Title _____

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Jnotes

Chapter 1

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：与环境反应相关

Basic information

Atomic structure: Bohr atomic model; wave-mechanical model.

Quantum number (n, l, ml, ms) P19-21

Electron configuration. (P22-24)

Atomic Bonding in solids

Structure of crystalline solids

crystalline structure: single; poly-crystalline.

noncrystalline structure

lattice and unit cell: SC (APF=0.54); BCC (APF=0.68); FCC (APF=0.74); HCP.

computation: Density $\left(\rho = \frac{nA}{V_c N_A}\right)$, APF $= \frac{n(\frac{4}{3}\pi r^3)}{a^3}$

(P46-47) crystallographic directions and Planes (用 integral index)

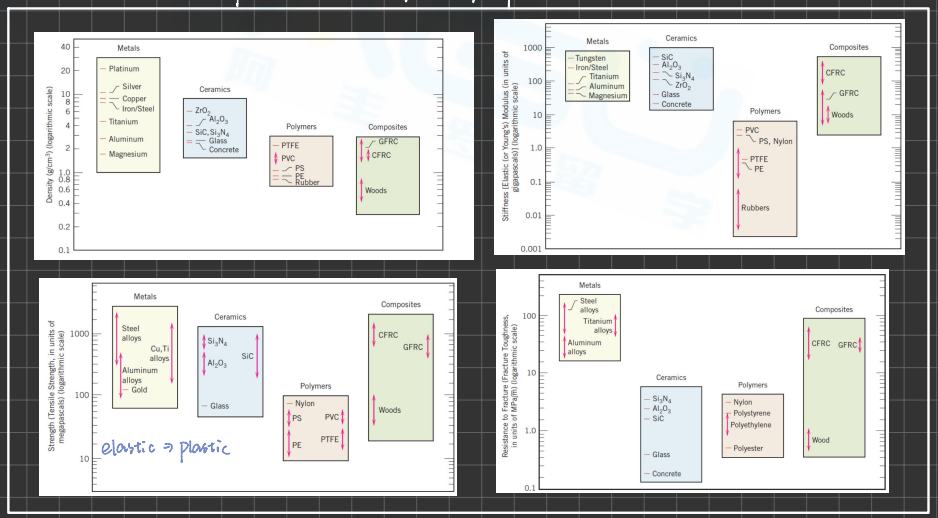
(P48-49) Linear and Planar Density.

X.Y.Z 轴方向点的倒数.

Classification of solid material

metal (P7); ceramics (P8); polymers (P9-10); composites (P11)

Comparision in Room-Temp.



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 ⇒ $\bar{1}$

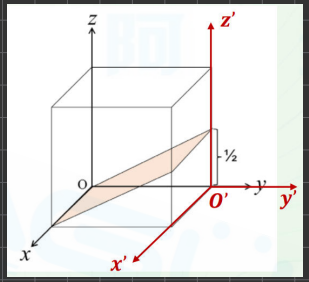
若出现分数 ⇒ 乘最大的分数，使 xyz 整数化.

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： $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$

设 (h k l)

Chapter 2
Imperfection in Solids

Line / Linear Defect (1维)

Types of dislocation
① Edge dislocation (t ⊥ b)
② screw dislocation (t ∥ b).
③ mixed dislocations (同时有 screw 和 edge)
(t: 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 ($\vec{t}$)
(有向)

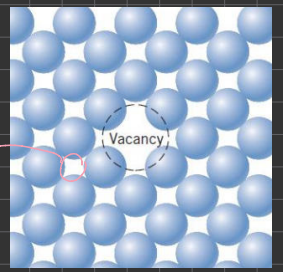
Interstitial defect.

self-interstitial
(晶体中的原子移来填补空隙)
interstitial of impurity atom
(空隙中插入其它原子).

Point defect (0维) — substitutional impurity atom

⇒ 指一个/两个原子.

△区分 interstice 和 vacancy.



Interstice.

① vacancy: $N_v = N\exp\left(-\frac{Q_v}{kT}\right)$.
energy required for formation of a vacancy
number of vacancy in equibrium.

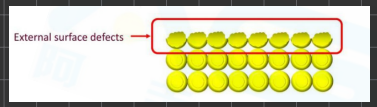
$N = \frac{N_A \cdot \rho}{A}$ (N: 每立方体木的晶体中有N个原. T: 开尔文温度.
(A: 相对原子质量. k: 玻尔兹曼常数. 数值为 1.38×10^{-23} J/k.
ρ: density).
△ T < melting point 时 $N_v/N \simeq 10^{-4}$

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

Plan Defect (2维)

(Interfacial Defect).

External surfaces
(表面原子没有原在和其它原子结合).



(特点: 能量高 ⇒ 不稳定)

Grain boundaries defect.

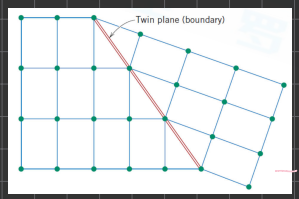
Grain boundary
(两个具有不同晶体方向的晶粒间的边界).

defect 产生原因: 边界原子由于晶粒方向不同即没有匹配上.

△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.

Twin boundaries.

(mirror lattice symmetry)



△形成于施加 shear forces.

Twin boundary and the adjacent atom positions

boundaries between two phases

(3维) Bulk (volume) Defect.

: pores, cracks, foreign inclusion, (broken)
other phases (include impurity.)

small spaces are empty.

Chapter 3 Diffusion

temperature, time dependent process.

Dependence

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

Basic information

(具体见下页)
Calculation

① $J = -D\frac{dc}{dx}$

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

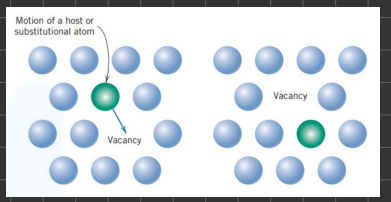
③ $D = D_0 \exp\left(-\frac{Q_d}{RT}\right)$

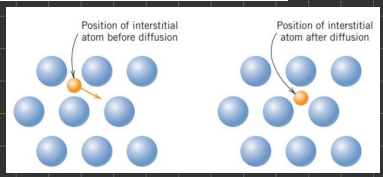
Bulk diffusion (caused by atomic motion).

vacancies diffusion

原子和相邻的vacancy发生位置

impurities 原子.





interstitial diffusion.

(impurity 原子插入晶体内原子间隙中.)

△ 相较 vacancies diff. 更容易发生: 所需能量小 ($Q_i < Q_v$)

Grain boundaries diffusion

△特点: Grain间有许原子的扩, 使得它发生的速率远大于 bulk diffusion (100 times greater).

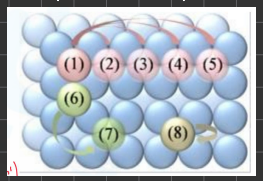
△当晶粒较小时, 该类diffusion起的作用较大.

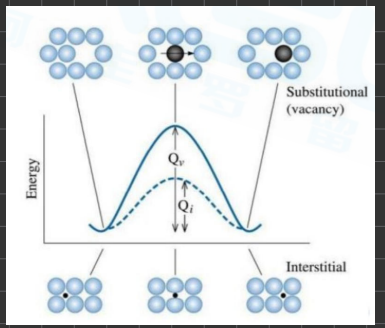
Surface diffusion

① 附着表面原子 (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.

[给左右两浓度时计算 diffusion flux, diffusion coefficient 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.

⇒ [J] = [kg/m²·s] or [atoms/m²·s]

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

使用条件: C变化与t不相关. (or 与x相关).

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

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

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

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

用周末对应得到数值.

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 coefficent

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

depends on atom

Q_d: 原子挣脱 bond 发生 diffusion 所需的能量.

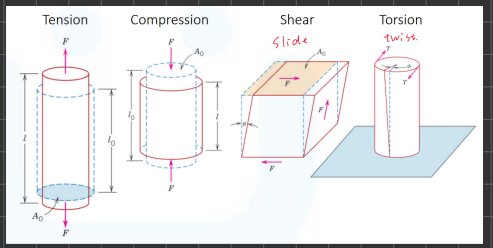
▵ D_0: 在无 activation energy 障碍情况下扩散的比限速率. 题目后给

T: 开尔文温度; R = 8.314 J/mol·K.

Chapter 4 ① Mechanical properties

Concept : response to an applied load or force. (在力的作用和下材料的不同反应).

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 strength (shear test 中): $\tau = \frac{F_s}{A}$ A: 剪切截面积

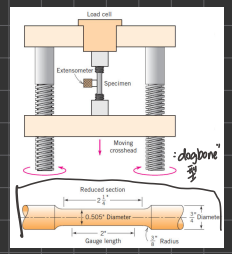
A_0: 试样的初始面积 σ_t, σ_c: 在 tensile 和 compressive tests 中的最大应力.

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

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

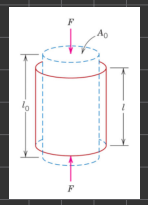
④ ductility: 表示材料在受到塑性形变下保持不破裂的性质.

- machine: 匀速拉伸样品, 测算: 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 和 true.
- 样品要求 (specimen): 常为 cylindrical, "dogbone" 构型.



tensile test 拉力

Compressive test. 压力

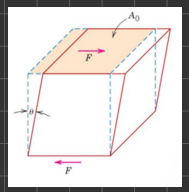


(和 tensile test 类似. 但施加的是压力).

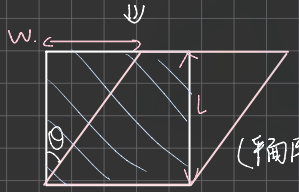
test

Shear test

shear force (施加于下面平行的力)



(立体图)



(横向图)

→ τ (stress)

initial specimen

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

Mohs hardness Test. (材料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材料确定硬度值.

△其它硬度测试方法.

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	t	b	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	

[a] P is the load in kg; D is the diameter of the spherical indenter in mm; d is the diameter of the impression in mm; d_1 is the average length of the diagonal of the impression in mm; l is the length of the impression in mm; b is the width of the impression in mm; t is a constant for the indenter-specimen combination.