ЕФЕКТИВНА МАСА НА ЗАРЕДЕНИТЕ ЧАСТИЦИ В КРИСТАЛА

1. Движение на електрон в кристала под действие на външно електрично поле.

$$Fa << E_g ,$$

$$U(r) = -e\mathrm{E}x .$$

$$\left[-\frac{\hbar^2}{2m}\Delta + (V(r)+U(r))\right]\psi(r) = E'\psi(r).$$

$$\left[-\frac{\hbar^2}{2m}\Delta + V(r)\right]\psi(r) = (E'-U)\psi(r) = E\psi(r)$$

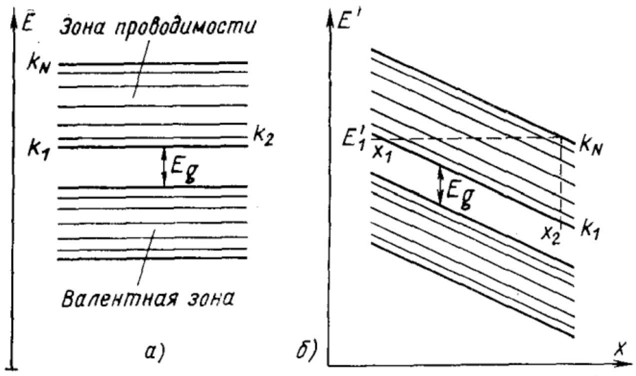
$$E' = E + U(r).$$

$$E' = E_a + C + 2A(\cos k_x a + \cos k_y a + \cos k_z a) - e\mathrm{E}x . \quad (1)$$

$$E_{\max} = E_a + C + 6A - e\mathrm{E}x ,$$

$$E_{\min} = E_a + C - 6A - e\mathrm{E}x .$$

$$E_{\max} - E_{\min} = 12A,$$



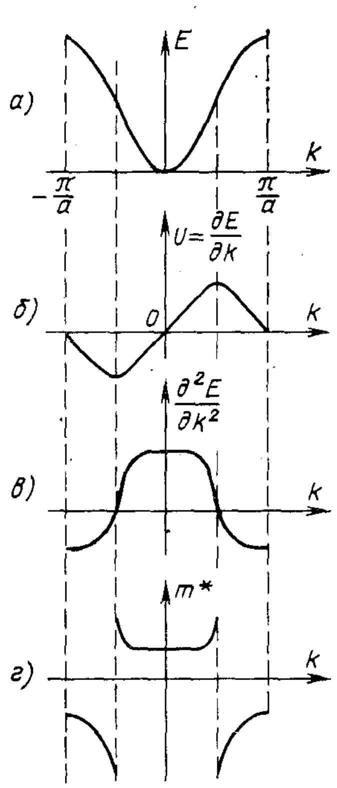
$$E' = E + U = const .$$

$$\Delta x = \frac{E_{\max} - E_{\min}}{e\mathrm{E}} = \frac{12A}{e\mathrm{E}} . \quad (2)$$

$$p = \hbar k , \qquad v = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk} = \frac{dE}{dp} . \quad (3)$$

$$E = -2A\cos ka, \quad (4)$$

$$v = \frac{2aA}{\hbar}\sin ka . \quad (5)$$



Фигура 2. Зависимост на енергията E (*а*), скоростта v (*б*), величината $\partial^2 E/\partial k^2$ (*в*) и ефективната маса m^* (*г*) от вълновия вектор *к* за кубична кристална решетка.

$$\langle v\rangle = \int_{-\pi/a}^{\pi/a} v(k)dk = \frac{2aA}{\hbar}\int_{-\pi/a}^{\pi/a}\sin kadk = 0\,.$$

$$\frac{dE}{dt} = Fv\,, \qquad \frac{dE}{dt} = \frac{dE}{dp}\frac{dp}{dt}\,, \qquad \frac{dp}{dt} = F \tag{6}$$

$$\frac{dp}{dt} = F_{\text{кр}} + F\,.$$

$$p(t) = p_0 + Ft$$

2. Ефективна маса

$$a = -\frac{1}{m}F = -\frac{1}{m}e\mathrm{E}\,,$$

$$a = \frac{dv}{dt} = \frac{\partial v}{\partial p}\frac{\partial p}{\partial t} = \frac{\partial^2 E}{\partial p^2}F \tag{7}$$

$$a_i = \frac{1}{\hbar^2}\sum_{i,j}^{3}\frac{\partial^2 E}{\partial k_i \partial k_j}.F_j\,,$$

$$\frac{1}{m_{ij}^*} = \frac{1}{\hbar^2}\sum_{i,j}^{3}\frac{\partial^2 E}{\partial k_i \partial k_j}\,. \tag{8}$$

$$\frac{1}{m_1}=\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_x^2}, \qquad \frac{1}{m_2}=\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_y^2}, \qquad \frac{1}{m_3}=\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_z^2}.$$

$$E(k)=E(k_0)+\frac{\hbar^2(k_x-k_{0x})^2}{2m_1}+\frac{\hbar^2(k_y-k_{0y})^2}{2m_2}+\frac{\hbar^2(k_z-k_{0z})^2}{2m_3}.$$

$$E(p)=E(p_0)+\frac{(p_x-p_{0x})^2}{2m_1}+\frac{(p_y-p_{0y})^2}{2m_2}+\frac{(p_z-p_{0z})^2}{2m_3}. \tag{9}$$

Изоенергетичната повърхност $E(p)-E(p_0)=const$

$$a^2=2m_1[E(p)-E(p_0)],$$
$$b^2=2m_2[E(p)-E(p_0)], \tag{10}$$
$$c^2=2m_3[E(p)-E(p_0)].$$

$$v_i=\frac{dE}{dp_i}=\frac{p_i-p_{0i}}{m_i}.$$

Ако $E(p)=E$ и $E(p_0)=E_0$, то: $p_i-p_{0i}=\sqrt{2m_i(E-E_0)}$,

$$v_i=\frac{p_i-p_{0i}}{m_i}=\sqrt{\frac{2(E-E_0)}{m_i}}. \tag{11}$$

За кристал с кубична симетрия

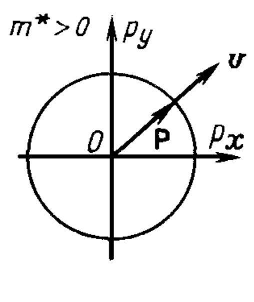
$$E(p)=E(p_0)+\frac{p^2}{2m^*}=const.$$

$$\frac{1}{m^*}=\frac{\partial^2 E}{\partial p^2}=\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}. \tag{12}$$

$$\frac{\partial^2 E}{\partial k^2}>0 \qquad \text{и} \qquad m^*=const>0, \tag{13}$$

$$F=m^*a \tag{14}$$

Като се има впредвид, че $a=dv/dt$ и $F=dp/dt$, то $p=m^*v$.



$$\frac{\partial^2 E}{\partial k^2}<0 \qquad \text{и} \qquad m^*=const<0, \tag{15}$$

$$a = -\frac{F}{m^*}, \qquad F = -e\mathrm{E}, \qquad a = \frac{-|e|\mathrm{E}}{-|m^*|} = \frac{e\mathrm{E}}{m^*}.$$

В точките на огъване $k = \pm\pi/2a$ $\quad \frac{\partial^2 E}{\partial k^2} = 0$ и $m^* \to \infty$.

$$m_p^* > m_n^*.$$

3. Метод на ефективната маса

$$\left[-\frac{\hbar^2}{2m}\Delta + V(r) + U(r)\right]\psi(r) = E\psi(r). \tag{16}$$

$$-\frac{\hbar^2}{2m}\Delta\psi_0(r) = E\psi_0(r). \tag{17}$$

$$-\frac{\hbar^2}{2m^*}\Delta\psi(r) = E\psi(r). \tag{18}$$

$$\left[-\frac{\hbar^2}{2m}\Delta + V(r)\right]\psi(r) = E\psi(r) \tag{19}$$

$$\left[-\frac{\hbar^2}{2m^*}\Delta + U(r)\right]\psi(r) = E\psi(r),$$

4. Елементарна теория на примесните състояния

4.1. Донорни примеси

$$U(r) = -\frac{Ze^2}{4\pi\varepsilon_0\varepsilon r}, \tag{20}$$

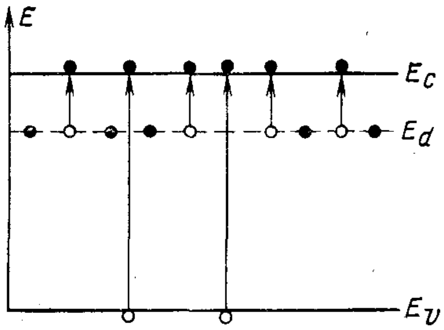
$$\left[-\frac{\hbar^2}{2m^*}\Delta - \frac{Ze^2}{4\pi\varepsilon_0\varepsilon r}\right]\psi_a = E_n\psi_a.$$

$$E_n = E_c - \frac{m^* Z^2 e^4}{8h^2\varepsilon_0^2\varepsilon^2}\frac{1}{n^2},$$

$$E_n = E_c - \frac{mZ^2e^4}{8h^2\varepsilon_0^2}\left(\frac{m^*}{m}\right)\frac{1}{\varepsilon^2 n^2}.$$

$$E_n = E_c - \frac{13{,}52Z^2}{\varepsilon^2}\left(\frac{m^*}{m}\right)\frac{1}{n^2} = E_c - \frac{E_d}{n^2} \tag{21}$$

$$E_d = \frac{13{,}52Z^2}{\varepsilon^2}\left(\frac{m^*}{m}\right) \tag{22}$$



4.2. Акцепторни примеси

$$E_p = E_v + \frac{m^* Z^2 e^4}{8h^2 \varepsilon_0^2 \varepsilon^2} \frac{1}{n^2} = E_v + \frac{E_a}{n^2} \qquad (23)$$

$$E_a = \frac{13{,}52 Z^2}{\varepsilon^2} \left(\frac{m^*}{m} \right), \qquad (24)$$