CH3.結晶固體的結構

基本概念

1. **crystalline** →material is one in which the atoms are situated in a repeating or periodic array over large atomic distances 長程有序排列!!
2. **crystal structure**→ the manner in which atoms, ions, or molecules are spatially arranged→就是 BCC.FCC.HCP 啦!
3. **lattice** →三維排列的點與原子位置(center)相符合(coincide)
4. **atomic hard sphere model**→ 表達了和鄰居的接觸，well-defined 直徑
5. 為了描述方便將 crystal structure 細分更小的重複實體→**unit cell**

FCC→金銀銅鋁鉛鉑鎳

HCP→Mg.Zn.Ti.Cd.Co(美新胎葛鬼)

Crystal structure→描述單位晶胞的幾何和原子排列

FCC	單位晶胞 4 個原子，CN=12，APF=0.74，最密面(111)
BCC	單位晶胞 2 個原子，CN=8，APF=0.68
HCP	單位晶胞 6 個原子(有時會算錯)，CN=12，APF=0.74，c/a=1.633*(pf) 最密面(0001) (*單位晶胞含 3 個 parallelepipeds)

金屬有較高的 APF 使自由電子雲提供的 shielding 最大化

Polymorphism→具有一種以上的 crystal structure→若為元素通常稱為→Allotropy

即同形體，同素異形體，不同狀況有不同晶體結構

EX. C(石墨.鑽石)，Fe(BBC.FCC)， White (β) tin→ Gray (α) tin

Crystal system→只描述單位晶胞的幾何，crystal structure 屬於他

Lattice parameters→六個參數來定義單位晶胞的幾何 a, b, c 和α ,β ,γ

七大晶系 14 種單位晶胞→all

都直角: Cubic(3 邊同)→tetragonal(2 邊同)→orthorhomic(都不同)

三邊同，三角同 but 非直角→菱→rhombohedral

Hexagonal

Monoclinc→單斜→三邊都不同，有一角非直角

Triclinic→三斜→三邊都不同，三角都不同

Crystallographic directions→中刮號[uvw]

若是六方→Miller-Bravais

$$[u'v'w'] \longrightarrow [uvtw]$$

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

*basal plane→六方中，a1.a2.a3 在同一面

CRYSTALLOGRAPHIC PLANES

Miller indices→小刮號(hkl)

遇六方→(hkil)

$i = -(h + k)$ 其它指數相同

取截距倒數(平行視為無窮遠截距)，再取最小整數組

有截距法求平面的味道，截距倒數為法向量

*在 cubic crystal 中，有個特性是方向和平面指數相同時，兩者互相垂直。

*有時候指數不會減化(X 光繞射)，對陶磁材料而言，減化指數和未減化指數代表的平面可能不同!

平面族→大刮號{…}

A “family” of planes contains all those planes that are crystallographically equivalent 有相同的原子堆積!!

EX.在 cubic，3 個數字無論順序和符號組成的平面都是同平面族

*[方向]→(平面)→{族}

$$\mathrm{LD} = \frac{\text{number of atoms centered on direction vector}}{\text{length of direction vector}}$$ 單位為長度倒數

$$\mathrm{PD} = \frac{\text{number of atoms centered on a plane}}{\text{area of plane}}$$ 單位為面積倒數

Close-packed

HCP→ABABABAB

FCC→ABCABCABC

For a crystalline solid, when the periodic and repeated arrangement of atoms is perfect or extends throughout the entirety of the specimen without interruption, the result is a single crystal.

atomic mismatch within the region where two grains meet; this area, called a grain boundary

Most crystalline solids are composed of a collection of many small crystals or grains; such materials are termed polycrystalline.

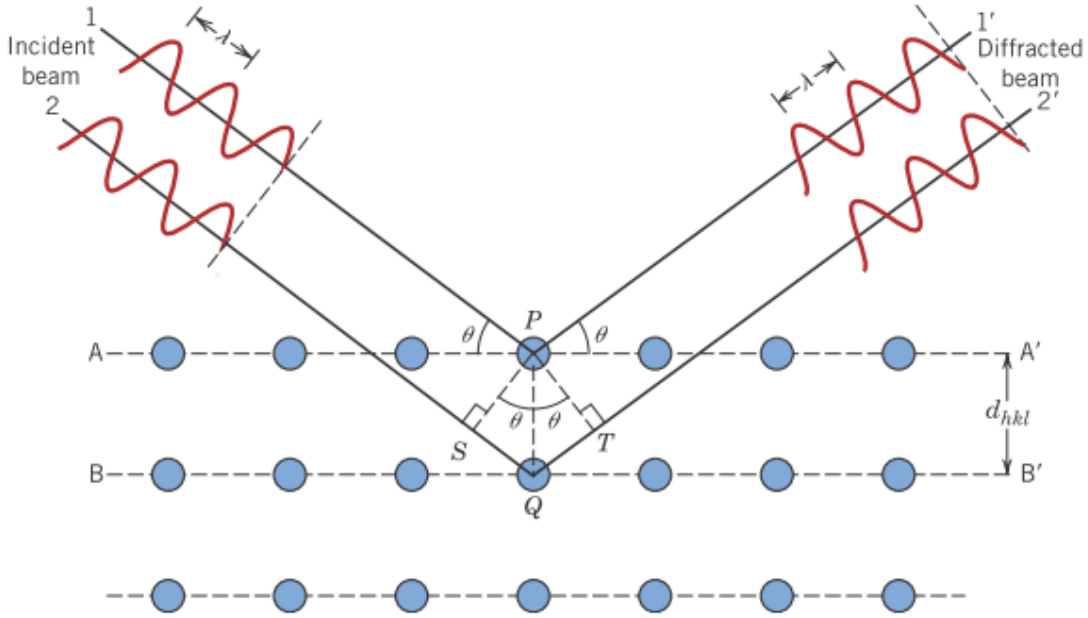
對多晶材料而言，即使每一晶粒都是異向性的，由晶粒組成的試片是等向行為因為個別晶粒的方向是隨機的。

Sometimes the grains in polycrystalline materials have a preferential crystallographic orientation, in which case the material is said to have a texture.

Ex. iron alloys 的[100]方向的 magnetic texture

Noncrystalline=amorphous，supercooled liquid *共價鍵方向性較易形成非晶 liquids

X-Ray Diffraction(這部分要去複習 smith)



$$n\lambda = d_{hkl}\sin\theta + d_{hkl}\sin\theta$$

$$= 2d_{hkl}\sin\theta$$

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$ (cubic symmetry)

上式為充分非必要，當 BCC 或 FCC，除了 corner 的位置，其他位置 may 成為散射中心。

繞射條件

BBC→h+k+l→偶

FCC→h.k.l→全奇或全偶

繞射角:2θ

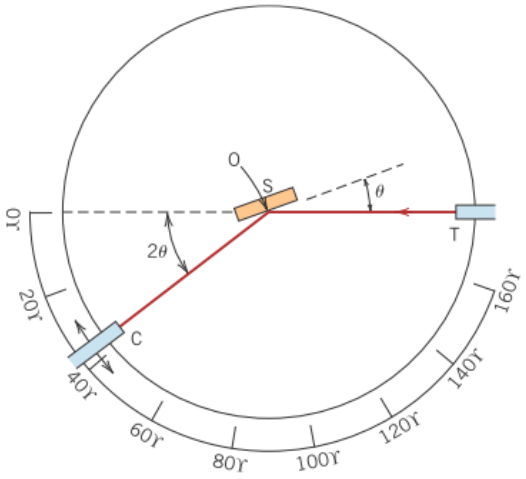
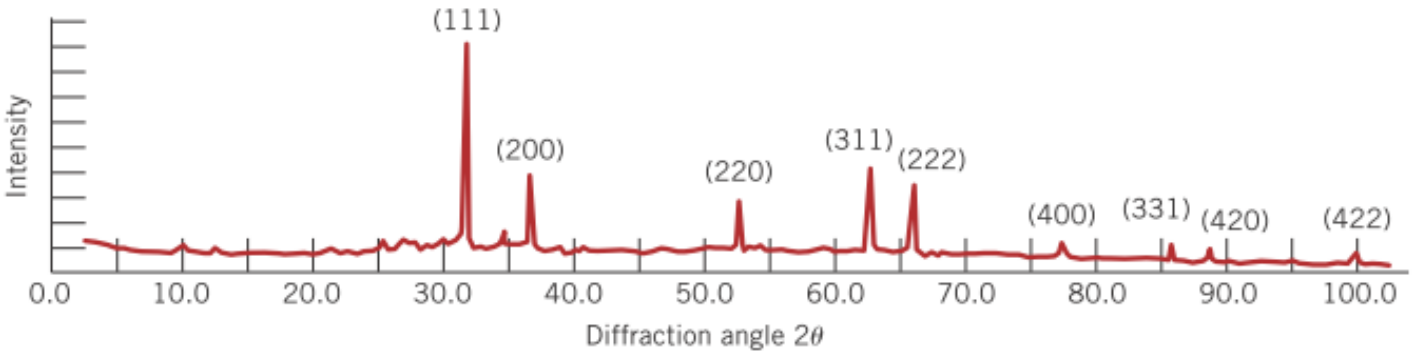


Figure 3.20 Schematic diagram of an x-ray diffractometer; T = x-ray source, S = specimen, C = detector, and O = the axis around which the specimen and detector rotate.



Smith 補充

LRO→long-range-order	
SRO→short-range-order	EX.水分子短程有序，但分子間以弱次級鍵隨機鍵結，長程無序
Crystalline solid	
Amorphous	全部原子位置都隨機的

Crystal structure	
Space lattice	3-D array of points，have same geometric environment
lattice points	Space lattice 中的一個點
Unit cell	Space lattice 中最小的重複 unit
Motif	A group of atoms that are organized relative to each other and are associated with a lattice point
Lattice constant	描述 unit cell 的長度和角度皆為 lattice conatant!

三個最 common→BCC.FCC.HCP 差不多占了 90%的金屬

HCP→一般是指 larger cell(為了方便)，再細分是 primitive cell
larger cell→含 6 個原子
primitive cell→含 2 個原子

方向[uvw]→<uvw>
平面(hkl)→{hkl} ； HCP 用 Miller-Bravais indices{hkil}

	BCC	FCC	HCP
最密堆積方向	<111>directions	<110>directions	<1120>directions
最密堆積平面	沒有	{111}directions	{0001}directions

注意是 directions

Polymorphic→一材料在不同狀況(溫度、壓力)，可形成不同的 crystalline form 或 allotropy 同素異形:EX. Fe 溫度要背!! 912→1394→1539

X-Ray→電磁波，波長約 0.05~0.25nm，藉由加速電子撞擊 target metal 產生

約 98%的動能會轉變成熱能，需要冷卻系統!

Characteristic radiation is an intense form of x-ray radiation which occurs at specific wavelengths for a particular element. The K_α radiation, the most intense characteristic radiation emitted, is caused by excited electrons dropping from the second atomic shell
(n = 2) to the first shell (n = 1). The next most intense radiation, K_β, is caused by excited electrons dropping from the third atomic shell (n = 3) to the first shell (n = 1).

最常用的 X-Ray 技術→powder method

*X-Ray 的複習翻一下 smith，講的比 callister 多

金屬玻璃→快速凝固→性質比結晶還好，用 X 光繞射沒清楚可見的峰值(因非晶)