Cr}; 0)$$

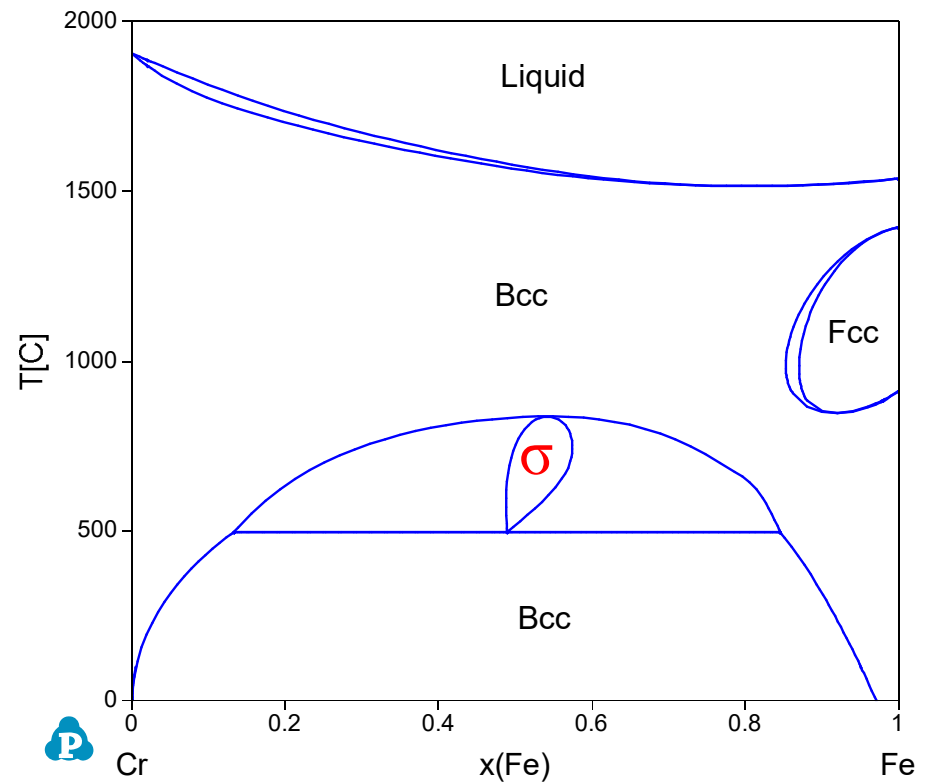
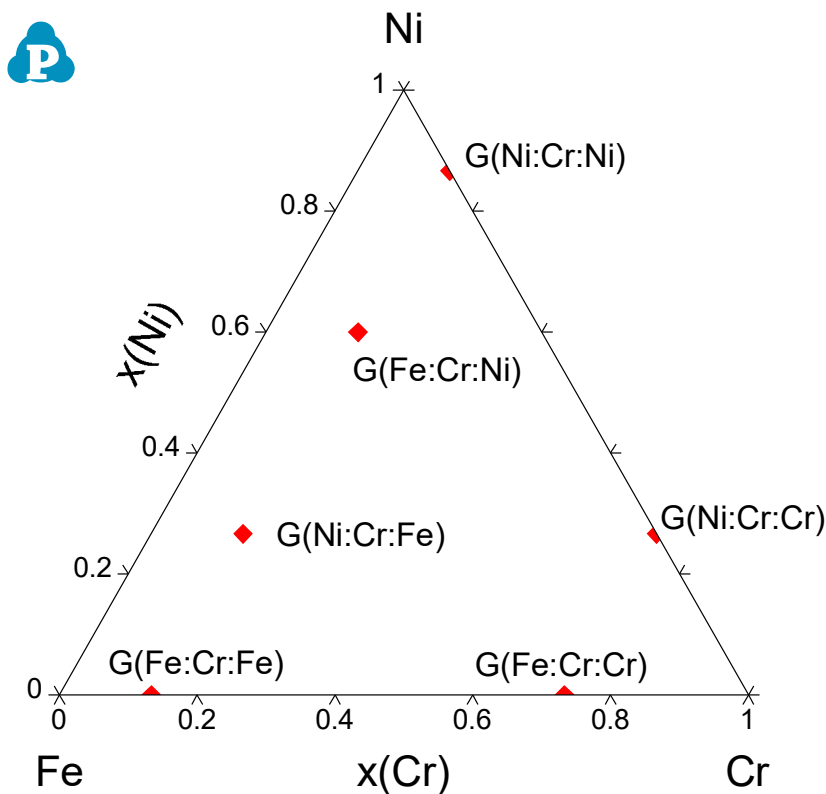
$$G_{\text{Ni:Cr:Fe}}^{0,\sigma} \quad G(\text{Sigma}, \text{Ni:Cr:Fe}; 0)$$

$$G_{\text{Fe:Cr:Ni}}^{0,\sigma} \quad G(\text{Sigma}, \text{Ni:Cr:Ni}; 0)$$



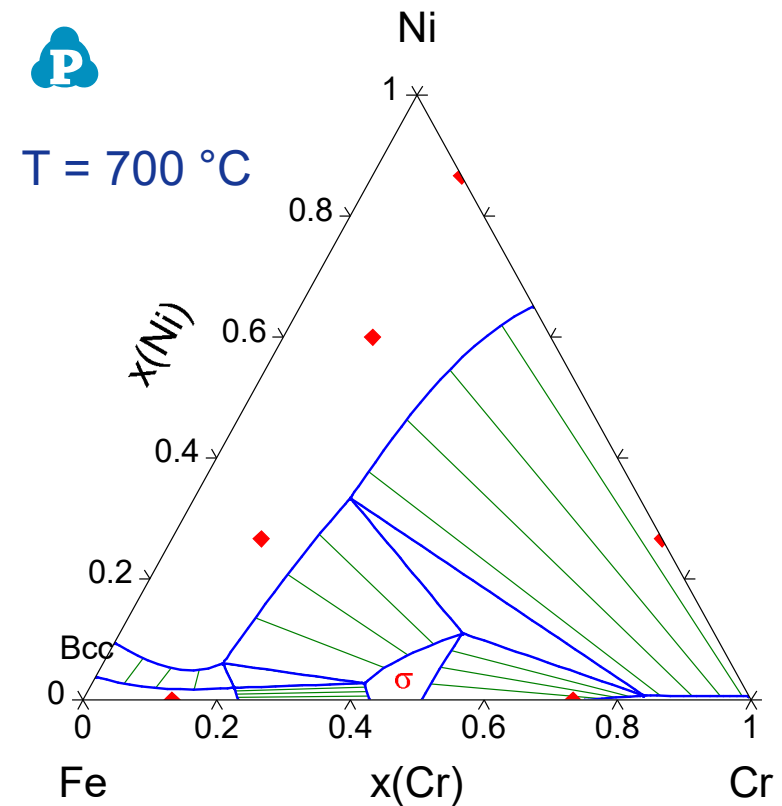
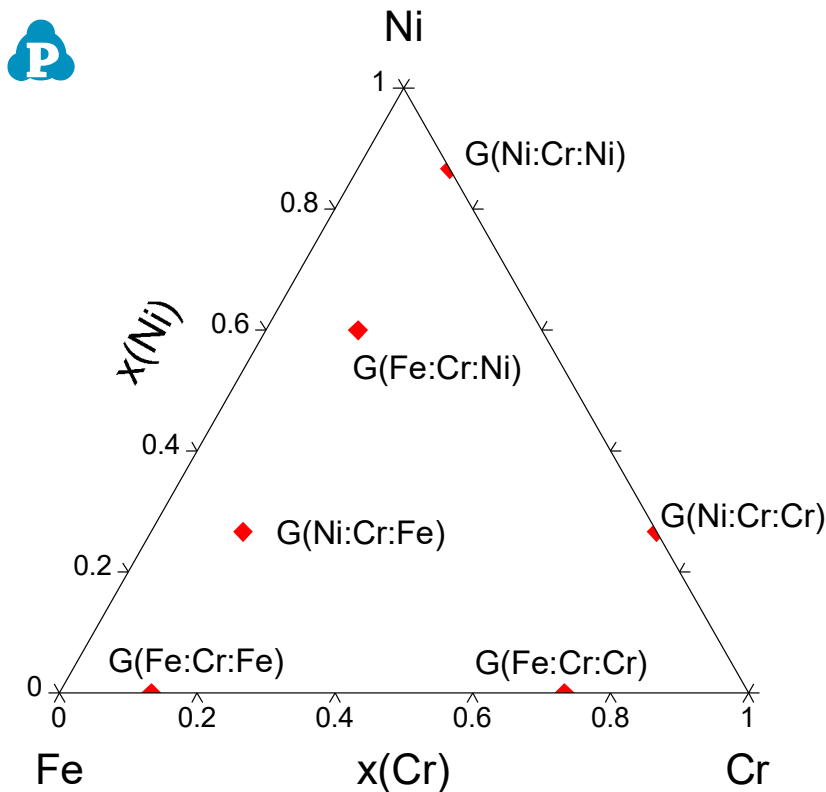
# Endmember 在相图中的位置

$\sigma$  相:  $(\text{Fe}, \text{Ni})_8(\text{Cr})_4(\text{Cr}, \text{Fe}, \text{Ni})_{18}$

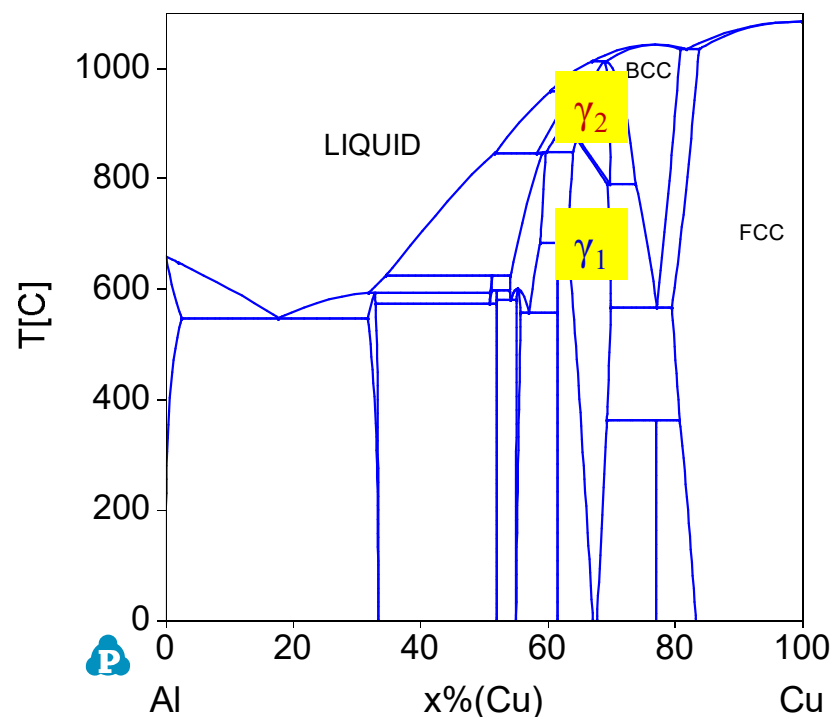
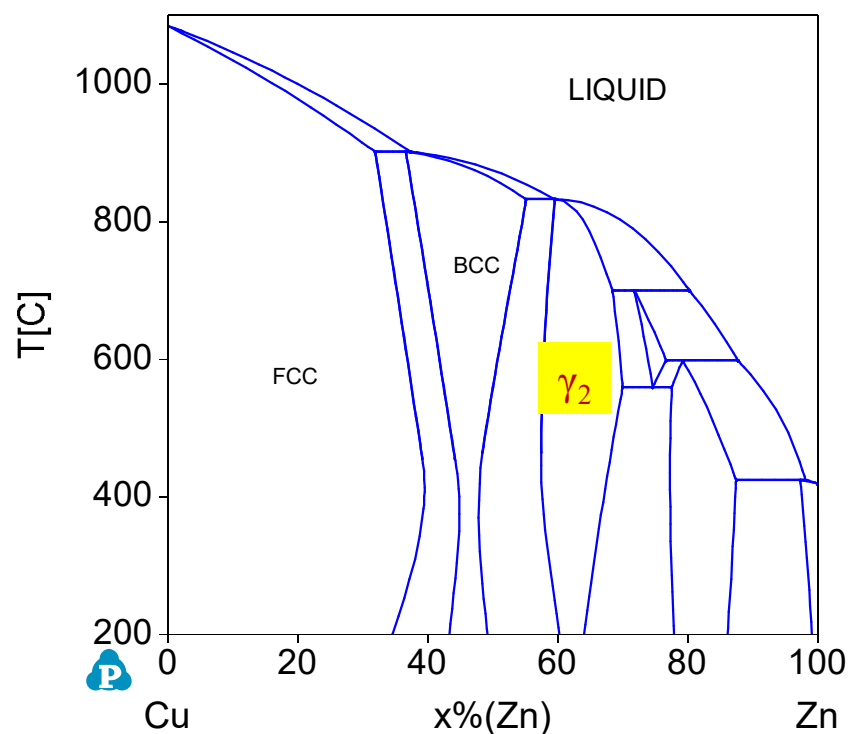


# Endmember 在相图中的位置

$\sigma$  相:  $(\text{Fe}, \text{Ni})_8(\text{Cr})_4(\text{Cr}, \text{Fe}, \text{Ni})_{18}$



# Endmember 在相图中的位置



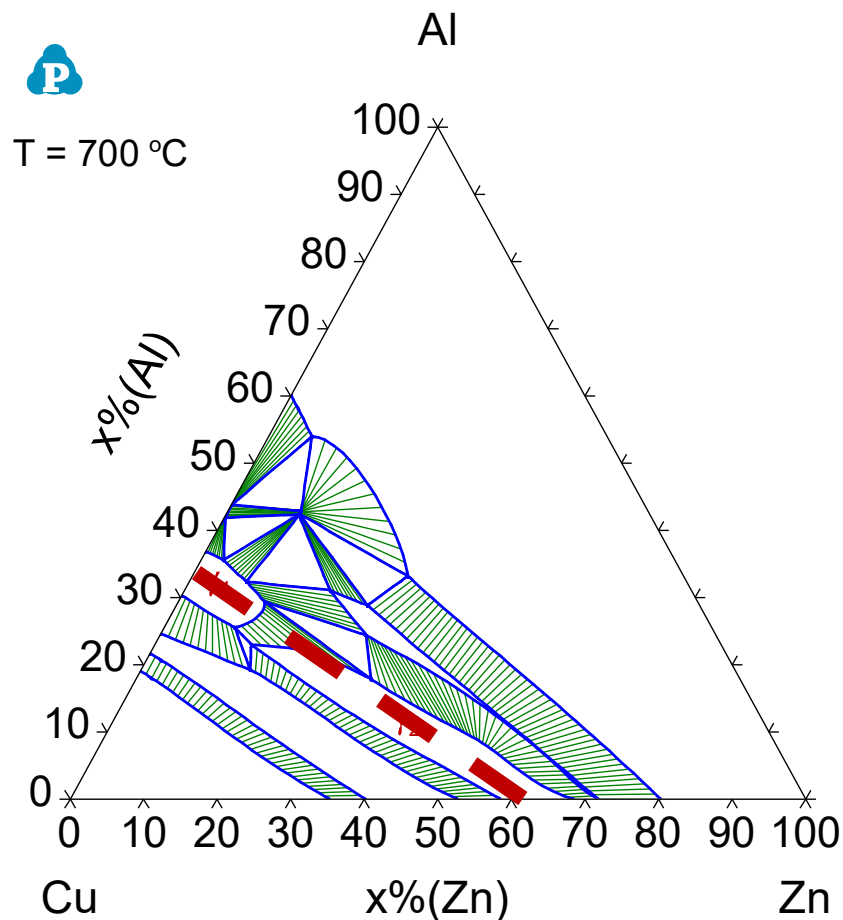
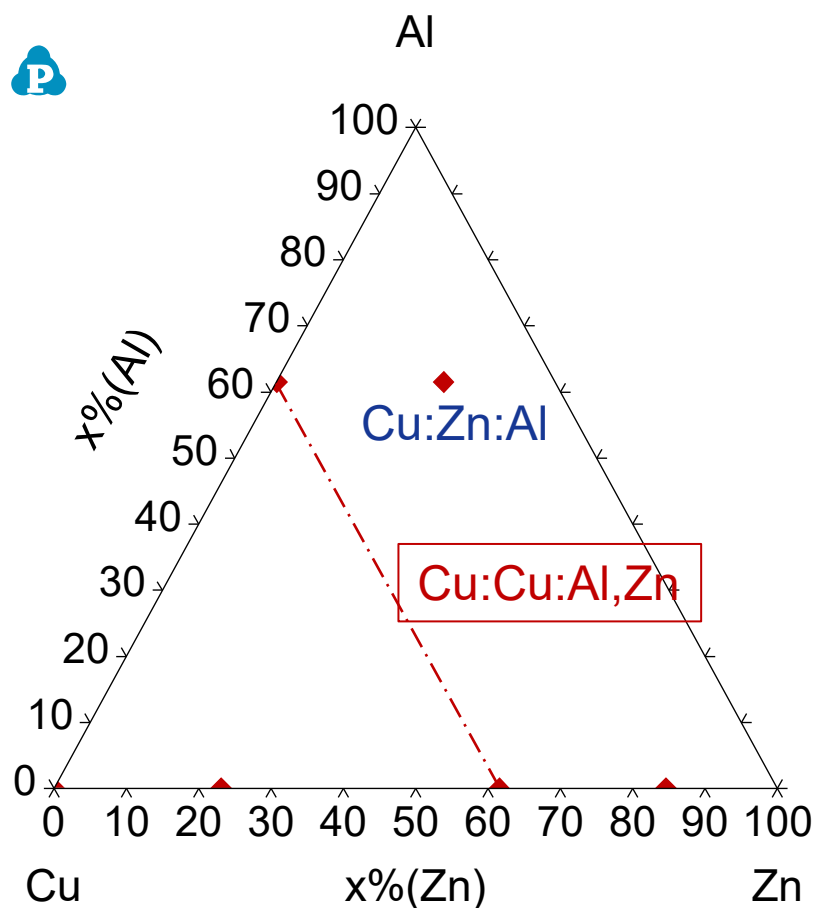
$(\text{Zn})_4 (\text{Cu})_4 (\text{Cu}, \text{Zn})_6 (\text{Cu}, \text{Zn})_{12} \longleftrightarrow (\text{Al}, \text{Cu})_4 (\text{Cu})_4 (\text{Cu})_6 (\text{Al}, \text{Cu})_{12}$

$(\text{Al}, \text{Cu}, \text{Zn})_4 (\text{Cu})_4 (\text{Cu}, \text{Zn})_6 (\text{Al}, \text{Cu}, \text{Zn})_{12}$  18 endmember

$(\text{Cu})_4 (\text{Cu}, \text{Zn})_6 (\text{Al}, \text{Cu}, \text{Zn})_{16}$  6 endmember

# Endmember 在相图中的位置

$\gamma$  phase: (Cu)<sub>4</sub> (Cu,Zn)<sub>6</sub> (Al,Cu,Zn)<sub>16</sub>



[2015Liang\\_Calphad\\_224\\_CuZn.pdf](#); [2015Liang\\_Calphad\\_252\\_AlCu.pdf](#); [2016Liang\\_Calphad\\_21\\_AlCuZn.pdf](#)



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# Questions?

