- **积分公式**.$\int_{-\infty}^{\infty} exp[ix^2]dx = \sqrt{\pi}exp[i\pi/4]$(Fresnel积分公式); $\int_{-\infty}^{\infty} dxexp[-\alpha x^2+\beta x] = \sqrt{\frac{\pi}{\alpha}}exp[\frac{\beta^2}{4\alpha}]$, $\int_0^{+\infty} x^n exp[-ax^2]dx = \frac{\Gamma(\frac{n+1}{2})}{2a^{\frac{n+1}{2}}}$, $\int_{-\infty}^{+\infty} xexp[-\frac{1}{2}ax^2+bx]dx = \frac{b}{a}\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$, $\int_{-\infty}^{+\infty} x^2 exp[-\frac{1}{2}ax^2+bx]dx = \frac{1}{a}(1+\frac{b^2}{a})\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$; $\int_{-\infty}^{+\infty} x^{2n}exp[-\frac{1}{2}ax^2]dx = \frac{(2n-1)!!}{a^n}\sqrt{\frac{2\pi}{a}}$(广义Guass积分式); $\int_0^{+\infty} x^{2n+1}exp[-ax^2]dx = \frac{n!}{2a^{n+1}}$; $(\frac{1}{\sqrt{2\pi\hbar}})^3\iiint exp[-\frac{i}{\hbar}\vec{p'}\cdot\vec{r}](p_z\frac{\partial}{\partial p_y} - p_y\frac{\partial}{\partial p_z})exp[\frac{i}{\hbar}\vec{p}\cdot\vec{r}]d\tau = (p_z\frac{\partial}{\partial p_y} - p_y\frac{\partial}{\partial p_z})(\frac{1}{\sqrt{2\pi\hbar}})^3\iiint exp[\frac{i}{\hbar}(\vec{p}-\vec{p'})\cdot\vec{r}]d\tau = (p_z\frac{\partial}{\partial p_y} - p_y\frac{\partial}{\partial p_z})\delta(\vec{p}-\vec{p'})$

- **晶格** (1)三斜(1;$a_1 \neq a_2 \neq a_3; \alpha \neq \beta \neq \gamma$);单斜(2;$a_1 \neq a_2 \neq a_3; \alpha = \gamma = \pi/2 \neq \beta$); 正交(4;$a_1 \neq a_2 \neq a_3; \alpha = \beta = \gamma = \pi/2$);四角(2,$a_1 = a_2 \neq a_3; \alpha = \beta = \gamma = \pi/2$); 立方(3;$a_1 = a_2 = a_3; \alpha = \beta = \gamma = \pi/2$);三角(1,$a_1 = a_2 = a_3; \alpha = \beta = \gamma \neq \pi/2$); 六角(1;$a_1 = a_2 \neq a_3; \alpha = \beta = \pi/2, \gamma = 2\pi/3$)(2)sc(简单立方);bcc(体心立方);fcc(面心立方);hcp(六角密堆积) (3)常见结构:NaCl(Cl^-面心&角+Na^+边中&体心);CsCl(Cs^+体心+Cl^-角); 金刚石结构(fcc+000&$\frac{1}{4}\frac{1}{4}\frac{1}{4}$);ZnS结构(Zn000, $0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0$; S$\frac{1}{4}\frac{1}{4}\frac{1}{4}, \frac{1}{4}\frac{3}{4}\frac{3}{4}, \frac{3}{4}\frac{1}{4}\frac{3}{4},, \frac{3}{4}\frac{3}{4}\frac{1}{4}$)

- **两种指标**设晶面截距为a_1, a_2, a_3(1)$(a_1^{-1}, a_2^{-1}, a_2^{-1})$;(2)$[a_1, a_2, a_3]$.上划线表示负号$[u\bar{v}w]$

- **布拉格条件**$2d\sin\theta = n\lambda; \Delta\vec{k} = \vec{G}; 2\vec{k}\cdot\vec{G} = \vec{G}^2$;

- **劳厄条件**$\vec{a_1}\cdot\Delta\vec{k} = 2\pi v_1; \vec{a_2}\cdot\Delta\vec{k} = 2\pi v_2; \vec{a_3}\cdot\Delta\vec{k} = 2\pi v_3$;

- **倒格子初基平移矢量**$\vec{b_1} = 2\pi\frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}, \vec{b_2} = 2\pi\frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}, \vec{b_3} = 2\pi\frac{\vec{a_1}\times\vec{a_2}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}$

- **倒格矢**$\vec{G} = v_1\vec{b_1} + v_2\vec{b_2} + v_3\vec{b_3}, v_i$:$\mathcal{Z}$

- **几何结构因子**前提:方向为$\vec{k'} = \vec{k} + \Delta\vec{k} = \vec{k} + \vec{G}$, $S_G = \sum_j f_j e^{-i\vec{r_j}\cdot\vec{G}} = \sum_j e^{-i2\pi(x_j v_1 + y_j y_2 + z_j v_3)}$, 其中$f_j = \int dV n_j(\vec{r})e^{-i\vec{G}\cdot\vec{r}}$

- **第一布里渊区**倒格子的维格纳-塞茨原胞(1)sc$-\rangle$sc($2\pi/a$);bcc$-\rangle$棱形十二面体($2\pi/a\sqrt{2}$); fcc$-\rangle$截角八面体(八面体的每个角都被切下,使得相邻三个面的正方形的边能围成正六边形)

- **声子** (1)单原子:$u_{s\pm1} = ue^{isKa}exp^{\pm iKa}$色散关系:$w^2 = (2C/M)(1-\cos Ka)$; $w^2 = (4C/M)\sin^2\frac{1}{2}Ka$;群速:$v_g = \frac{dw}{dK} = \sqrt{\frac{Ca^2}{M}}\cos\frac{1}{2}Ka$; 长波极限($Ka << 1$):$w^2 = (C/M)K^2a^2$ (2)双原子:原胞p个原子,3个声学支,3p-3个光学支.$M_1\frac{d^2u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s); M_2\frac{d^2v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$. $u_s = ue^{isKa}e^{-iwt}, v_s = ve^{isKa}e^{-iwt}$,行列式系数为0:$M_1M_2w^4 - 2C(M_1+M_2)w^2 + 2C^2(1-\cos Ka) = 0$;长波极限: 光学支$w^2 = 2C(\frac{1}{M_1} + \frac{1}{M_2})$,声学支$w^2 = \frac{C}{2(M_1+M_2)}K^2a^2$