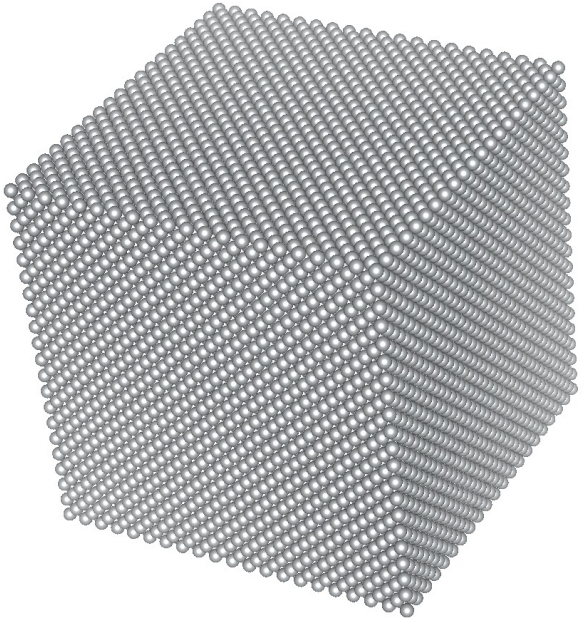
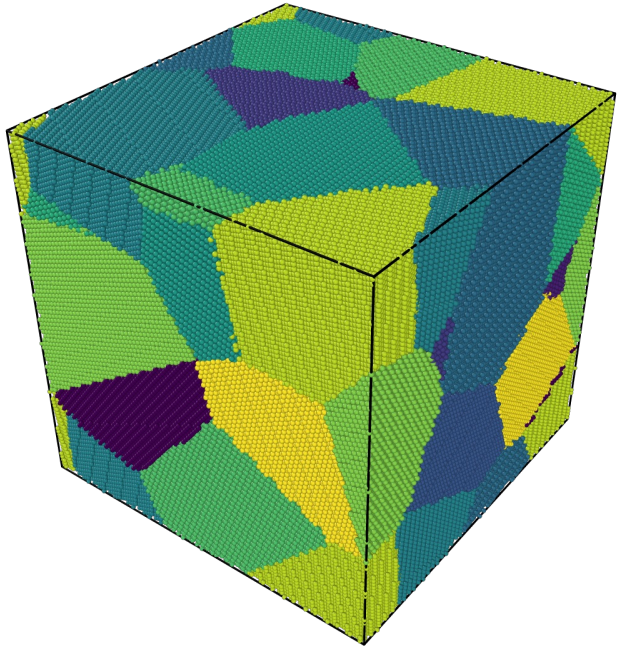
3. X射线与晶体的相互作用

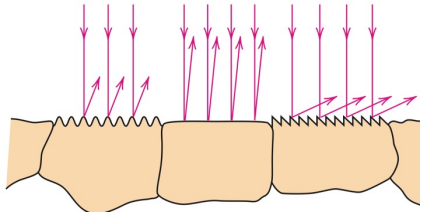
Dongsheng Wen

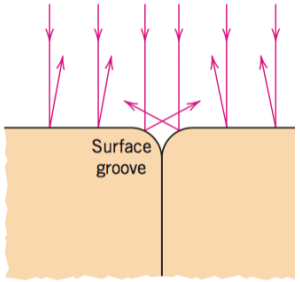
单晶与多晶材料 (polycrystalline materials)

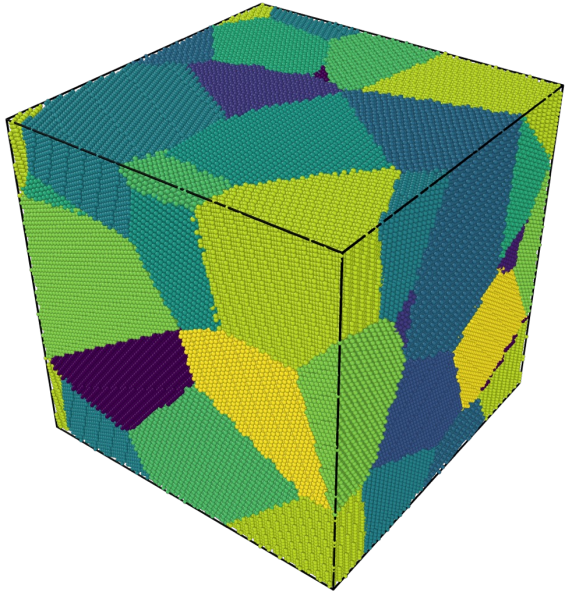


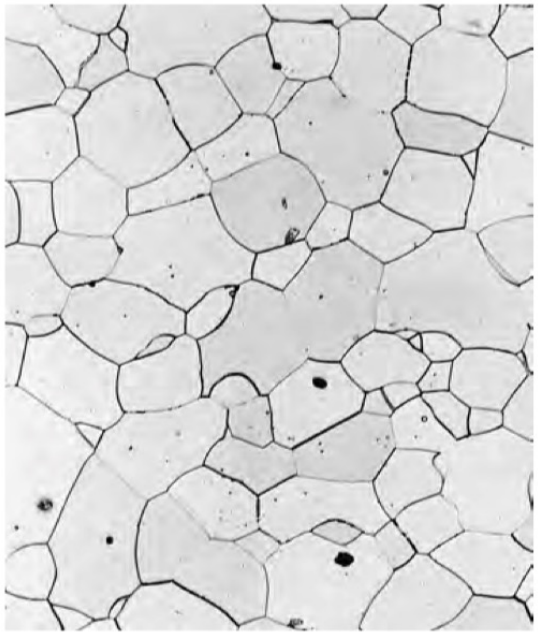


多晶材料

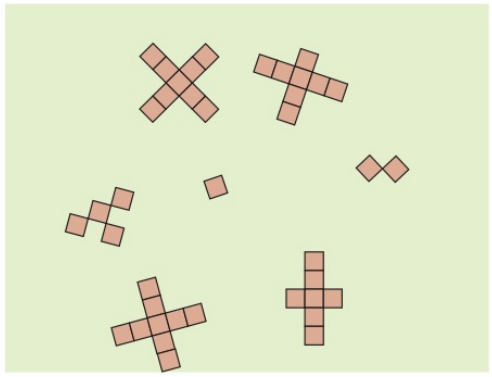




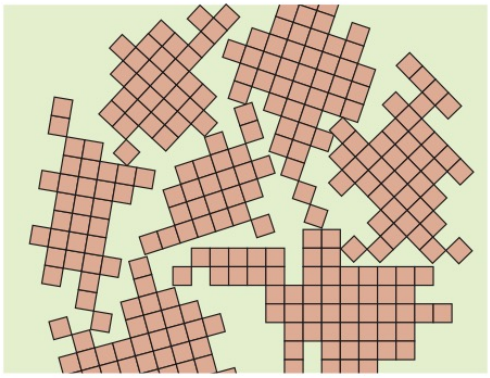




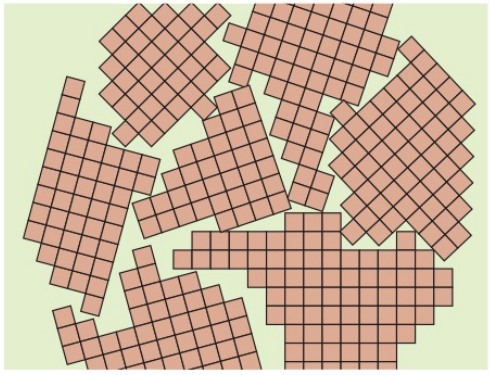
多晶材料形成



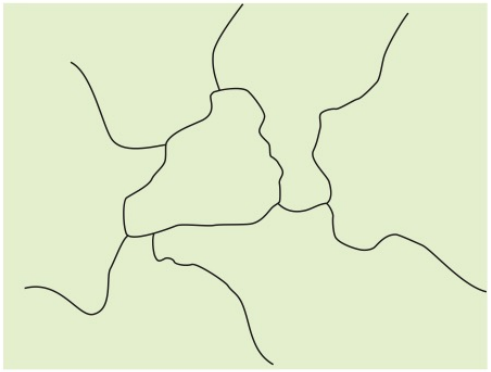
(a)



(b)

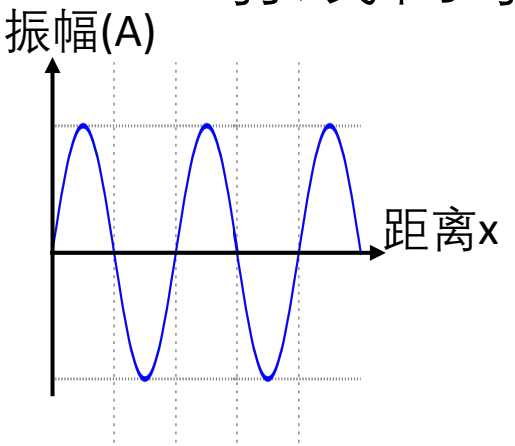


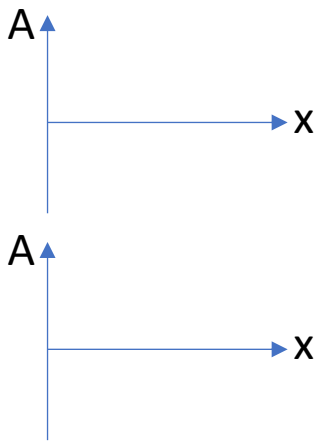
(c)

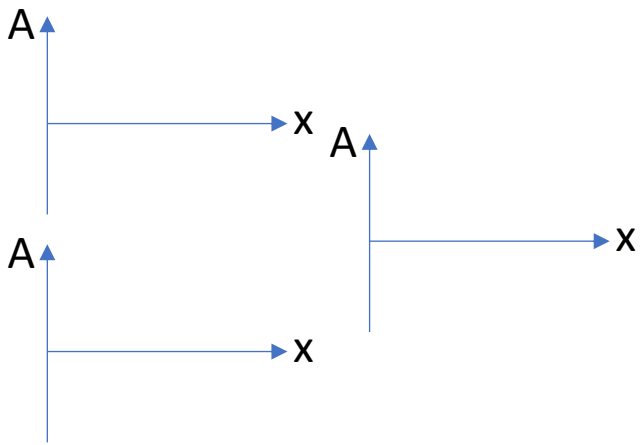


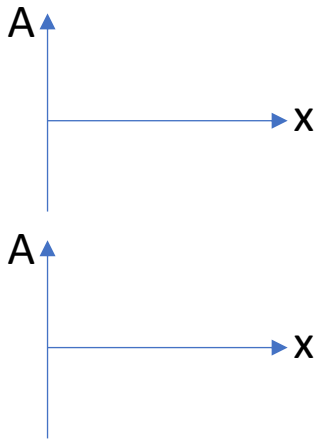
(d)

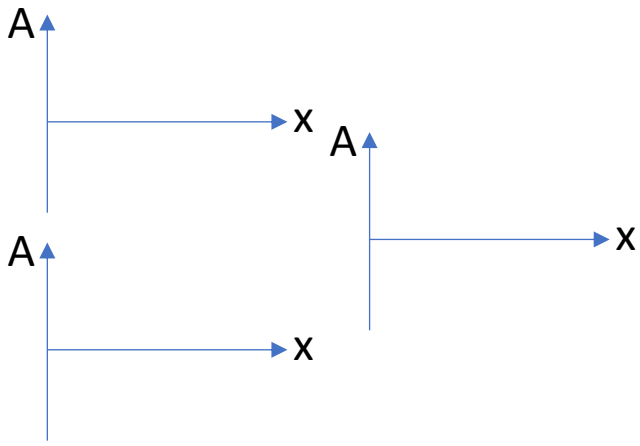
X-射线衍射 (X-ray diffraction)

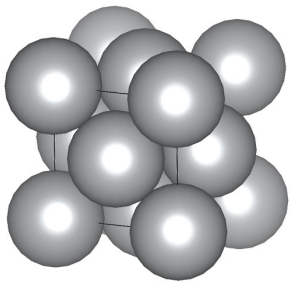






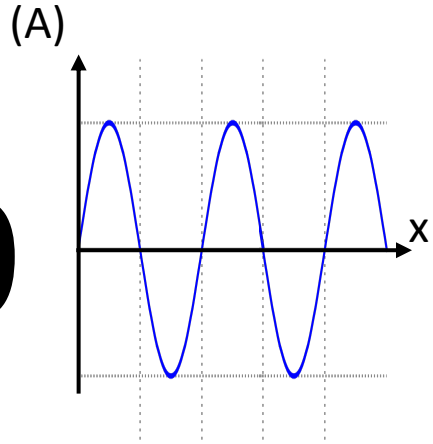


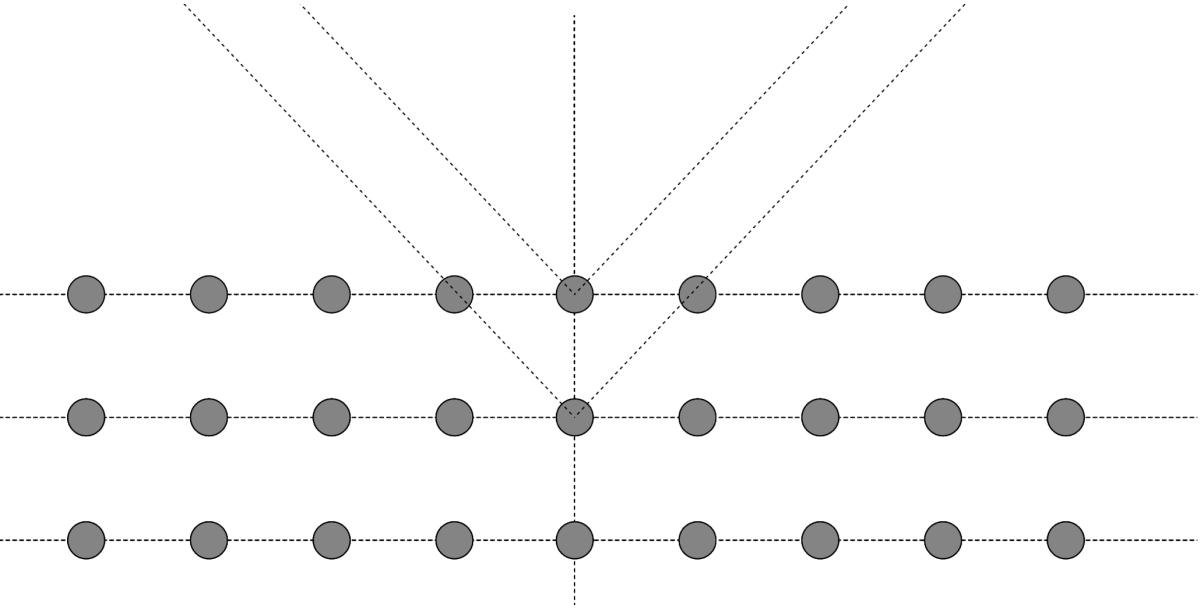




X-射线衍射 (X-ray diffraction)

布拉格方程 (Bragg's law): $\lambda = 2d\sin\theta$





X-射线衍射 (X-ray diffraction) $\lambda = 2d\sin\theta$

晶面(hkl)的晶面间距：$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

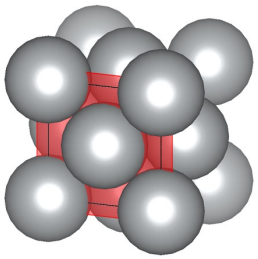
晶面间距d 取决于：

- 晶体结构
- 晶格常数 a
- 外界条件：温度，压力，形变

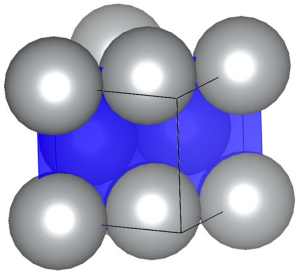
晶面(hkl)的晶面间距d_{hkl}

练习：FCC-Al, $a = 4.04\text{Å}$

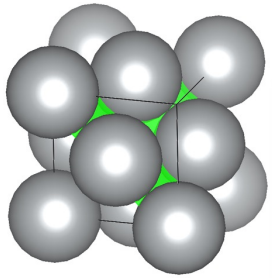
{100}面



{110}面



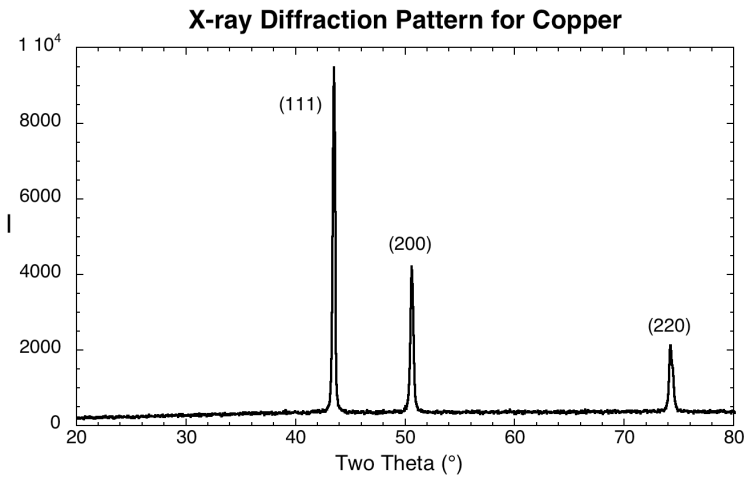
{111}面



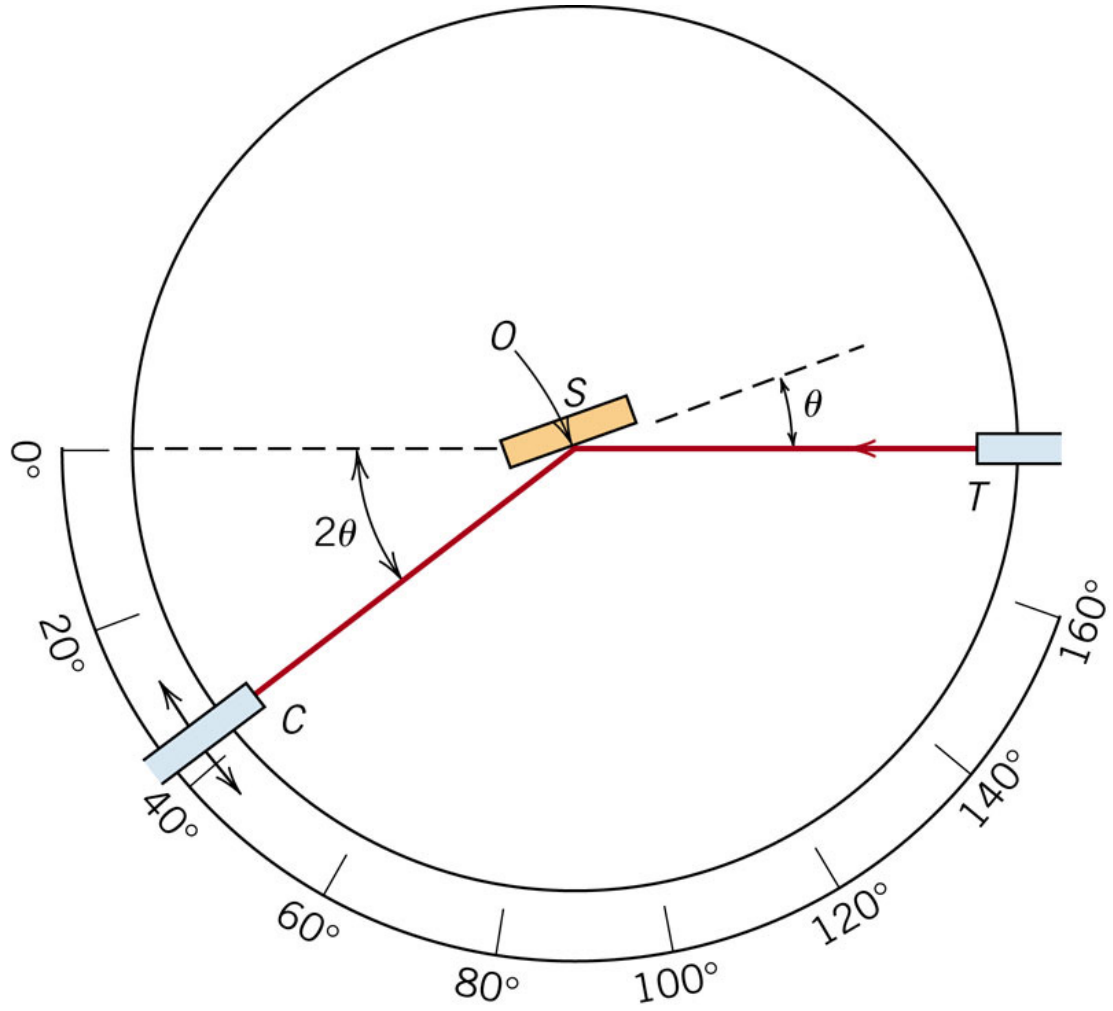
XRD设备工作原理


D8 ADVANCE

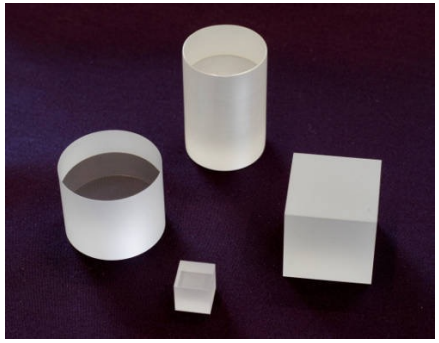

BRUKER

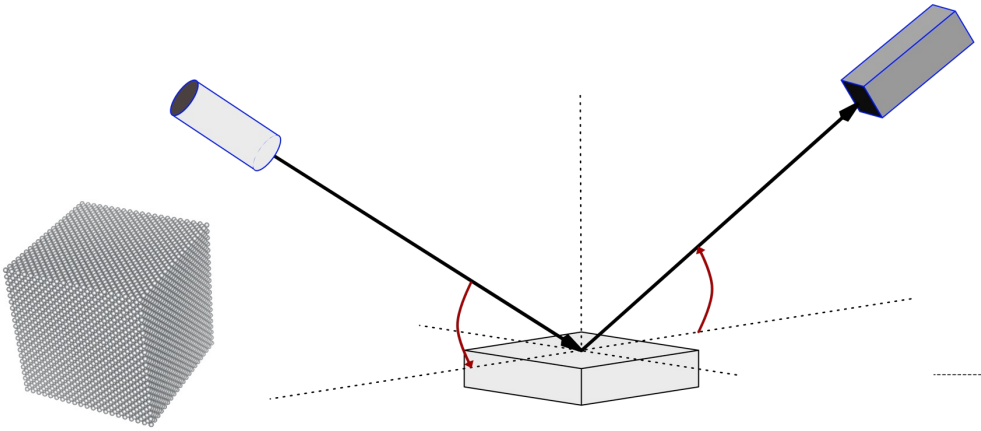

X-ray Diffraction Pattern for Copper
1 10^4
8000
6000
I
4000
2000
0
(111)
(200)
(220)
20
30
40
50
60
70
80
Two Theta (°)

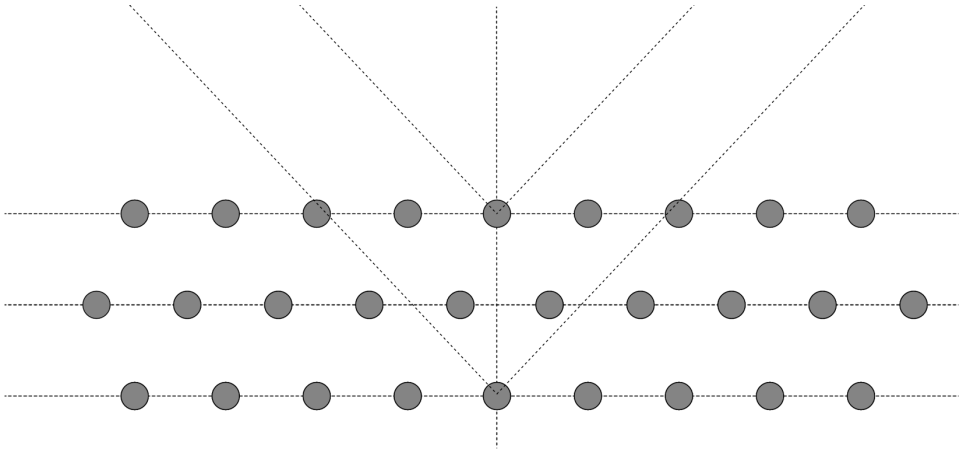
XRD设备工作原理



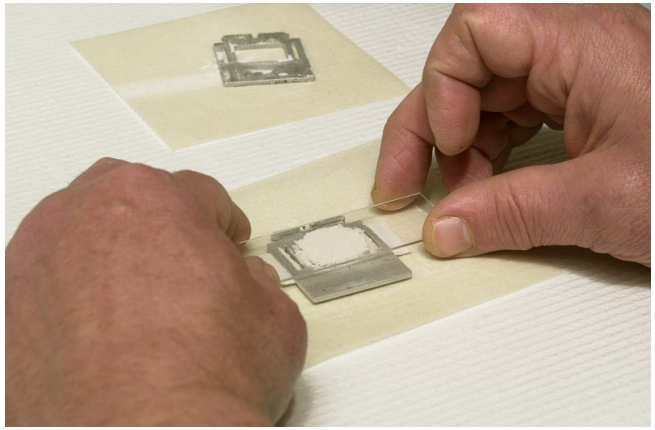
X射线衍射: 单晶

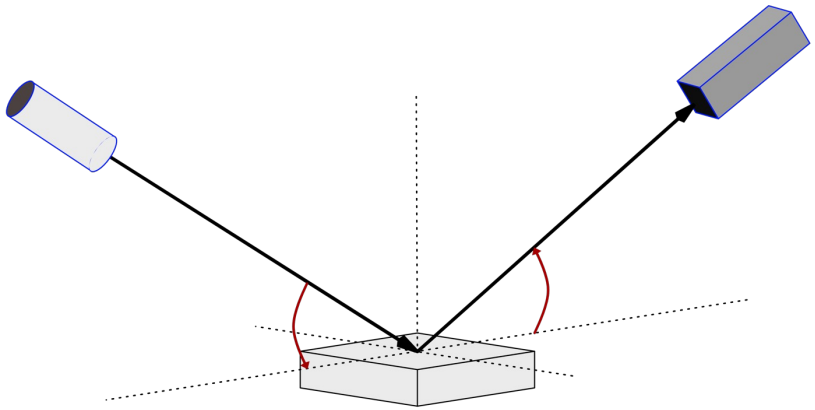


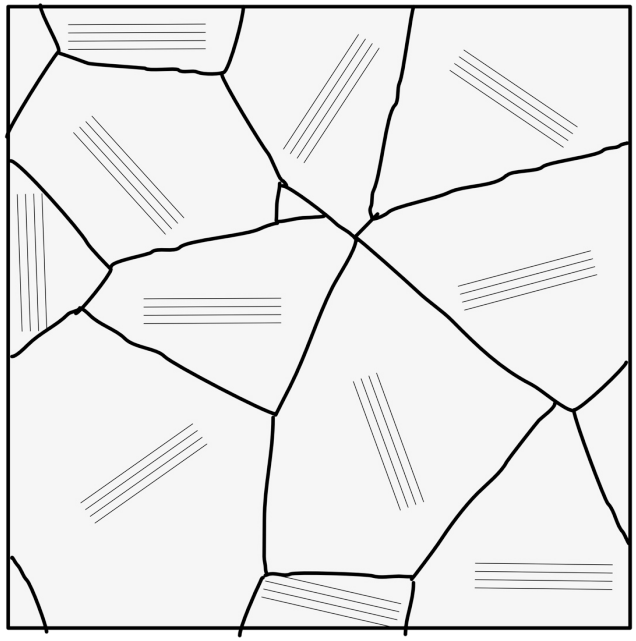




X射线衍射: 多晶/粉末







结构因素

	FCC (hkl)	BCC (hkl)
可以发生衍射的面	h, k, l 全是奇数或者全是偶数	h+k+l=偶数
不可以发生衍射的面	h, k, l 奇数偶数混杂	h+k+l=奇数

FCC (hkl)

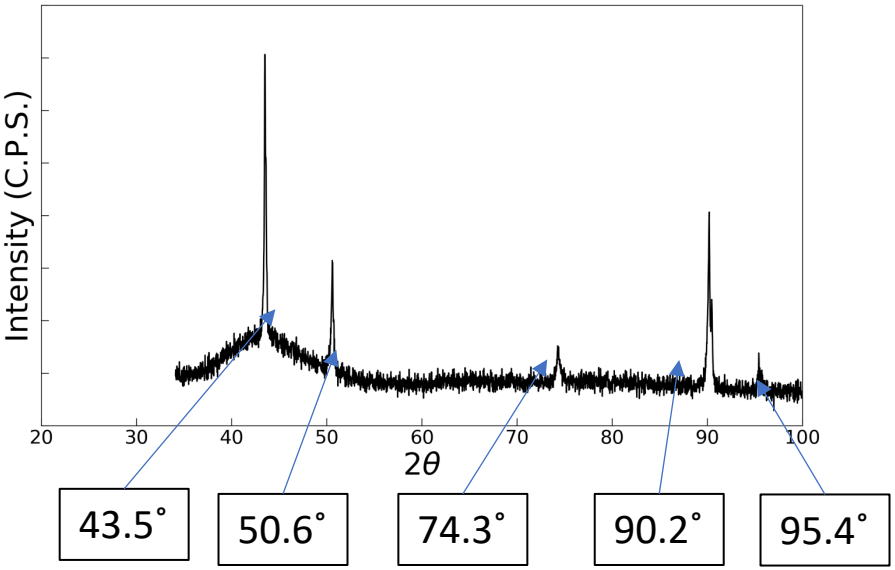
$(h^2 + k^2 + l^2)$	hkl	衍射？

BCC (hkl)

hkl	衍射？

XRD练习

已知该材料是FCC结构的多晶材料，利用铜激发出来的X射线 ($\lambda = 1.54$ Å) 获得了以下的X射线衍射峰。
标出该材料的衍射面，并且求晶格常数a。提示：FCC可发生衍射的面，h, k, l 全是奇数或者全是偶数。



2θ	θ	(hkl)	d_{hkl}
43.5˚			
50.6˚			
74.3˚			
90.2˚			
95.4˚			

如果是你不知道的结构呢？

- 和已有的XRD数据库比对

International Center for Diffraction Data

Cambridge Crystallographic Data Centre

- 如果还是找不到呢？

部分图片来源

- https://waferpro.com/about-silicon-wafers/
- https://www.homedepot.com/p/Benzara-Iron-Bucket-Design-Toilet-Paper-Holder-Wall-Rack-in-Gray-I305-HGM017/307632368
- https://pubs.usgs.gov/of/2001/of01-041/htmldocs/images/romount/
- https://www.rigaku.com/
- https://www.indiamart.com/proddetail/sto-single-crystal-substrate-11134759533.html

4. 合金，相