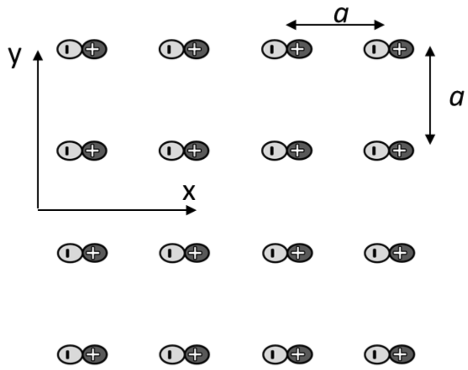
Condensed Matter Physics May 18th 2020

1) The sites of a simple square lattice are occupied by single atoms with one valence electron. This latter is in a p_x-type orbital with wavefunction $\phi_{p_x}(\vec{r})$ real. The lattice is shown in the figure (lattice parameter a=0.5 nm).

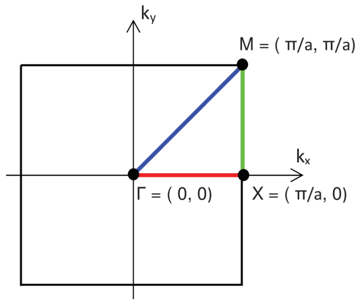


Assume valid the tight-binding approximation and let the orbital energy E_p=5 eV, the overlap integral $\alpha(\vec{R}) = \int d\vec{r}\phi_{p_x}(\vec{r})\phi_{p_x}(\vec{r}-\vec{R}) = 0$,
the integral $\beta = -\int d\vec{r}\phi_{p_x}^2(\vec{r})\Delta U(\vec{r}) = 0$, where $\Delta U(\vec{r})$ is the crystal potential, and finally the transfer integral $\gamma(\vec{R}) = -\int d\vec{r}\phi_{p_x}(\vec{r})\Delta U(\vec{r})\phi_{p_x}(\vec{r}-\vec{R})$.

a) Assuming *only first-neighbor interaction* and *repulsive* crystal potential $\Delta U(\vec{r})$, say the sign of the transfer integrals γ_x and γ_y for the different first neighbors.

b) Determine the dispersion relationship between energy and crystal momentum $\vec{k} = (k_x, k_y)$.

c) Plot the dispersion relationship along the Γ-X, Γ-M and M-X directions of the first Brillouin zone according to the notation shown in the figure.



Set $|\gamma_x| = 0.6$ eV and $|\gamma_y| = 0.8$ eV .

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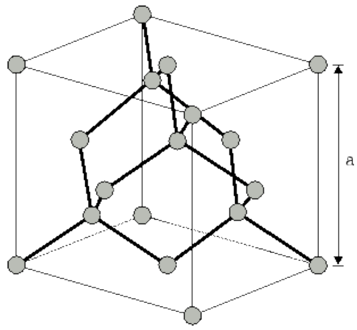
2) Diamond features a face-centered cubic lattice structure with two atom basis. By performing a diffraction measurement using an x-ray beam with λ=0.100 nm, the fourth Bragg reflection compatible with the diamond structure is observed at the angle θ=34.07°. Evaluate:



a) the lattice parameter *a* of the conventional cubic cell of diamond;

b) the Debye temperature of diamond knowing that the longitudinal and transverse sound velocities are equal to 3.06×10^6 cm/s and 1.28×10^6 cm/s, respectively;

c) the specific heat at 5 K in the Debye approximation.

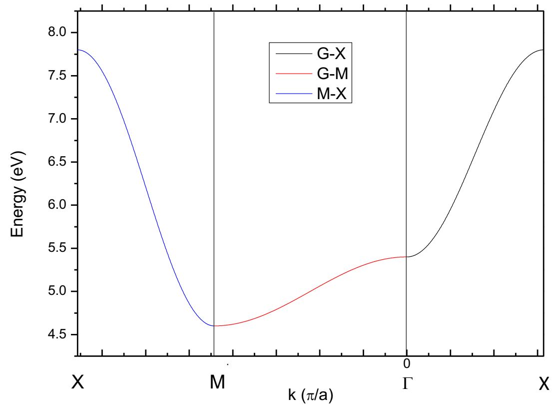
Solution

1)

a) $\gamma(\vec{R_l}) = -\int d\vec{r}\phi_{p_x}(\vec{r})\Delta U(\vec{r})\phi_{p_x}(\vec{r}-\vec{R_l})$ with $\Delta U(\vec{r}) > 0$ (repulsive crystal potential).

Therefore, we have $\gamma_x = -\int d\vec{r}\phi_{p_x}(\vec{r})\Delta U(\vec{r})\phi_{p_x}(\vec{r}-\vec{R_l}) > 0$ 

and $\gamma_y = -\int d\vec{r}\phi_{p_x}(\vec{r})\Delta U(\vec{r})\phi_{p_x}(\vec{r}-\vec{R_l}) < 0$ 



b) Let henceforth $\gamma_{x,y} = |\gamma_{x,y}|$, to simplify the notation. Then

$$E(\vec{k}) = E_p - 2[\gamma_x \cos k_x a - \gamma_y \cos k_y a]$$

c) Γ-X

$k_y = 0$ and $k_x \in \left[0, \frac{\pi}{a}\right]$.

$$E(\vec{k}) = E_p - 2[\gamma_x \cos k_x a - \gamma_y]$$

Γ-M

$k_x = k_y = k/\sqrt{2}$ and $k \in \left[0, \frac{\pi}{a}\sqrt{2}\right]$. $E(\vec{k}) = E_p - 2\left[(\gamma_x - \gamma_y)\cos\frac{ka}{\sqrt{2}}\right]$

M-X

$k_x = \frac{\pi}{a}$ and $k_y \in \left[\frac{\pi}{a}, 0\right]$. $E(\vec{k}) = E_p - 2[-\gamma_x - \gamma_y \cos k_y a]$

2)

a) $2d\sin\theta = \lambda$, and for diamond the selection rule-compatible fourth peak is for (hkl)=(400).

Thus, $a = d(4^2 + 0^2 + 0^2)^{1/2} = \frac{4\lambda}{2\sin\theta} = 0.357\ \mathrm{nm}$

b) The Debye temperature is given by $\vartheta_D = \frac{\hbar}{k_B}(6\pi^2 n)^{\frac{1}{3}}\langle v_s\rangle$, where $n=8/a^3=1.758\cdot 10^{29}\ \mathrm{m}^{-3}$, and

$\langle v_s\rangle = \frac{1}{\left[\frac{1}{3}\left(\frac{1}{v_l}+\frac{2}{v_t}\right)\right]^{\frac{1}{3}}} = 1.45\cdot 10^6\ \mathrm{cm/s}$. One finds $\vartheta_D = 2412\ \mathrm{K}$.

c) At 5 K, $c_V = 234\left(\frac{T}{\vartheta_D}\right)^3 n k_B = 5.06\ \frac{\mathrm{J}}{\mathrm{K\cdot m^3}}$.