

Contents of Today

热力学研究热功转换的方向、限度以及能量的衡算。

- Review
- Gibbs自由能的计算

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判断过程方向之等温等压过程

等温定压的体系

$$(\Delta G)_{T,p} < 0$$
 表示自发

$$(\Delta G)_{T,p} = 0$$
 表示平衡

$$(\Delta G)_{T,p} > 0$$
 表示不自发

$$(\Delta G)_{T,p} > W'$$
 表示不可能进行

在等温定压条件下,一个自发过程发生时,系统的Gibbs自由能总要减少,当减少到不能再减少时,系统即达平衡,这是系统的Gibbs自由能应为极小值

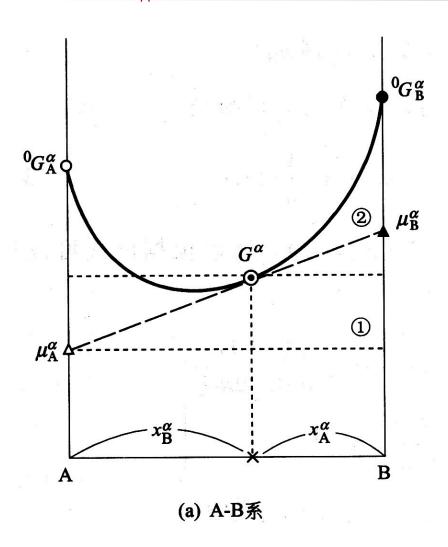
思考题:试推导在何种条件下,可用U和H来判断过程的方向和限度。

$$TdS - dU - p_{\beta \mid} dV \ge -\delta W'$$



Phase Transformation and Applications

Binary



A-B二元自由能和化学势 之间的关系

$$G^{\alpha} = \mu_{A}^{\alpha} \cdot x_{A} + \mu_{B}^{\alpha} \cdot x_{B}$$

$$\mu_{A}^{\alpha} = G^{\alpha} - \left(\frac{\partial G^{\alpha}}{\partial x_{B}}\right) \cdot x_{B}$$

$$\mu_{B}^{\alpha} = G^{\alpha} - \left(\frac{\partial G^{\alpha}}{\partial x_{B}}\right) \cdot x_{B} + \left(\frac{\partial G^{\alpha}}{\partial x_{B}}\right)$$

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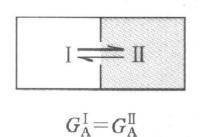


单元系

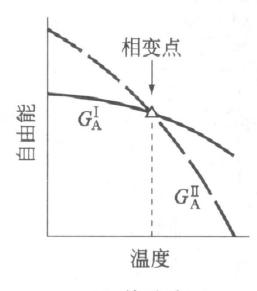
- F=C-P+2=3-P
- 两相共存F=1
 - 给定温度或压力,体 系就已确定,因为两 相均为纯物质

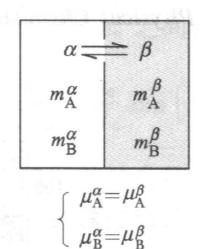
二元系

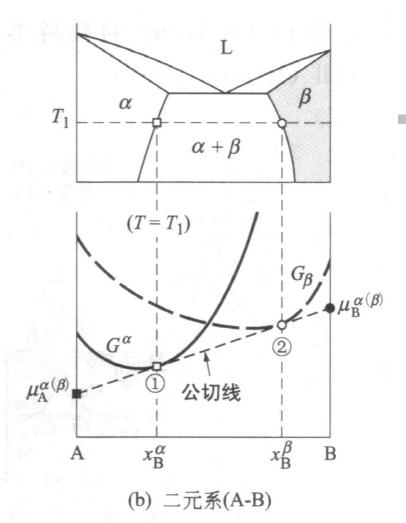
- F=C-P+1=3-P
- 两相共存F=1
 - 给定温度或压力,体 系如果要确定,必须 给定两相中的组成, 即浓度
 - 多相平衡条件给出,



.....







(a) 单元系(A)

图 4.1 单元系和二元系的两相平衡条件

(a) 单元系中自由能的交叉点是平衡温度; (b) 二元系中公切线的切点 ①和②是平衡成分

T. Nishizawa

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Review

- 可逆过程/熵/判断过程方向性
- 热力学函数关系式
- 多相平衡
- 溶液/溶体
- 相律
- 二元、三元相图



今天: 体系自由能的计算

- 能量
- · Gibbs自由能定义及其作用
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 - 二元系
 - 溶液模型



Energy

Phase Transformation and Applications

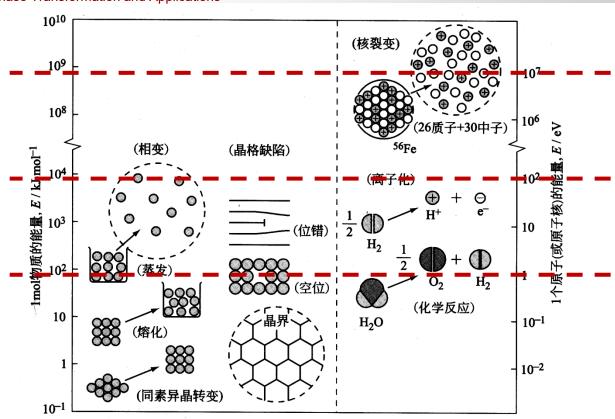


图 2.1 与材料的微观组织有关的能量(位错和晶界的能量已经换算成对应于1个原子的能量)与化学能的比较

1 eV/atom=1.602 · 10^{-19} C · V×6.022 · 10^{23} /mol

$$=9.648 \times 10^4 \text{ J/mol}$$

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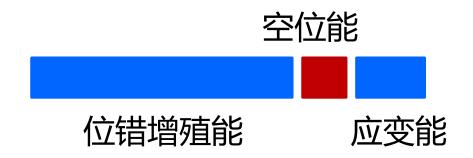
塑性加工过程中能量的分配(1/3)

Phase Transformation and Applications

将纯铁片进行强烈塑性加工所需的能量(约8 kJ·mol⁻¹)的大部分以热能形式消耗掉,其余的5%(400 J·mol⁻¹)左右以晶格缺陷的形式储存在试样中。

存储能量的大体比例为:

- 1) 约75%为位错增殖能;
- 2) 约10%为过剩空位能;
- 3) 其余的15%是应变能。



如果假设位错能量为 $\Delta e_d = 5 \times 10^{-9} \text{ J·m}^{-1}$

空位形成能是 $\Delta e_v = 1.5 \text{ ev}$

计算:由于强塑性加工所产生的位错密度和空位浓度?

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塑性加工过程中能量的分配(2/3)

Phase Transformation and Applications

能量 (约8 kJ·mol⁻¹) 的5% (400 J·mol⁻¹) 储存在试样中。

存储能量的大体比例为: 1) 约75%为位错增殖能;

如果假设位错能量为 $\Delta e_d = 5 \times 10^{-9} \text{ J·m}^{-1}$

计算: 1) 由于强塑性加工所产生的位错密度?

$$\rho_{\rm d} = \frac{\Delta E_{\rm d}}{V \cdot \Delta e d} = \frac{300 \ J \cdot mol^{-1}}{7 \times 10^{-6} m^3 \cdot mol^{-1} \cdot 5 \times 10^{-9} \ J \cdot m^{-1}} = 9 \times 10^{15} \ {\rm m}^{-2}$$

空位能

位错增殖能

应变能



塑性加工过程中能量的分配(3/3)

Phase Transformation and Applications

能量(约8 kJ·mol⁻¹)的5%(400 J·mol⁻¹)储存在试样中。

存储能量的大体比例为: 2) 约10%为过剩空位能;

空位形成能是 $\Delta e_v = 1.5 \text{ ev}$

计算:由于强塑性加工所产生的空位浓度?

$$\rho_v = \frac{\Delta E_v}{\Delta e v} = \frac{40 \ J \cdot mol^{-1}}{1.5 \times 96480 \ J \cdot m^{-1}} = 3 \times 10^{-4}$$

空位能

 $1 \text{ eV/atom} = 1.602 \cdot 10^{-19} \text{ C} \cdot \text{V} \times 6.022 \cdot 10^{23} / \text{mol}$ $=9.648\times10^{4}\,\text{J/mol}$

位错增殖能

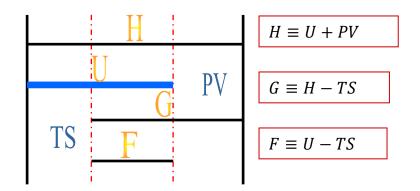


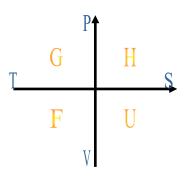
今天: 体系自由能的计算

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Gibbs函数与化学势





 μ_i The chemical potential of the component i.

$$\left(\frac{\partial \mathbf{G}}{\partial \mathbf{n_i}}\right)_{\mathbf{T},\mathbf{P},\mathbf{n_j}\neq\mathbf{n_i}} = \left(\frac{\partial F}{\partial n_i}\right)_{T,V,n_j\neq n_i} = \left(\frac{\partial H}{\partial n_i}\right)_{P,S,n_j\neq n_i} = \left(\frac{\partial U}{\partial n_i}\right)_{V,S,n_j\neq n_i} = \mu_i$$

偏摩尔量



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P, V, Xi影响化学势

1,温度的影响

$$\left(\frac{\partial G}{\partial T}\right)_{P,x_i} = -S$$

$$\underline{S_{298}^0} = \int_{0}^{298} \frac{C_P}{T} dT$$

2, 压力的影响

$$\left(\frac{\partial G}{\partial P}\right)_{T,x_i} = V$$

气相

$$\underline{V} = \frac{RT}{P}$$

$$d\underline{G} = RTd \ln P$$

3, 组成的影响: 偏摩尔Gibbs自由能

$$\Delta G = \Delta H - T \cdot \Delta S$$



1.13 Heat Capacity at Constant Pressure

Phase Transformation and Applications

Heat (energy) capacity: defined as the amount of thermal energy required to change the temperature of a material.

$$\delta Q = dU - \delta W = dU + PdV = dH = mCdT$$

$$CdT = \frac{dH}{m} = d\underline{H}$$

$$C_P \equiv \left(\frac{\partial \underline{H}}{\partial T}\right)_P$$

No other forms of work (except volume work) involved

$$dH = mC_P dT$$

Need to specify Path / Condition

A function of both temperature and presure

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Entropy Changes (1)

The specific entropy change for a material heated between two temperature, T1 and T2, at constant pressure. (no change of state between the two temperatures)

$$d\underline{S} = \frac{\delta Q_{rev}}{T} = \frac{C_P dT}{T}$$

$$\underline{S}_{2} - \underline{S}_{1} = \int_{S_{1}}^{S_{2}} d\underline{S} = \int_{T_{1}}^{T_{2}} \frac{C_{P}dT}{T}$$

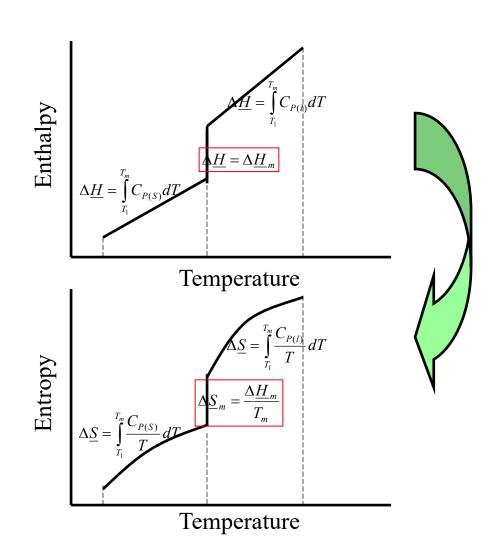
In the case of change of state between

$$\Delta \underline{S}_{melting} = \frac{\Delta H_{melting}}{T_{melting}}$$

Reversible process: at the melting temperature



Entropy Changes (2)





2.10 Entropy change in chemical reactions and the third law (1)

Phase Transformation and Applications

The calculation of entropy changes for a chemical reaction is similar to the calculation in the case of enthalpy changes.

One very important difference:

Nernst 1906

The entropy change in any chemical reaction involving only pure, crystalline ZERO at the ABSOLUTE Zero of temperature. substances:

Pure: pure elements and stoichiometrically balanced compounds that are perfectly crystalline.

Planck

The entropy of a pure, perfectly crystalline substances: ZERO at the ABSOLUTE Zero of temperature.

Superscript zero: standard state, 1 atm

Subscript zero: temperature ZERO

$$\Delta S_0^0 = 0$$

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2.10 Entropy change in chemical reactions and the third law (2)

Phase Transformation and Applications

The third law provides a great simplification in the calculation of entropies of reaction.

$$\Delta S_T^0 = \Delta S_0^0 + \int_0^T \frac{C_P}{T} dT = \int_0^T \frac{C_P}{T} dT$$

The entropy changes near room temperature are often needed in thermodynamic calculations, the integral in above equation has been evaluated for many substance at 298 K.

$$S_{298}^{0} = \int_{0}^{T_{m}} \frac{C_{P}}{T} dT + \frac{\Delta \underline{H}_{m}}{T_{m}} + \int_{T_{m}}^{T_{b}} \frac{C_{P}}{T} dT + \frac{\Delta \underline{H}_{b}}{T_{b}} + \int_{T_{b}}^{298} \frac{C_{P}}{T} dT$$

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2.10 Entropy change in chemical reactions and the third law (3)

Phase Transformation and Applications

The entropy change for a chemical reaction at 298 K.

$$\Delta S_{298}^{0} = \sum_{products} n_{P} \underline{S}_{298,p}^{0} - \sum_{reac \tan ts} n_{r} \underline{S}_{298,r}^{0}$$

The entropy change for a chemical reaction at other temperature.

$$\Delta S_T^0 = \Delta S_{298}^0 + \int_{298}^T \frac{n_p C_{p,prod} - n_r C_{p,react}}{T} dT$$



相变焓

潜热;熔化焓;蒸发焓:相变焓

水的气化焓 40.7 kJ·mol⁻¹

气化体积膨胀所需能量

 $P \cdot \Delta V \approx P \cdot V_{x, x, x} \approx RTb$ = $3.1 \, kJ \cdot mol^{-1}$

水分子分开的内能变化 (约90%) $40.7 - 3.1 = 37.6 kJ \cdot mol^{-1}$

水的熔化焓 $6.0 kJ \cdot mol^{-1}$

冰到水体积<mark>收缩</mark>所需能量 内能变化约等于其熔化焓

$$P \cdot \Delta V \approx -0.17 J \cdot mol^{-1}$$

$$6.0 kJ \cdot mol^{-1}$$



相变焓

水的气化焓 40.7 kJ⋅mol⁻¹

水的熔化焓 $6.0 kJ \cdot mol^{-1}$

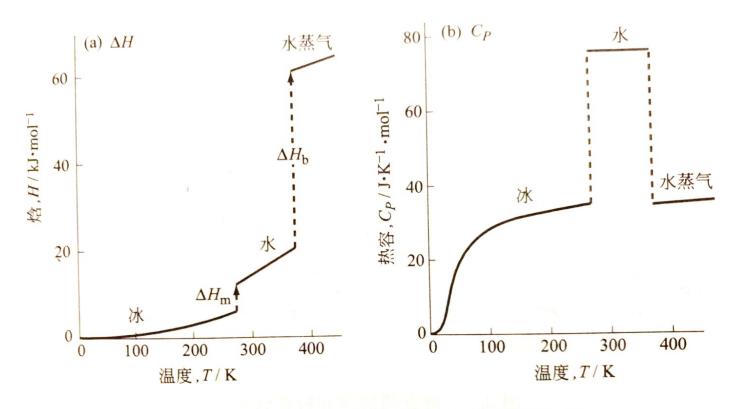


图 2.4 常压下 H_2O 的焓 (a) 和定压热容 (b) (可知水的热容异常巨大,水银的热容也只不过是 27.7 $J \cdot K^{-1} \cdot mol^{-1}$)



Phase Transformation and Applications

$$\Delta H_m \approx RTm$$

$$\Delta H_b \approx 92Tb$$

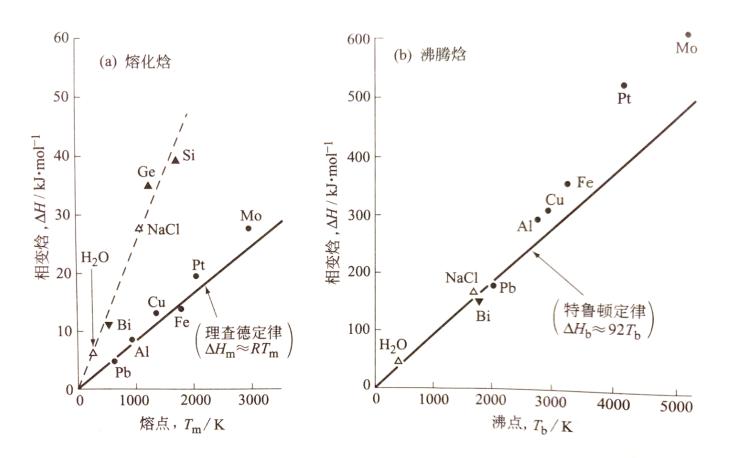


图 2.5 理查德定律和特鲁顿定律



P, V, Xi影响化学势

1,温度的影响

$$\left(\frac{\partial G}{\partial T}\right)_{P,x_i} = -S$$

$$\underline{S_{298}^0} = \int_{0}^{298} \frac{C_P}{T} dT$$

2,压力的影响

$$\left(\frac{\partial G}{\partial P}\right)_{T,x_i} = V$$

气相

$$\underline{V} = \frac{RT}{P}$$

$$d\underline{G} = RTd \ln P$$

3,组成的影响:偏摩尔Gibbs自由能

$$\Delta \underline{G} = \Delta \underline{H} - T \cdot \Delta \underline{S}$$

 $G = H-T \cdot S$



Variation of vapor pressure of a condensed phase with total applied pressure

Phase Transformation and Applications

Increasing the pressure on the liquid increases the vapor pressure $\pi_{\text{e}}\text{:}$ equilibrium vapor pressure

 π : the vapor pressure of the liquid under a total pressure p_T . The specific Gibbs free energy changes when the liquid is pressurized from π_e to p_T

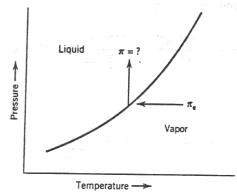


Figure 4.6 Effect of total pressure on vapor pressure.

$$d\underline{G}_l = \underline{V}_l dp$$

$$\Delta \underline{G}_l = \underline{V}_l \Delta p = \underline{V}_l (p_T - \pi_e)$$

The Gibbs free energy of the gas must also change, assuming it is an ideal gas

$$\Delta \underline{G}_V = RT \ln \frac{\pi}{\pi_e}$$

$$\underline{V}_{l}(p_{T} - \pi_{e}) = RT \ln \frac{\pi}{\pi_{e}}$$

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Variation of vapor pressure of a condensed phase with total applied pressure (2)

Phase Transformation and Applications

$$\underline{V}_{l}(p_{T} - \pi_{e}) = RT \ln \frac{\pi}{\pi_{e}}$$

$$\Delta \underline{G}_{l} = \underline{V}_{l} \Delta p = \underline{V}_{l}(p_{T} - \pi_{e})$$
If $p_{T} >> \pi_{e}$

$$\underline{V}_{l} p_{T} = RT \ln \frac{\pi}{\pi_{e}}$$

The fractional change of the vapor pressure of water at 298 K when the total pressure of the system is increased to 10 atm

The equilibrium vapor pressure of water is 0.031 atm

$$\ln \frac{\pi}{\pi_e} = \ln \left(1 + \frac{\Delta \pi}{\pi_e} \right) = \frac{\Delta \pi}{\pi_e} = 0.0074$$

$$= \ln \left(1 + \frac{\Delta \pi}{\pi_e} \right) = \frac{\Delta \pi}{\pi_e} = 0.0074$$

$$= \frac{1 \text{ atm } -> 10 \text{ atm}}{\text{Vapor pressure changes by 0.74 %}}$$

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今天: 体系自由能的计算

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溶液 (2)

Fugacity is defined for gases:

$$d\overline{G}_i = RTd(\ln f_i)$$

Thermodynamic activity of a component, i, is defined as:

$$\alpha_i \equiv \frac{f_i}{f_i^{\circ}}$$

 f_i° The fugacity of the component i in its standard state.

The fugacity of a condensed phase is equal to the fugacity of the vapor phase in equilibrium with it.

The fugacity of the vapor is equal to the pressure of the vapor, if the vapor in equilibrium with the condensed phase is ideal.



体系自由能的计算

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Dilute Solution and Colligative Properties (1)

Phase Transformation and Applications

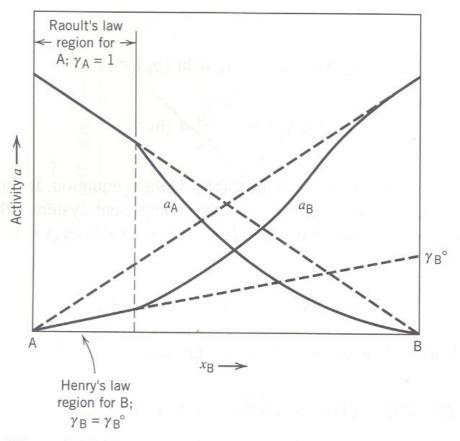


Figure 7.11 Henry's law and Raoult's law regions for the nonideal solution.

Henry's law region:

$$\gamma_B = \gamma_B^{\circ} \qquad d(\ln \gamma_B^{\circ}) = 0$$

$$\gamma_B^{\circ} = Cons \tan t$$

Raoult's law region:

$$\gamma_A^{\circ} = 1$$

$$x_A = 1, a_A = 1$$

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4.常用热力学模型

Phase Transformation and Applications

- 纯组元和化学计量比化合物
- 溶体和中间化合物
 - 理想溶体
 - 正规溶体
 - 亚正规溶体
 - 缔合溶液模型
 - 亚点阵模型
- 磁性有序无序和化学有序无序对热力学性质的贡献
 - 磁性有序无序
 - 化学有序无序
- 多元系热力学性质的外推关系
 - 对称方法
 - 非对称方法
 - 周国治模型



Regular Solution (1)

$$\underline{G}_{M} = x_{A}\overline{G}_{A}^{rel} + x_{B}\overline{G}_{B}^{rel}$$

$$\overline{G}_A^{rel} = \overline{G}_A - \underline{G}_A^{\circ} = RT \ln \alpha_A$$

$$\underline{G}_{M} = x_{A}RT \ln(\gamma_{A}x_{A}) + x_{B}RT \ln(\gamma_{B}x_{B})$$

$$\underline{G}_{M} = RT(x_{A} \ln x_{A} + x_{B} \ln x_{B}) + RT(x_{A} \ln \gamma_{A} + x_{B} \ln \gamma_{B})$$

$$\underline{G}_{M} = \underline{G}_{M}^{ideal} + \underline{G}_{M}^{xs}$$

$$\underline{G}_{M}^{ideal} = RT(x_A \ln x_A + x_B \ln x_B)$$

$$\underline{G}_{M}^{xs} = RT(x_{A} \ln \gamma_{A} + x_{B} \ln \gamma_{B})$$



Regular Solution (2)

Phase Transformation and Applications

$$\ln \gamma_A = \frac{\omega}{RT} x_B^2 = \frac{\omega}{RT} (1 - x_A)^2$$

$$\underline{G}^{xs} = \underline{H}^{xs}$$

regular solution

$$\underline{G}_{M} = RT(x_{A} \ln x_{A} + x_{B} \ln x_{B}) + RT(x_{A} \ln \gamma_{A} + x_{B} \ln \gamma_{B})$$

$$\underline{G_M} = RT(x_A \ln x_A + x_B \ln x_B) + \underbrace{x_A \omega x_B^2 + x_B \omega x_A^2}_{(x_A + x_B)(\omega x_A x_B)}$$

$$\underline{G}_M = RT(x_A \ln x_A + x_B \ln x_B) + \omega x_A x_B$$

$$\underline{H}_{M} = \omega x_{A} x_{B}$$

$$\underline{G}_{M} = \underline{G}_{M}^{ideal} + \underline{G}_{M}^{xs}$$

$$\underline{H}_{M} = \underline{H}_{M}^{ideal} + \underline{H}_{M}^{xs}$$

$$\underline{H}_{M}^{ideal} = 0$$



Regular Solution (3)

For the regular solution: $\underline{S}^{xs}_{M} = 0$

$$\underline{S}^{xs}_{M} = 0$$
 $\underline{G}^{xs}_{M} = \underline{H}^{xs}_{M} = \omega x_{A} x_{B}$

$$\overline{H}_{B}^{xs} = \underline{H}_{M}^{xs} + x_{A} \left(\frac{\partial \underline{H}_{M}^{xs}}{\partial x_{B}} \right)_{T}$$

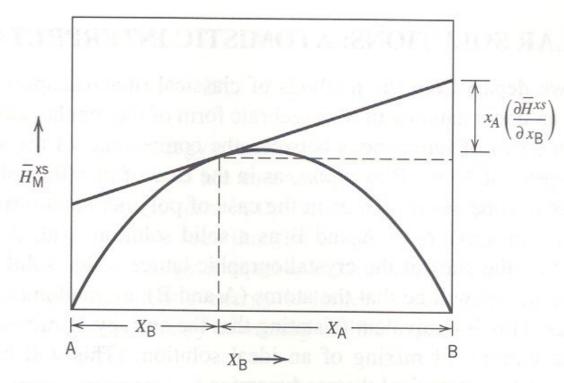


Figure 7.13 Plot of excess enthalpy of mixing versus composition for a nonideal solution.



Regular Solution (4)

For the regular solution:

$$\underline{S}^{xs}_{M} = 0$$

$$\underline{S}^{xs}_{M} = 0 \qquad \underline{G}_{M}^{xs} = \underline{H}_{M}^{xs} = \omega x_{A} x_{B}$$

$$\overline{H}_{B}^{xs} = \underline{H}_{M}^{xs} + x_{A} \left(\frac{\partial \underline{H}_{M}^{xs}}{\partial x_{B}} \right)_{T}$$

$$\overline{H}_{B}^{xs} = \underline{H}_{M}^{xs} + x_{A} \left(\frac{\partial \underline{H}_{M}^{xs}}{\partial x_{B}} \right)_{T} \qquad \overline{H}_{B}^{xs} = \omega x_{A} x_{B} + x_{A} \left(\frac{\partial (\omega x_{A} x_{B})}{\partial x_{B}} \right)_{T}$$

$$\overline{H}_B^{xs} = \omega x_A x_B + x_A \omega (x_A - x_B)$$

$$\overline{H}_B^{xs} = \omega x_A^2$$

$$\overline{G}_B^{XS} = RT \ln \gamma_B$$

$$\overline{H}_B^{xs} = \omega x_A^2 \qquad \overline{G}_B^{xs} = RT \ln \gamma_B \qquad \underline{G}_M^{xs} = RT(x_A \ln \gamma_A + x_B \ln \gamma_B)$$

$$\ln \gamma_B = \frac{\omega}{RT} x_A^2$$

Justify the algebraic form of the activity coefficient in a regular solution.

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Regular Solution: Atomistic Interpretation (1)

Phase Transformation and Applications

A,B二元完全无序分布 只考虑最近邻原子间的相互作用

N_A个A原子与N_B个B原子混合形成规则溶液

Random distribution

Z: coordination number

E_{AA}: bonding energy

Table 7.1 Bond Energies After Mixing Atoms A and B in a Solid Solution

	Number of Bonds	Energy per Bond	Energy
$N_{ m AB}$	$N_{ m A}rac{N_{ m B}}{N_{ m T}}Z$	$E_{ m AB}$	$rac{N_{ m A}N_{ m B}}{N_{ m T}}~Z~E_{ m AB}$
N_{AA}	$rac{1}{2}rac{N_{ m A}^2}{N_{ m T}}$	$E_{\scriptscriptstyle{\mathrm{AA}}}$	$rac{1}{2}rac{N_{ m A}^2}{N_{ m T}}~Z~E_{ m\scriptscriptstyle AA}$
$N_{ m AB}$	$rac{1}{2}rac{N_{\mathrm{B}}^{2}}{N_{\mathrm{T}}}\mathbf{Z}$	$E_{ m BB}$	$rac{1}{2}rac{N_{ m B}^2}{N_{ m T}}E_{ m BB}$

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Regular Solution: Atomistic Interpretation (2)

Phase Transformation and Applications

$$\frac{N_A Z}{2} \times \frac{N_A}{N_T}$$

$$E_{M} = Z \left[\frac{N_{A}^{2}}{2N_{T}} E_{AA} + \frac{N_{B}^{2}}{2N_{T}} E_{BB} + \frac{N_{A}N_{B}}{N_{T}} E_{AB} - \frac{N_{A}}{2} E_{AA} - \frac{N_{B}}{2} E_{BB} \right]$$

$$E_{M} = ZN_{T} \left\{ \frac{[x_{A}^{2} - x_{A}]E_{AA} + [x_{B}^{2} - x_{B}]E_{BB}}{2} \right\} + x_{A}x_{B}E_{AB}$$

$$E_M = ZN_T x_A x_B [E_{AB} - 1/2(E_{AA} + E_{BB})]$$

$$\varpi = 0$$
, ideal $\varpi \neq 0$, $\underline{S}_{M}^{xs} = 0$, regular

$$E_M = \omega x_A x_B$$

$$\omega = ZN_T[E_{AB} - 1/2(E_{AA} + E_{BB})]$$

$$\underline{G}_{M}^{xs} = \underline{H}_{M}^{xs} - T\underline{S}_{M}^{xs} = \varpi x_{A}x_{B}$$

$$H = U + PV = E + PV$$

$$S_M^{xs} = 0$$

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Regular Solution Atomistic Interpretation (3)

Phase Transformation and Applications

For the regular solution: $\underline{S}_M = 0$

$$\underline{S}_M = 0$$

$$\underline{G}_{M}^{xs} = \underline{H}_{M}^{xs} = \omega x_{A} x_{B}$$

$$\overline{H}_{B}^{xs} = \underline{H}_{M}^{xs} + x_{A} \left(\frac{\partial \underline{H}_{M}^{xs}}{\partial x_{B}} \right)_{T} \qquad \overline{H}_{B}^{xs} = \omega x_{A} x_{B} + x_{A} \left(\frac{\partial (\omega x_{A} x_{B})}{\partial x_{B}} \right)_{T}$$

$$\overline{H}_{B}^{xs} = \omega x_{A} x_{B} + x_{A} \omega (x_{A} - x_{B})$$

$$\overline{H}_{B}^{xs} = \omega x_{A}^{2}$$

$$\ln \gamma_{B} = \frac{\omega}{RT} x_{A}^{2}$$

$$\ln \gamma_B = \frac{\omega}{RT} x_A^2$$

$$\overline{G}_B^{xs} = RT \ln \gamma_B$$

Justify the algebraic form c in a regular solution.

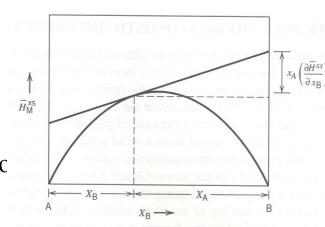


Figure 7.13 Plot of excess enthalpy of mixing versus composition for a nonideal solution.

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Example 3.7

[**例题 3.7**] 试根据正规溶体模型,求出 A-B 二元系α溶体中组元 A 和

根据式 (3.15), A-B 二元系 α 溶体自由能的正规溶体近似表达式为

$$G^{\alpha} = {}^{0}G_{A}^{\alpha}(1-x_{B}) + {}^{0}G_{B}^{\alpha}x_{B} + \Omega_{AB}^{\alpha}(1-x_{B})x_{B} + RT[(1-x_{B})\ln(1-x_{B}) + x_{B}\ln x_{B}]$$

将上式求 $(\partial G^{\alpha}/\partial x_{\rm B})$, 并代人式 (3.39) 中, 可得式 (3.43)。

$$\mu_{A}^{\alpha} = {}^{0}G_{A}^{\alpha} + \Omega_{AB}^{\alpha} \cdot x_{B}^{2} + RT \ln(1 - x_{B})$$

$$\mu_{B}^{\alpha} = {}^{0}G_{B}^{\alpha} + \Omega_{AB}^{\alpha} \cdot (1 - x_{B})^{2} + RT \ln x_{B}$$
(3.43)

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Example 3.7

Phase Transformation and Applications

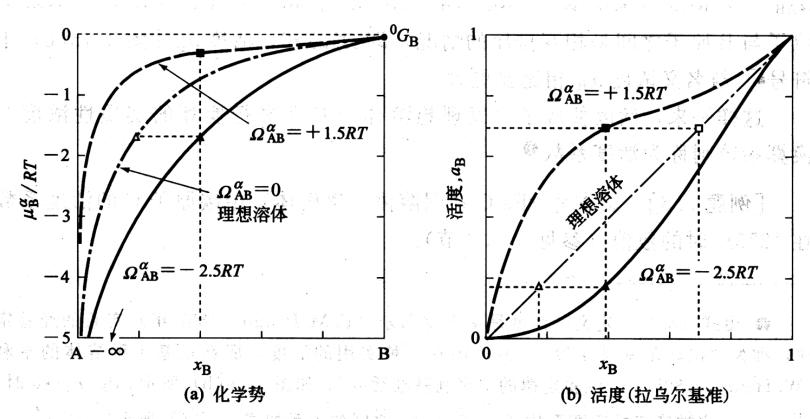


图 3.15 A-B 系正规溶体 B 组元的化学势($\mu_{\rm B}$)和活度 $(a_{\rm B})$,其中 $\mu_{\rm B}$ 的数值 是令 $^{\rm O}G_{\rm B}=0$ 并除以 RT 时的数值



Review: 体系自由能的计算

Phase Transformation and Applications

- 能量
- · Gibbs自由能定义及其作用
- Gibbs自由能的计算
 - **纯物质**
 - 二元系
 - 溶液模型(规则溶液)



Review

- 自由能的计算
- 溶液模型 (规则)

思考题

- 磁转变带来自由能的变化
- 非晶相的自由能

下次主要内容

- 溶液模型(亚点阵)
- 钢中碳的自由能计算
- 钢中第二相析出浓度积



作业

试分析纯铁的A₃点相变温度,在引入磁场中时,将发生下述哪一种变化? 并叙述其理由。

①上升;②下降;③不变。

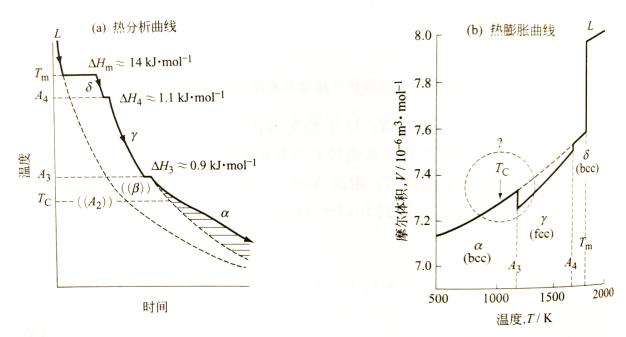


图 2.18 纯铁的热分析曲线和热膨胀曲线 (A₃ 点相变是反向的由疏排到密排的"异常相变")

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