- **积分公式**.$\int_{-\infty}^{\infty}exp[ix^2]dx=\sqrt{\pi}exp[i\pi/4]$(Fresnel积分公式); $\int_{-\infty}^{\infty}dxexp[-\alpha x^2+\beta x]=\sqrt{\frac{\pi}{\alpha}}exp[\frac{\beta^2}{4\alpha}]$, $\int_0^{+\infty}x^n exp[-ax^2]dx=\frac{\Gamma(\frac{n+1}{2})}{2a^{\frac{n+1}{2}}}$, $\int_{-\infty}^{+\infty}xexp[-\frac{1}{2}ax^2+bx]dx=\frac{b}{a}\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$, $\int_{-\infty}^{+\infty}x^2exp[-\frac{1}{2}ax^2+bx]dx=\frac{1}{a}(1+\frac{b^2}{a})\sqrt{\frac{2\pi}{a}}exp[b^2/(2a)]$; $\int_{-\infty}^{+\infty}x^{2n}exp[-\frac{1}{2}ax^2]dx=\frac{(2n-1)!!}{a^n}\sqrt{\frac{2\pi}{a}}$(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$\vec{k'}=\vec{k}+\Delta\vec{k}=\vec{k}+\vec{G}$, $S_G=\sum_j f_je^{-i\vec{r_j}\cdot\vec{G}}=\sum_j e^{-i2\pi(x_jv_1+y_jy_2+z_jv_3)}$, 其中$f_j=\int dVn_j(\vec{r})e^{-i\vec{G}\cdot\vec{r}}$
- **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-振动** (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$w^2=\frac{C}{2(M_1+M_2)}K^2a^2$;光学支下原子反向震动即质心固定,由光的电场来激发. (3)波矢选择定则:波矢$\vec{k}$非弹性散射到$\vec{k'}$,同时产生/吸收波矢为$\vec{K}$的声子,那么$\vec{k}=\vec{k'}\pm\vec{K}+\vec{G}$,$\vec{G}$是倒格矢; (4)声子能量:$\epsilon=(n+\frac{1}{2})\hbar\omega$;动能守恒:$\frac{\hbar^2k^2}{2M_n}=\frac{\hbar^2k'^2}{2M_n}\pm\hbar\omega$
- **声子-热学** (0)定容热容$C_V=(\frac{\partial U}{\partial T})_V(1)$