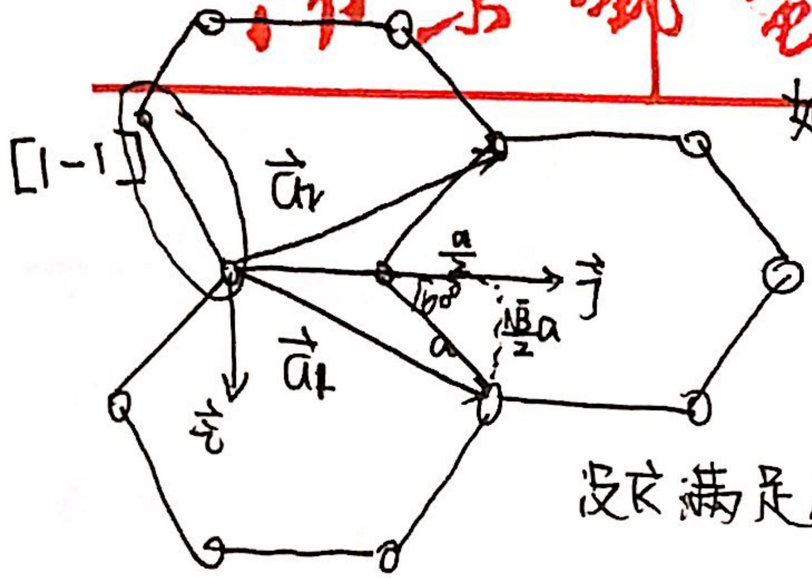
[1-1]




如图选择 $\vec{i}$、$\vec{j}$.

$$\vec{a_1} = \frac{\sqrt{3}}{2}a\vec{i} + \frac{3}{2}a\vec{j}$$

$$\vec{a_2} = -\frac{\sqrt{3}}{2}a\vec{i} + \frac{3}{2}a\vec{j}.$$

设 $\vec{k}$ 满足右手系 $\vec{i}\times\vec{j} = \vec{k}$.

$$\Rightarrow \vec{a_3} = c\cdot\vec{k}.$$

$$\Rightarrow \Omega_d = \vec{a_3}\cdot(\vec{a_1}\times\vec{a_2}) = \frac{3\sqrt{3}}{4}a^2c.$$

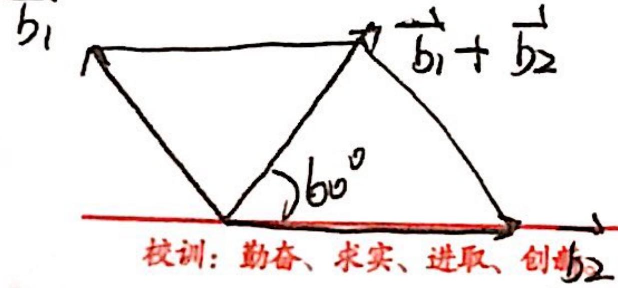
$$\Rightarrow \vec{b_1} = \frac{\vec{a_2}\times\vec{a_3}}{\Omega_d}2\pi = \frac{\vec{a_2}\times\vec{a_3}}{\frac{3}{4}\sqrt{3}a^2c}$$

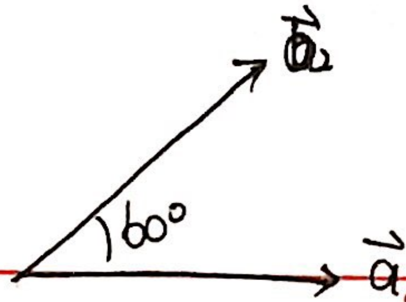
$$= \frac{2\sqrt{3}}{3a}\vec{i} + \frac{2}{3a}\vec{j}.$$

$$\vec{b_2} = \frac{\vec{a_3}\times\vec{a_1}}{\Omega_d}\cdot 2\pi = \frac{\vec{a_3}\times\vec{a_1}}{\frac{3}{4}\sqrt{3}a^2c}$$

$$= \frac{-2\sqrt{3}}{3a}\vec{i} + \frac{2}{3a}\vec{j}.$$

$\Rightarrow \cos\langle\vec{b_1},\vec{b_2}\rangle = 120°$




加上基元

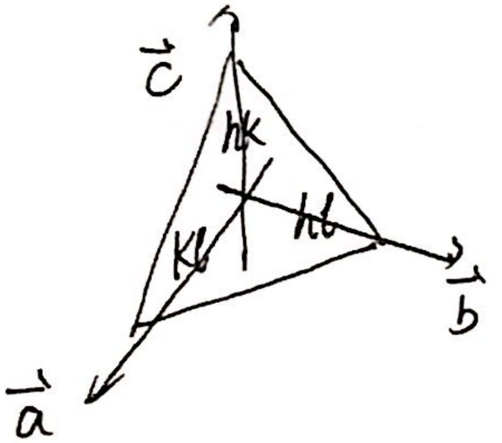


如图所示不难证明 $\vec{b_1}$、$\vec{b_2}$ 同样也是正六方格

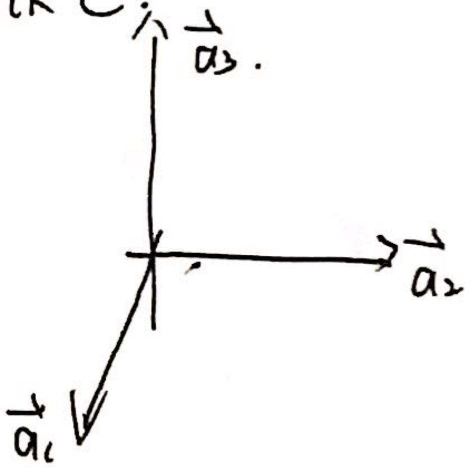
[1-2] 在面心立方晶格中，用晶胞基矢坐标系中，某一晶面族的密勒指数为$(hkl)$，求原胞基矢坐标系中，该晶面族的晶面指数。

$$\frac{1}{h}:\frac{1}{k}:\frac{1}{l} \Rightarrow kl:hl:hk$$

该面过 $kl\vec{a}$，$hl\vec{b}$，$hk\vec{c}$。




$\Rightarrow$




由 $\vec{a} = a\vec{i}$，$\vec{b} = a\vec{j}$，$\vec{c} = a\vec{k}$.

$$\vec{a_1} = \frac{a}{2}(\vec{j}+\vec{k}) \qquad \vec{a} = \vec{a_2}+\vec{a_3}-\vec{a_1}$$

$$\vec{a_2} = \frac{a}{2}(\vec{i}+\vec{k}) \quad \Rightarrow \quad \vec{b} = \vec{a_1}+\vec{a_3}-\vec{a_2}$$

$$\vec{a_3} = \frac{a}{2}(\vec{i}+\vec{j}) \qquad \vec{c} = \vec{a_2}+\vec{a_1}-\vec{a_3}.$$

$\Rightarrow$ 该面过 $kl(\vec{a_2}+\vec{a_3}-\vec{a_1})$、$hl(\vec{a_1}+\vec{a_3}-\vec{a_2})$

$hk(\vec{a_2}+\vec{a_1}-\vec{a_3})$

即过 $(-kl, kl, kl)$, $(hl, -hl, hl)$

$(hk, hk, -hk)$

代入 $\frac{x}{h_1}+\frac{y}{h_2}+\frac{z}{h_3}=1$

$\Rightarrow$ 解得 $h_1=\frac{2hkl}{k+l}$ 晶胞坐标系下

$h_2=\frac{2hkl}{h+l}$ $\Rightarrow \frac{1}{h_1}:\frac{1}{h_2}:\frac{1}{h_3}$

$h_3=\frac{2hkl}{k+h}$

$=(k+l):(h+l):(k+h)$

$\Rightarrow$ 设 $p$ 为三个值的最大公约数.

则 $\left(\frac{k+l}{p}\right):\left(\frac{h+l}{p}\right):\left(\frac{k+h}{p}\right)=(h_1 h_2 h_3)$

[习题解法② 倒格矢坐标互换]

晶胞基矢：$\vec{a} = a\vec{i}$，$\vec{b} = a\vec{j}$，$\vec{c} = a\vec{k}$.

倒基矢：$\vec{a}^* = \frac{2\pi}{a}\vec{i}$，$\vec{b}^* = \frac{2\pi}{a}\vec{j}$，$\vec{c} = \frac{2\pi}{a}\vec{k}$.

~~晶基~~

原胞：$\vec{a}_1 = \frac{a}{2}(\vec{j}+\vec{k})$，$\vec{a}_2 = \frac{a}{2}(\vec{i}+\vec{k})$，$\vec{a}_3 = \frac{a}{2}(\vec{i}+\vec{j})$

倒基矢：$\vec{b}_1 = \frac{2\pi}{a}(-\vec{i}+\vec{j}+\vec{k})$

$\vec{b}_2 = \frac{2\pi}{a}(\vec{i}-\vec{j}+\vec{k})$

$\vec{b}_3 = \frac{2\pi}{a}(\vec{i}+\vec{j}-\vec{k})$

$\vec{a}^* = \frac{1}{2}(\vec{b}_2+\vec{b}_3)$

$\vec{b}^* = \frac{1}{2}(\vec{b}_1+\vec{b}_3)$

$\vec{c}^* = \frac{1}{2}(\vec{b}_1+\vec{b}_2)$

$\Longrightarrow$ 由 $\vec{G}_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$

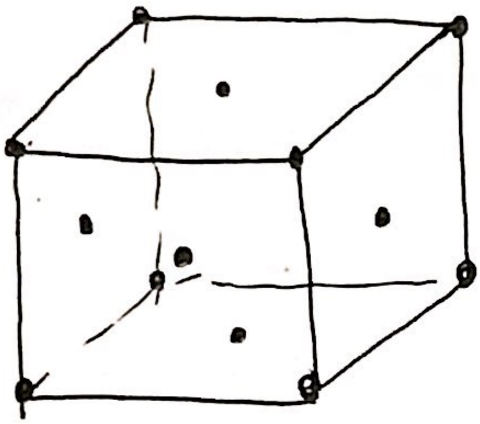
$= \frac{1}{2}[(k+l)\vec{b}_1 + (h+l)\vec{b}_2 + (h+k)\vec{b}_3]$

$\Rightarrow k+l : h+l : h+k \Rightarrow p$ 为最大公约数

$\left(\frac{k+l}{p} : \frac{h+l}{p} : \frac{k+h}{p}\right) = (h_1 h_2 h_3)$

面心立方

[1-4] 求面密度 $\sigma_{max}$ ⇒ $\rho=\sigma/d$ ⇒ $\sigma_{max}$ ⇒ $d_{max}$　　$\rho=Const.$



※倒空间对应k空间，以最小面间距作为 $\vec{b}_1$、$\vec{b}_2$、$\vec{b}_3$.(三维有三个方向的最小间距).或称最近波前距离完备？

$$\vec{K}_h=h_1\vec{b}_1+h_2\vec{b}_2+h_3\vec{b}_3.$$

$$\Rightarrow \vec{b}_1=\frac{2\pi}{a}(-\vec{i}+\vec{j}+\vec{k})$$

$$\vec{b}_2=\frac{2\pi}{a}(\vec{i}-\vec{j}+\vec{k})$$

$$\vec{b}_3=\frac{2\pi}{a}(\vec{i}+\vec{j}-\vec{k})$$

$$\Rightarrow \vec{K}_h=\frac{2\pi}{a}\left[(h_2+h_3-h_1)\vec{i}+(h_1+h_3-h_2)\vec{j}+(h_2+h_1-h_3)\vec{k}\right]$$

$$\Rightarrow d=\frac{2\pi}{|\vec{K}_h|}\Rightarrow d_{max}\Rightarrow |\vec{K}_h|_{min}\Rightarrow \begin{matrix}(1\ 0\ 0)\\(1\ 1\ 1)\end{matrix}$$

$(h_1,h_2,h_3\in Z^+)$

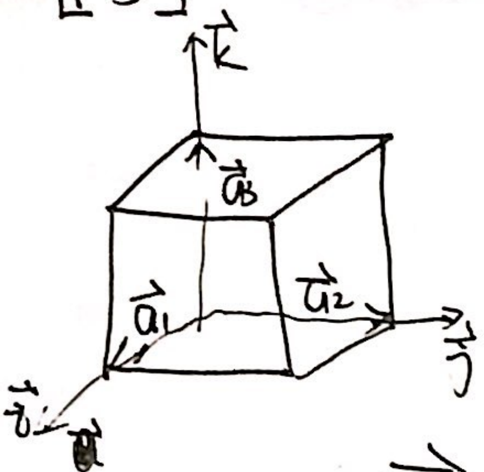
$$\Rightarrow d_{max}=\frac{a}{\sqrt{3}}$$

$$\rho=\frac{4}{a^3}$$



$$\Rightarrow \sigma_{max}=\rho\cdot d=\frac{4}{\sqrt{3}a^2}$$

[1-5]




$\vec{a}_1 = a\vec{i}$. $\vec{a}_2 = a\vec{j}$. $\vec{a}_3 = a\vec{k}$.

$\vec{b}_1 = \frac{2\pi}{a}\vec{i}$, $\vec{b}_2 = \frac{2\pi}{a}\vec{j}$. $\vec{b}_3 = \frac{2\pi}{a}\vec{k}$.

$\cancel{\vec{G}_h = h}$

$\vec{a} = \vec{a}_1$, $\vec{a}_2 = \vec{b}$. $\vec{a}_3 = \vec{c}$

$\Rightarrow$ $\vec{b}_1 = \vec{a}^*$, $\vec{b}_2 = \vec{b}^*$, $\vec{b}_3 = \vec{c}^*$

$$\Rightarrow \vec{G}_h = (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3.)\cdot\frac{2\pi}{a.}$$

$$d = \frac{2\pi}{|\vec{G}_H|} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$\boxed{\text{II.1}}$

$$U(r) = -\frac{A}{r^m} + \frac{B}{r^n}$$

$$\left.\frac{\partial U(r)}{\partial r}\right|_{r=r_0} = 0$$

$\Rightarrow$

$$\frac{mA}{r^{m+1}} = \frac{nB}{r^{n+1}} \quad ①$$

$$\left.\frac{\partial^2 U(r)}{\partial r^2}\right|_{r=r_0} \geq 0$$

$\Rightarrow$

$$-\frac{m(m+1)A}{r^{m+2}} + \frac{n(n+1)B}{r^{n+2}} > 0$$

代入①式

$$-\frac{(m+1)B\cdot n}{r^{n+2}} + \frac{n(n+1)B}{r^{n+2}} > 0.$$

由$r>0$得 $nB(n-m) > 0. \Rightarrow n > m.$

排斥能有效距离更短

$\boxed{II.11}$

$$U(r) = -\frac{N}{2}\left[\frac{\alpha Z_1 Z_2 e^2}{4\pi\varepsilon r} - \frac{B}{r^n}\right]$$

$$\left.\frac{\partial U}{\partial r}\right|_{r=r_0} = -\frac{N}{2}\left[\frac{-\alpha Z_1 Z_2 e^2}{4\pi\varepsilon r^2} + \frac{nB}{r^{n+1}}\right] = 0$$

$$\Rightarrow \quad r_0^{n-1} = \frac{4\pi\varepsilon nB}{Z_1 Z_2 \alpha e^2} \quad \Rightarrow \quad r_0 = \left(\frac{4\pi\varepsilon nB}{Z_1 Z_2 \alpha e^2}\right)^{\frac{1}{n-1}}$$

$\Rightarrow$

~~$r_0$ ∝~~ Suppose $\alpha, B = $ Const. & ~~minimum~~. satisfy minimum energy condition

$$\Rightarrow \quad r_0 \propto (Z_1 Z_2)^{-\frac{1}{n-1}} = (Z_1 Z_2)^{\frac{1}{1-n}}$$

$$\Rightarrow \quad \frac{r_0'}{r_0} = \frac{(4 Z_1 Z_2)^{\frac{1}{1-n}}}{(Z_1 Z_2)^{\frac{1}{1-n}}} = 4^{\frac{1}{1-n}}$$

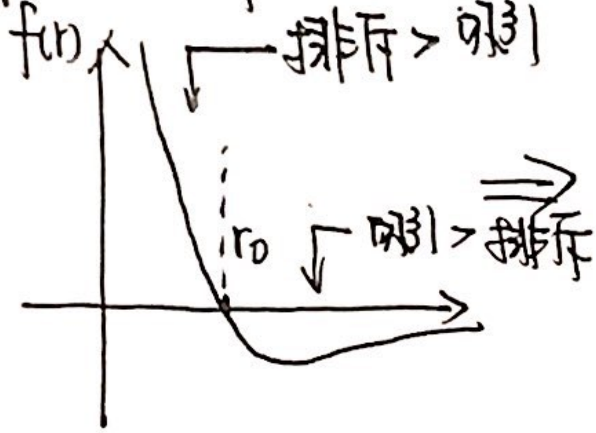
由 $B = \frac{\alpha Z_1 Z_2}{4\pi\varepsilon r} \cdot r^{n-1} \Rightarrow E_b = -U(r_0)$

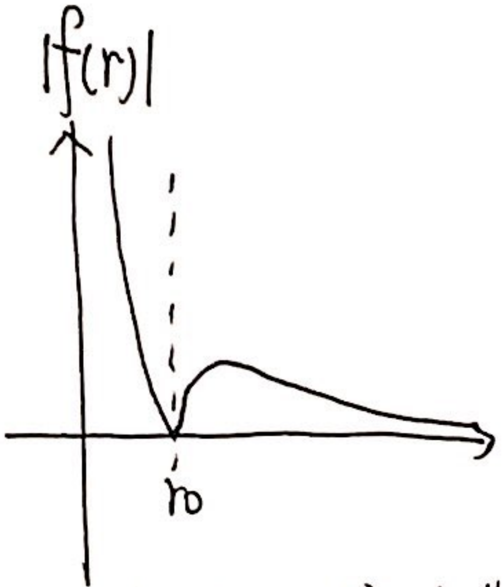
$$= -\frac{N}{2}\left(1 - \frac{1}{n}\right)\frac{Z_1 Z_2 \alpha e^2}{4\pi\varepsilon r_0}$$

$$\frac{E_b'}{E_b} \propto \frac{Z_1' Z_2'}{Z_1 Z_2} \cdot \frac{r_0}{r_0'} = 4^{-\frac{1}{1-n}+1}$$

$$= 4^{\frac{n}{n-1}}$$

II.III




固体受外力发生形变，外力撤消后形变消失的性质称为弹性.

在 $r=r_0$ 时 $f_a=f_p$

$r>r_0$ 时 $f_\alpha>f_p$

$r<r_0$ 时 $f_\alpha<f_p$

⇒

当物体受挤压时 排斥力起主导作用

当物体受拉伸时 吸引力起主导作用

弹性的宏观本质对应原子间存在吸引和排斥两种作用力的微观本质.