Title ____________________

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Jnotes

Chapter 1

Basic information

atomic structure
- Bohr atomic model
- wave-mechanical model.
  - quantum number (n, l, m_l, m_s) P19-21

Electron configuration. (P22-24)

Atomic Bonding in solids

Introduction: material science & engineer

Distinguish
- science: develop or synthesize new materials
- engineer: create new products or system using existing materials

Components: processing ⇒ structure ⇒ properties ⇒ Performance.

(mechanical, electrical, thermal. magnetic, optical, deteriorative)

变质性：与化学反应相关.

Classification of solid material

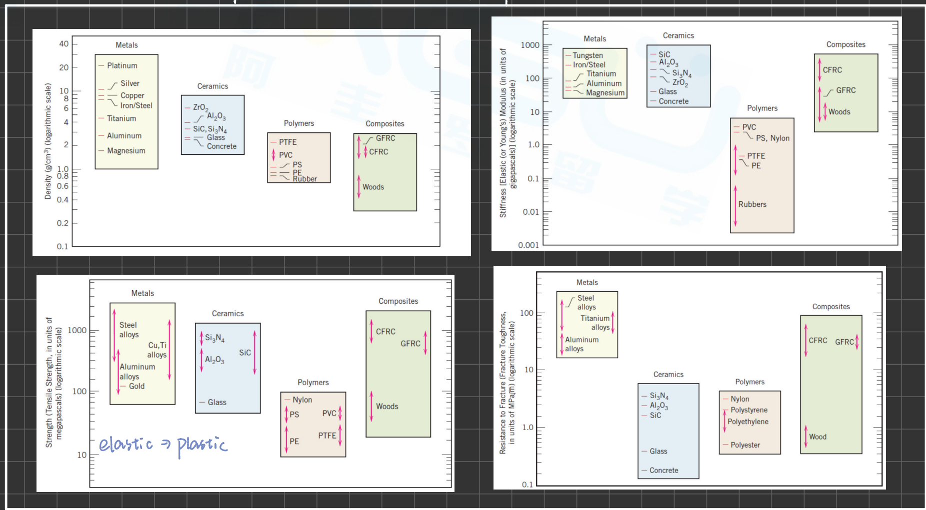
metal (P7)

ceramics (P8)

polymers. (P9.10).

composites. (P11)

Comparision in Room-Temp.



structure of crystalline solids

crystalline structure
- single
- poly-crystalline.
- lattice and unit cell
  - SC (APF=0.52)
  - BCC (APF=0.68)
  - FCC (APF=0.74)
  - HCP.

noncrystalline structure

○ Computation: Density $(\rho = \frac{nA}{V_C/N_A})$, $APF = \frac{n(\frac{4}{3}\pi R^3)}{a^3}$

(P46.47) crystallographic directions and planes
- 用 integral index
- X.Y.Z 轴交点的倒数.

(P48.49) Linear and Planar Density.

Crystallographic Directions & Planes

①. Crystallographic Direction. ⇒ 用方括号.

△ [x y z] : 以原点为起点, x. y. z 为 x, y, z 轴的 vector projection

若出现负值: 在数值上加 "–" eg: $-1 \Rightarrow \bar{1}$

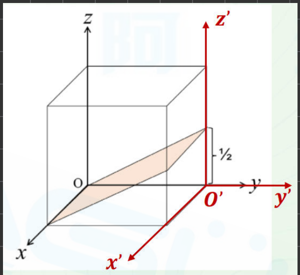
若出现分数 ⇒ 求最大倍数, 使 xyz 整数化.

②. Miller Indices : notation for crystal planes ⇒ 用圆括号.

a) 确定面坐标的过程.

i). 看是否过原点, 若过原点则改变坐标系 ⇒ ii). 找面在 x, y, z 轴上的投影, 取其倒数.

eg:



△若和某一坐标轴平行, 则投影为∞, 倒数为0.

⇓

iii) 把所有坐标均化为整数.

b). 两个 miller index 相同的面间距: $d = \dfrac{a}{\sqrt{h^2+k^2+l^2}}$

设 (h k l)

Chapter 2
Imperfection in Solids

Line / Linear Defect (1维)

Types of dislocation
- ① Edge dislocation ($\ell \perp b$)
- ② screw dislocation ($\ell \parallel b$)
- ③ mixed dislocations (同时有screw和edge)

(ℓ: dislocation line. b: burger vector).

Burger vector ($\vec{b}$)
(与slip方向平行. 可以想象成和施加的外力平行的方向)

dislocation line ($\vec{\ell}$)
(看图)

Point defect (0维)

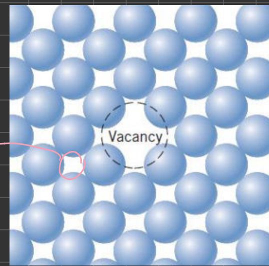
∃ 指一个/两个原子.

Interstitial defect.
- self-interstitial
(晶体中的原子种类本身插入空隙)
- interstitial of impurity atom
(空隙中插入其它原子).

— substitutional impurity atom

△区分 interstice 和 vacancy.

interstice.



① vacancy: $N_v = N\exp\left(-\frac{Q_v}{kT}\right)$.

N_v: number of vacancy in equibrium.

Q_v: energy required for formation of a vacancy

$N = \frac{N_A \cdot \rho}{A}$
(A: 相对原子质量. ρ: density).

N: 每立方厘米的晶体中有N个原. T: 开尔文温度.

k: 玻尔兹曼常数. 数值为 1.38×10^{-23} J/k.

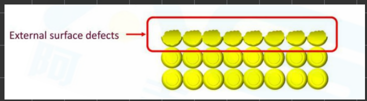
△ T< melting point 时 $N_v/N \simeq 10^{-4}$.

②. concentration of absences: $\frac{N_v}{N} = \exp\left(-\frac{Q_v}{kT}\right)$.

Plan Defect (2维)
(interfacial Defect).

(特点：能量高且不稳定)

External surfaces



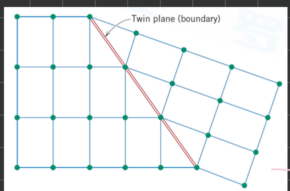
(表面原子没有周围和其它原子结合).

Grain boundaries defect.
- Grain boundary
(两个具有不同晶体方向的晶粒间的边界).
- defect产生原因：边界原子由于晶粒方向不同所没有匹配上.

△特点：可以被光学显微镜及精度更小的显微镜观察到.
不稳定. 易发生化学反应.

boundaries between two phases

Twin boundaries.
(mirror lattice symmetry)



○ 形成于施加 shear forces.

Twin boundary and the adjacent atom positions

(3维) Bulk (volume) Defect.

: pores, cracks, foreign inclusion, other phases

small spaces are empty.

broken

include impurity.

Chapter 3 Diffusion

Basic information

Dependence

temperature, time dependent process.

concept

① material transport by atomic motion (in specific solid)
② transport in different phases.

Calculation

(具体见下页)

① $J = -D\dfrac{dc}{dx}$

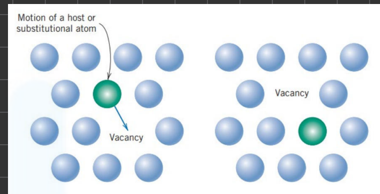
② $\dfrac{C_x - C_0}{C_s - C_0} = 1 - \mathrm{erf}\left(\dfrac{x}{2\sqrt{Dt}}\right)$

③ $D = D_0 \exp\left(-\dfrac{Q_d}{RT}\right)$

Bulk diffusion (caused by atomic motion).

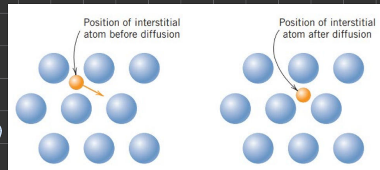
vacancies diffusion

原子和相邻的vacancy交换位置. impurities 原子.

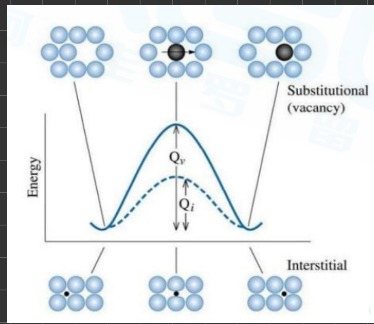


interstitial diffusion.

(impurity 原子插入晶体内原子间缝隙中.)



△ 相较 vacancies diff. 更快发生: 所需能量小 ($Q_i < Q_v$)



Grain boundaries diffusion

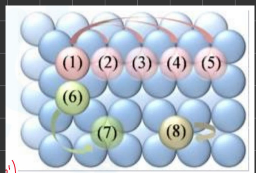
△特点: Grain间有少个原子密、使得它发生的速率远大于 bulk diffusion (10^6 times grater).

△当晶粒极小时. 该类diffusion起的作用极大.

surface diffusion

① 涉及表面原子 (adatoms) 和原子团簇 (atomic clusters) 运动

② surface diffusion jump mechanisms.



(三种不同的表面扩散的跳跃机制)

Chapter 3 计算

eg: T, 浓度 C, t.

[给左右侧浓度时计算 diffusion flux, diffusion coeffition 及相关量]

∘ diffusion is a time dependent process. (Fick's law)

Def

Diffusion flux (J): $J = \frac{M}{At} = \frac{1}{A}\frac{dM}{dt}$ ∘ 质量在面上的变化率.

$\Rightarrow [J] = [kg/m^2 \cdot s]$ or $[atoms/m^2 \cdot s]$

① Fick's 1st law (steady state diffusion).

使用条件: C变化与t不相关 (or 仅与x相关).

$J = -D\frac{dc}{dx}$ $\left(J = -D\frac{C_2 - C_1}{\Delta x}\right)$. D: diffusion coefficent

② Fick's second law (non-steady). (与t相关)

① ∘ $\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$ (C变化同时与t, x相关)

② $\frac{C_x - C_0}{C_s - C_0} = 1 - erf\left(\frac{x}{2\sqrt{Dt}}\right)$ 　$erf\left(\frac{x}{2\sqrt{Dt}}\right)$: Gaussian error function

用图表对应得到数值.

C_0: 最终 C_s: 开始时. C_x: 中间时刻浓度.

Table 5.1 Tabulation of Error Function Values

z	erf(z)	z	erf(z)	z	erf(z)
0	0	0.55	0.5633	1.3	0.9340
0.025	0.0282	0.60	0.6039	1.4	0.9523
0.05	0.0564	0.65	0.6420	1.5	0.9661
0.10	0.1125	0.70	0.6778	1.6	0.9763
0.15	0.1680	0.75	0.7112	1.7	0.9838
0.20	0.2227	0.80	0.7421	1.8	0.9891
0.25	0.2763	0.85	0.7707	1.9	0.9928
0.30	0.3286	0.90	0.7970	2.0	0.9953
0.35	0.3794	0.95	0.8209	2.2	0.9981
0.40	0.4284	1.0	0.8427	2.4	0.9993
0.45	0.4755	1.1	0.8802	2.6	0.9998
0.50	0.5205	1.2	0.9103	2.8	0.9999

∘ **Diffusion coefficient**

$D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$

depends on atom

Q_d: 原子挣脱 bond 发生 diffusion 所需的能量.

∘ D_0: 在无 activation energy 障碍情况下扩散的上限速率. 题目会给

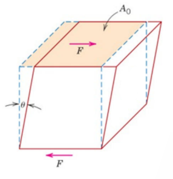
T: 开尔文温度; R = 8.314 J/mol·K.

Chapter 4 ① Mechanical properties

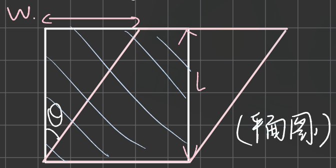
test

shear test

shear force
(施加于上下面平行的力)



(原图)



(平面图)

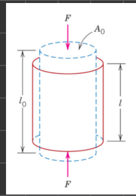
→ τ (stress)

initial specimen

- A_0 : initial specimen area.
- shear stress (τ) : $\tau = \frac{F}{A_0}$.
- shear strain : tangent of strain angle θ.

Comperissive test.

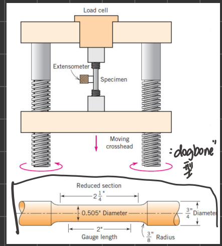
压力



同 tensile test 类似，但施加的是压力).

tensile test

拉力



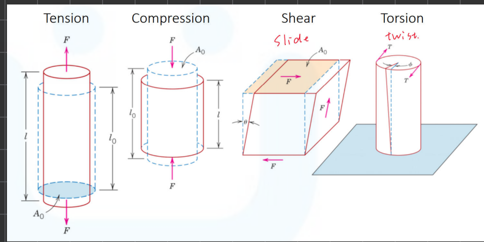
:"dogbone" 型

- machine：匀速拉伸样品，测某一瞬时时刻下的力 (load) 和伸长量 (elongation)
- output：load，elongation
- 用于定义 σ (机械应力) 和 ε (机械应变)
  engineer stress、engineer strain
  分为 engineer ~，true ~.
- 样品要求 (specimen)：常为 cylindrical，"dogbone" 构型.

Concept : response to an applied load or force.

(在力的影响下材料的不同反应).

Type of loads:



Types : strength, hardness, ductility, Stiffness

①. strength：材料在外力作用下抵抗破坏或抵抗永久变形的能力 (用应力衡量).

- tensile strength. $\sigma_t = \frac{F}{A_0}$
- yield strength $\sigma_y = \frac{F_y}{A_0}$
- compressive strength $\sigma_c = \frac{F_c}{A_0}$
- shear test 中. shear strength $\tau = \frac{F_s}{A}$ 剪切截面积

A_0：试样的初始面积　σ_t，σ_c：在 tensile 和 compressive test 中的最大应力.

②. hardness：材料抵抗局部塑性变形的能力. (eg：嵌入. 划痕，压痕).

③. stiffness：$K = \frac{F}{\Delta L}$　(F：外力；ΔL：外力产生的变形)

④. ductility：表示材料在受到塑性形变下保持不破裂的性质.

Mohs hardness Test. (矿物学中的一种硬度测试方法)

- Mohs hardness：定义为材料抵抗划痕的能力
- 通过比对材料和已知硬度的标准矿物确定硬度值.

◦ 其他硬度测试方法.

Table 6.5 Hardness-Testing Techniques

Test	Indenter	Shape of Indentation: Side View	Shape of Indentation: Top View	Load	Formula for Hardness Number[a]
Brinell	10-mm sphere of steel or tungsten carbide	D, d	d	P	$HB = \frac{2P}{\pi D[D - \sqrt{D^2 - d^2}]}$
Vickers microhardness	Diamond pyramid	136°	d_1, d_1	P	$HV = 1.854P/d_1^2$
Knoop microhardness	Diamond pyramid	$l/b = 7.11$, $b/t = 4.00$, t	b, l	P	$HK = 14.2P/l^2$
Rockwell and Superficial Rockwell	Diamond cone; $\frac{1}{16}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2}$ in. diameter steel spheres	120°		60 kg, 100 kg, 150 kg Rockwell; 15 kg, 30 kg, 45 kg Superficial Rockwell	