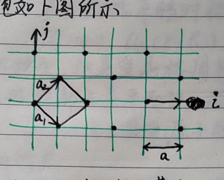
固体物理

第一节 晶体结构

1.1. (1) 原胞如下图所示



设方格边长为a
则原胞基矢为
$a_1 = a(i-j)$
$a_2 = a(i+j)$

(2) 设$a_i\,(i=1,2)$为正格子基矢，则由关系式

$$a_i \cdot b_j = \begin{cases} 2\pi, & i=j \\ 0, & i\neq j \end{cases}$$

所确定的$b_i\,(i=1,2)$为基矢的点阵，称为正格子的倒格子

在倒格子空间，布拉格反射条件为：反射波波矢K与入射波波矢K_0相差一个或几个倒格矢nG_h，即

$$K-K_0 = nG_h$$

(3) i与j是相互垂直的单位矢量，取单位矢量K垂直于i和j，则a_1, a_2和K构成的体积

$$\Omega = a_1\cdot(a_2\times K) = (ai-aj)\cdot(ai-aj) = 2a^2$$

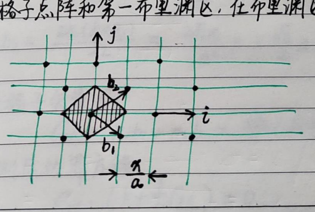
根据倒格子基矢定义

$$b_1 = \frac{2\pi(a_2\times K)}{\Omega} = \frac{2\pi}{2a^2}\times(ai-aj) = \frac{\pi}{a}(i-j)$$

$$b_2 = \frac{2\pi(K\times a_1)}{\Omega} = \frac{2\pi}{2a^2}\times(ai+aj) = \frac{\pi}{a}(i+j)$$

显然这将构成二维正方倒格子点阵

图示出倒格子点阵和第一布里渊区，在布里渊区边界上将发生布拉格反射



(4) 在点阵周期势场中运动的电子波函数是布洛赫波，即

$$\psi_k(r) = e^{ik\cdot r}u_k(r)$$

式中函数$u_k(r)$具有晶格平移对称性

$$u_k(r) = u_k(r+R)$$

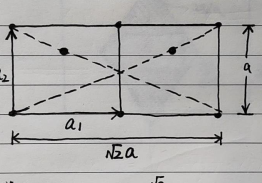
其中R是晶格格矢，这是受晶格周期势场调制的平面波，此即布洛赫定理。布洛赫波的指数部分是平面波，描述了晶体中电子的共有化运动，而周期函数则描述了晶体中电子围绕原子核的运动，因而布洛赫波正是反映晶体中电子运动的特点。

布洛赫定理必须采用玻恩-冯卡门周期性边界条件。

Born-von Karman boundary condition

即：$\psi(r+N_ia_i) = \psi(r)$

1.2 (1)



原胞基矢为 $a_1 = \frac{\sqrt{2}}{2}ai$，$a_2 = aj$

原胞体积 $\Omega = a_1\cdot a_2 = \frac{\sqrt{2}}{2}a^2$

引入垂直于i和j单位矢量K，则金刚石结构$(1,1,0)$面二维格子的倒格子基矢

$$b_1 = \frac{2\pi(a_2\times K)}{\Omega} = \frac{2\sqrt{2}\pi}{a^2}aj\times K = \frac{2\sqrt{2}\pi}{a}i$$

$$b_2 = \frac{2\pi(K\times a_1)}{\Omega} = \frac{2\sqrt{2}\pi}{a^2}K\times\frac{\sqrt{2}}{2}ai = \frac{2\pi}{a}j$$

(2) 倒格子矢量G_h

$$G_h = n_1b_1 + n_2b_2 = \frac{2\pi}{a}(\sqrt{2}n_1i + n_2j)$$

布里渊区边界方程

$$G_h\cdot\left(K+\frac{1}{2}G_h\right) = 0$$

此处$K(k_x, k_y)$表示二维矩形晶格中电子状态，上述方程可写成

$$\frac{4\pi^2}{a^2}(2n_1^2+n_2^2) = \frac{4\pi}{a}(\sqrt{2}n_1k_x + n_2k_y)$$

即

$$\sqrt{2}n_1k_x + n_2k_y = \frac{\pi}{a}(2n_1^2+n_2^2)$$

$\Rightarrow$

$n_1=\pm1,\ n_2=0$时，$k_x = \pm\frac{\sqrt{2}\pi}{a}$ (1)

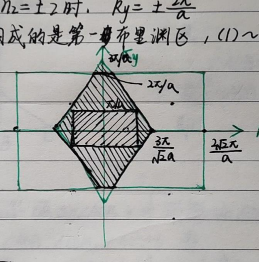
$n_1=0,\ n_2=\pm1$时，$k_y = \pm\frac{\pi}{a}$ (2)

$n_1=\pm1,\ n_2=\pm1$时，$\pm\sqrt{2}k_x + k_y = \frac{3\pi}{a}$ (3)

$n_1=\pm2,\ n_2=0$时，$k_x = \pm\frac{2\sqrt{2}\pi}{a}$ (4)

$n_1=0,\ n_2=\pm2$时，$k_y = \pm\frac{2\pi}{a}$ (5)

(1),(2)两式围成的是第一布里渊区，(1)~(5)围成第二布里渊区



1.3 ~~(1) 布拉维格子有~~

(2) 依照倒格子基矢定义

第一种 $b_1 = 2\pi\frac{a_2\times K}{\Omega}$，$b_2 = 2\pi\frac{K\times a_1}{\Omega}$

第二种 $b_1' = 2\pi\frac{a_2'\times K}{\Omega} = 2\pi\frac{(a_1+a_2)\times K}{\Omega}$

$$= 2\pi\frac{a_1\times K}{\Omega} + 2\pi\frac{a_2\times K}{\Omega} = b_1 - b_2$$

$$b_2' = 2\pi\frac{K\times a_1'}{\Omega} = 2\pi\frac{K\times a_1}{\Omega} = b_2$$

第三种 $b_1'' = 2\pi\frac{a_2''\times K}{\Omega} = 2\pi\frac{(2a_1+a_2)\times K}{\Omega} = b_1 - 2b_2$

$$b_2'' = 2\pi\frac{K\times a_1''}{\Omega} = 2\pi\frac{K\times a_1}{\Omega} = b_2$$

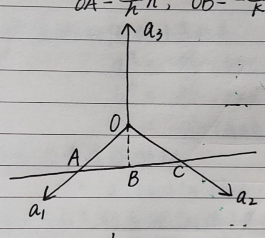
(3) 这三组倒格子基矢不是互相独立而是可以相互线性转化的

这反映它们都只是表示同一倒格子点阵

倒格子空间平移对称性使得，在以$b_1^{(l)}, b_2^{(l)}, b_3^{(l)}$为基的倒格子空间中的一个倒格矢量$G_h^{(l)}$，也是基矢$b_1^{(l)}, b_2^{(l)}, b_3^{(l)}$线性转换而来的基矢$b_1^{(m)}, b_2^{(m)}, b_3^{(m)}$为基的倒格子空间中的一个倒格矢量。这表明虽然一个布拉维格子的基矢选择有任意性，相应的倒格子基矢也有任意性，但倒格子却是由布拉维正格子所唯一确定的。

1.4. (1) 如图所示，某一晶面MN与六角形平面基矢a_1, a_2, a_3轴上的截距

$$\overline{OA} = \frac{a}{h}n,\quad \overline{OB} = -\frac{a}{k}n,\quad \overline{OC} = \frac{a}{l}n$$



且

$\angle AOB = \angle COB = 60°$，$\angle AOC = 120°$

有$S_{\triangle AOB} + S_{\triangle COB} = S_{\triangle AOC}$

即

有 $\frac{1}{2}\overline{OA}\cdot\overline{OB}\sin\angle AOB + \frac{1}{2}\overline{OC}\cdot\overline{OB}\cdot\sin\angle COB = \frac{1}{2}\overline{OA}\cdot\overline{OC}\cdot\sin\angle AOC$

代入$\overline{OA}, \overline{OC}, \overline{OB}$和$\angle AOB, \angle COB, \angle AOC$值，有

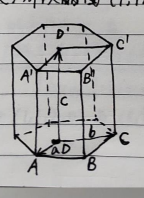
$$\frac{1}{2}\frac{a}{h}\cdot n\cdot\left(-\frac{a}{k}\right)\cdot n\cdot\sin60° + \frac{1}{2}\left(\frac{a}{l}\right)\cdot n\cdot\left(-\frac{a}{k}\right)\cdot n\cdot\sin60°$$

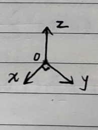
$$= \frac{1}{2}\left(\frac{a}{h}\right)\cdot n\left(\frac{a}{l}\right)\cdot n\cdot\sin120°$$

$$-\frac{1}{hk} - \frac{1}{lk} = \frac{1}{hl}$$

方程两边乘以(hkl)，移项得 $h+k+l=0$

(2) $h+k+l=0$表明，h, k, l不是独立的，$l=-h-k$，可以用(h,k,m)来表示六角晶系的面指数，所以晶面$(1,1,\bar{2},0)$即晶面$(1,1,0)$，晶面$(1,\bar{1},0,1)$即晶面$(1,\bar{1},1)$。





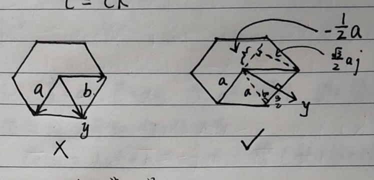
x, y, z 彼此垂直

引进直角坐标系$Oxyz$，使x与z轴分别与基矢a, c重合，基矢a, b, c表示为

$$\vec{a} = ai$$

$$\vec{b} = -\frac{1}{2}ai + \frac{\sqrt{3}}{2}aj$$

$$\vec{c} = ck$$



该原胞的倒格子基矢是

$$a^* = \frac{2\pi}{\Omega}(b\times c) = \frac{2\pi}{\Omega}\left(\frac{\sqrt{3}}{2}aci + \frac{1}{2}acj\right)$$

$$b^* = \frac{2\pi}{\Omega}(c\times a) = \frac{2\pi}{\Omega}acj$$

$$c^* = \frac{2\pi}{\Omega}(a\times b) = \frac{2\pi}{\Omega}\left(\frac{\sqrt{3}}{2}a^2k\right)$$

式中，Ω是晶胞体积

$$\Omega = |a\cdot(b\times c)| = |b\cdot(c\times a)| = \left|\left(-\frac{1}{2}ai + \frac{\sqrt{3}}{2}aj\right)\cdot(acj)\right| = \frac{\sqrt{3}}{2}a^2c$$

故六角晶系的晶胞倒格子基矢

$$a^* = \frac{2\pi}{a}\left(i + \frac{1}{\sqrt{3}}j\right)$$

$$b^* = \frac{2\pi}{a}\frac{2}{\sqrt{3}}j$$

$$c^* = \frac{2\pi}{c}k$$

根据上面的讨论，六角晶系的$(1,1,\bar{2},0)$晶面，也即$(1,1,0)$晶面，则其法线矢量$G_{(110)}$为

$$G_{(110)} = \frac{2\pi}{a}\left(i+\frac{1}{\sqrt{3}}j\right) + \frac{2\pi}{a}\frac{2}{\sqrt{3}}j = \frac{2\pi}{a}(i+\sqrt{3}j)$$

同样，六角晶系中$(1,\bar{1},0,1)$晶面也既$(1,\bar{1},1)$晶面，其法线矢量$G_{(1\bar{1}1)}$为

$$G_{(1\bar{1}1)} = \frac{2\pi}{a}\left(i+\frac{1}{\sqrt{3}}j\right) - \frac{2\pi}{a}\frac{2}{\sqrt{3}}j + \frac{2\pi}{c}k$$

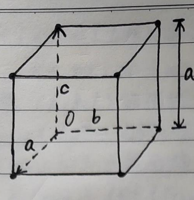
$$= \frac{2\pi}{a}\left(i-\frac{1}{\sqrt{3}}j\right) + \frac{2\pi}{c}k$$

设$G_{(110)}$与$G_{(1\bar{1}1)}$的夹角为α，有

$$\cos\alpha = \frac{\left(\frac{2\pi}{a}\right)^2\left(1\times1+\sqrt{3}\times\left(-\frac{1}{\sqrt{3}}\right)+0\times0\right)}{|G_{(110)}|\cdot|G_{(1\bar{1}1)}|} = \frac{\left(\frac{2\pi}{a}\right)^2(1-1)}{|G_{(110)}|\cdot|G_{(1\bar{1}1)}|} = 0$$

所以六角晶系中$(1,1,\bar{2},0)$与$(1,\bar{1},0,1)$两晶面的法线方向相互垂直。

1.5



立方晶系的晶胞

$$\vec{a} = ai,\ \vec{b} = aj,\ \vec{c} = ak \Rightarrow a^* = \frac{2\pi}{a}i,\ b^* = \frac{2\pi}{a}j,\ c^* = \frac{2\pi}{a}k$$

(1) 由倒格矢性质可知，倒格矢量

$$G_{hkl} = ha^* + kb^* + lc^* = \frac{2\pi}{a}(hi+kj+lk)$$

代表晶面族(h,k,l)的法线方向

晶列指数为$[h,k,l]$的晶列方向上的格矢

$$R_{hkl} = ha + kb + lc = a(hi+kj+lk)$$

$$= a\cdot\frac{a}{2\pi}\cdot\frac{2\pi}{a}(hi+kj+lk)$$

$$= \frac{a^2}{2\pi}\left(h\cdot\frac{2\pi}{a}i + k\cdot\frac{2\pi}{a}j + l\cdot\frac{2\pi}{a}k\right)$$

$$= \frac{a^2}{2\pi}(ha^* + kb^* + lc^*)$$

$$= \frac{a^2}{2\pi}G_{hkl} \propto G_{hkl}$$

故格矢R_{hkl}与倒格矢G_{hkl}互相平行，所以晶面族(h,k,l)的法线上的晶列指数为$[h,k,l]$。

(2) 晶向$[u_1,v_1,w_1]$与$[u_2,v_2,w_2]$上的正格矢量分别写成

$$R_1 = u_1a + v_1b + w_1c = u_1ai + v_1aj + w_1ak$$

和

$$R_2 = u_2a + v_2b + w_2c = u_2aj + v_2aj + w_2ak$$

设两晶向间夹角为α，则

$$R_1\cdot R_2 = |R_1\cdot R_2|\cdot\cos\alpha$$

故

$$\cos\alpha = \frac{R_1\cdot R_2}{|R_1|\cdot|R_2|} = \frac{(u_1ai+v_1aj+w_1ak)\cdot(u_2ai+v_2aj+w_2ak)}{|R_1|\cdot|R_2|}$$

$$= \frac{(u_1u_2+v_1v_2+w_1w_2)\cdot a^2}{\sqrt{u_1^2+v_1^2+w_1^2}\cdot a\cdot\sqrt{u_2^2+v_2^2+w_2^2}\cdot a}$$

$$= \frac{u_1u_2+v_1v_2+w_1w_2}{\sqrt{u_1^2+v_1^2+w_1^2}\cdot\sqrt{u_2^2+v_2^2+w_2^2}}$$

(3) 晶向$[u,v,w]$方向上的正格矢量可表示为

$$R = ua + vb + wc = uai + vaj + wak$$

晶面族(h,k,l)的法线方向，即与此晶面族对应的倒格矢G_{hkl}方向

$$G_{hkl} = ha^* + kb^* + lc^* = \frac{2\pi}{a}(hi+kj+lk)$$

设晶列$[u,v,w]$与晶面族(h,k,l)的法线之间夹角为β则

$$R\cdot G_{hkl} = |R|\cdot|G_{hkl}|\cdot\cos\beta$$

故

$$\cos\beta = \frac{R\cdot G_{hkl}}{|R|\cdot|G_{hkl}|} = \frac{(uai+vaj+wak)\cdot\left(h\frac{2\pi}{a}i + k\frac{2\pi}{a}j + l\frac{2\pi}{a}k\right)}{|R|\cdot|G_{hkl}|}$$

$$= \frac{(uh+vk+wl)\cdot2\pi}{\sqrt{(ua)^2+(va)^2+(wa)^2}\cdot\sqrt{\left(h\frac{2\pi}{a}\right)^2+\left(k\frac{2\pi}{a}\right)^2+\left(l\frac{2\pi}{a}\right)^2}}$$

$$= \frac{uh+vk+wl}{\sqrt{u^2+v^2+w^2}\cdot\sqrt{h^2+k^2+l^2}}$$

(4) 倒格矢量

$$G_{h_1k_1l_1} = h_1a^* + k_1b^* + l_1c^* = \frac{2\pi}{a}(h_1i+k_1j+l_1k)$$

$$G_{h_2k_2l_2} = h_2a^* + k_2b^* + l_2c^* = \frac{2\pi}{a}(h_2i+k_2j+l_2k)$$

分别表示晶面族(h_1,k_1,l_1)和(h_2,k_2,l_2)的法线方向，设两法线之间的夹角为γ，则

$$G_{h_1k_1l_1}\cdot G_{h_2k_2l_2} = |G_{h_1k_1l_1}|\cdot|G_{h_2k_2l_2}|\cdot\cos\gamma$$

故

$$\cos\gamma = \frac{G_{h_1k_1l_1}\cdot G_{h_2k_2l_2}}{|G_{h_1k_1l_1}|\cdot|G_{h_2k_2l_2}|} = \frac{\left(\frac{2\pi}{a}\right)^2\cdot(h_1h_2+k_1k_2+l_1l_2)}{\frac{2\pi}{a}\cdot\sqrt{h_1^2+k_1^2+l_1^2}\cdot\frac{2\pi}{a}\cdot\sqrt{h_2^2+k_2^2+l_2^2}}$$

$$= \frac{h_1h_2+k_1k_2+l_1l_2}{\sqrt{h_1^2+k_1^2+l_1^2}\cdot\sqrt{h_2^2+k_2^2+l_2^2}}$$