

# X 射线基础

第二次作业

姓名

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1. 半导体砷化镓 (GaAs) 是闪锌矿结构, Ga, As 原子在晶胞中的位置分别为:

Ga (0,0,0) (1/2,1/2,0) (1/2,0,1/2) (0,1/2,1/2)

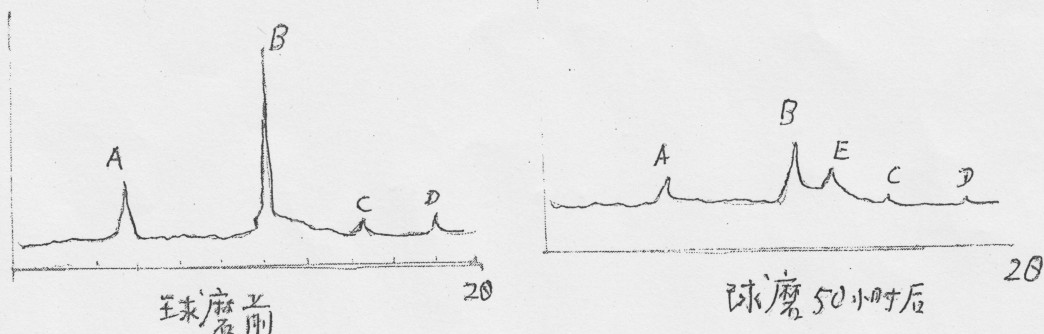
As (1/4,1/4,1/4) (3/4,3/4,1/4) (3/4,1/4,3/4) (1/4,3/4,3/4)

计算其结构因子  $F(hkl)$ , 并讨论其结构消光规律。

2. 金属 Nb 为体心立方晶体, 晶格常数  $a=0.329\text{nm}$ , 有铜  $K_\alpha$  X 射线作 Nb 粉末衍射实验, 列出可能存在的衍射峰的位置 (即  $\theta$  值) 及相应的衍射指数 ( $hkl$ ), 计算前两个峰的相对强度。

3. 将  $\alpha\text{-Fe}$  (30%), Si (70%) 的混合粉末球磨 50 小时, 球磨前后的 X 射线粉末衍射花样如下图所示。请标出各衍射峰的来源 (物相, 衍射指数), 并讨论样品球磨前后的物相变化。

$\alpha\text{-Fe}$  为体心立方晶体,  $a=0.286\text{nm}$ ; Si 为金刚石结构,  $a=0.357\text{nm}$ , X 射线用  $\text{Cu } K_\alpha$ 。



各衍射峰位置 A ( $2\theta=28.4^\circ$ ) B ( $2\theta=44.8^\circ$ ) C ( $2\theta=56.2^\circ$ )  
D ( $2\theta=65.2^\circ$ ) E ( $2\theta=49.2^\circ$ )

## 4. Patterson function of Tl atoms

We construct the Patterson function of Tl atoms as follows:

$$P(x) = \sum_{h=1}^8 |F_{2,h}^n|^2 \cos(2\pi hx/D), \quad (15)$$

where  $D=43.1 \text{ \AA}$  is the lamellar spacing. The function (Fig. 2) shows five distinct peaks on the Patterson coordinate, approximately at 0, 11.8, 18.7, 24.4, 31.3  $\text{\AA}$ . In order to interpret this pattern, let us consider a unit cell consisting of 20 DLPC molecules, 2 gramicidin monomers (which form one channel), 2 thallium acetate molecules and a number of water molecules. If the electron density of the unit cell is plotted on the  $x$  axis (normal to the plane of the membrane) with the origin set at the mid-plane of the bilayer, the cell will range from  $-D/2$  to  $D/2$  and a centrosymmetric bilayer from  $-H/2$  to  $H/2$  ( $H < D$ ); from  $-D/2$  to  $-H/2$  and  $H/2$  to  $D/2$  is water; the gramicidin channel (whose length is less than  $H$ ) is centrosymmetrically embedded in the bilayer. Thus the positions of Tl ions must also be symmetrically distributed; that is, potentially there are pairs of symmetric ion sites ( $x$  and  $-x$ ) and unpaired sites at  $x=0$  and  $D/2$  (equivalently  $-D/2$ ).

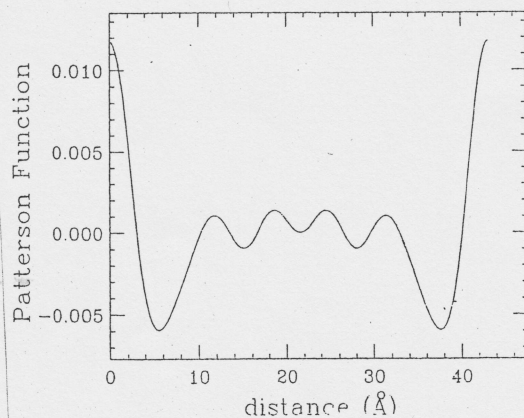


Fig. 2. The Patterson function of the Tl ions.

试确定 Tl 在单胞中的位置。