Level 3 Condensed Matter Physics- Part II
Examples Class 1 Answers

(1) (i) The Bloch wavefunction is given by $\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$, where $u_{n\mathbf{k}}(\mathbf{r})$ has the periodicity of the crystal (i.e. $u_{n\mathbf{k}}(\mathbf{r}+\mathbf{T}) = u_{n\mathbf{k}}(\mathbf{r})$ for any lattice translation vector $\mathbf{T}$). $\mathbf{k}$ is the wavevector and n the band index. Bloch functions differ from the plane wave, free electron solution by the additional term $u_{n\mathbf{k}}(\mathbf{r})$. This ensures that the electron *intensity* has the same periodicity as the crystal (i.e. $|\psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{T})|^2 = |\psi_{n\mathbf{k}}(\mathbf{r})|^2$). Note that $|\psi|^2$ is a measurable quantity, but not the wavefunction ψ.

(ii) The momentum operator is given by $\mathbf{p} = -i\hbar\nabla$. Applying this to a Bloch function:

$$-i\hbar\nabla\left[u_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}\right] = -i\hbar e^{i\mathbf{k}\cdot\mathbf{r}}\nabla u_{n\mathbf{k}} + \hbar\mathbf{k}\psi_{n\mathbf{k}}(\mathbf{r}) \neq \mathbf{p}\,\psi_{n\mathbf{k}}(\mathbf{r})$$

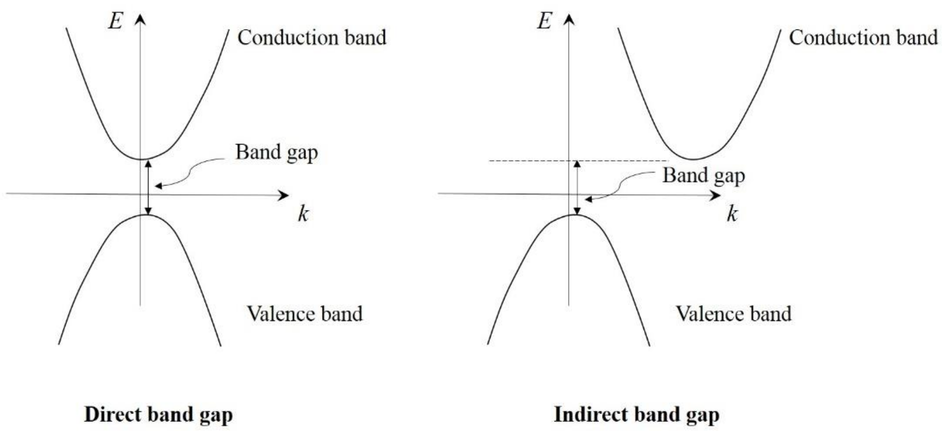
Therefore $\mathbf{k}$ in the Bloch function does not represent electron momentum.

(iii) From de Broglie's equation $\lambda = h/p$, so that the photon momentum at 500 nm wavelength is 1.3 x 10^{-27} kgm/s.

The Brillouin zone boundary is at π/a or 0.63 Å^{-1}. The crystal momentum $\hbar\mathbf{k}$ is therefore 6.6 x10^{-25} kgm/s.

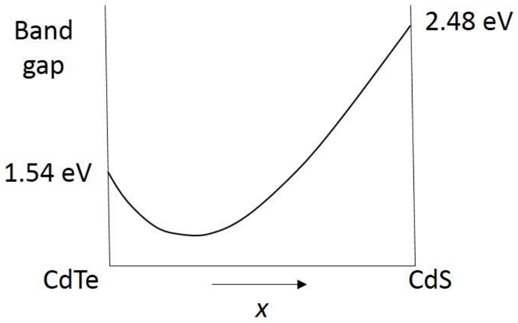
Photon momentum is several orders of magnitude smaller than the crystal momentum. We shall see in the lectures that this has implications for photoabsorption in indirect band gap semiconductors.

(2) (i) Energy-wavevector diagrams:



The photodiode must have a high light absorption coefficient. This is satisfied for direct band gap semiconductors and is therefore the material of choice. Light absorption in indirect band gap semiconductors requires both photon and phonon participation (the latter for momentum conservation) and is therefore weaker.

(ii) The band gap vs. composition curve looks like:



Using $E = hc/\lambda$ the energy of a 700 nm photon is 1.77 eV. For the solid to be transparent its band gap must be larger than 1.77 eV. We can determine the composition values where the band gap is equal to 1.77 eV, i.e.

$$1.77 = 1.54 - 0.90x + 1.84x^2$$

Solving for x we get $x = 0.67$ and $x = -0.19$. The latter is not physical (since $0 \leq x \leq 1$) so that from the graph above the composition range is $0.67 < x \leq 1$.

(iii) The conduction band minimum and valence band maximum are obtained from $dE_c/dk = 0$ and $dE_v/dk = 0$ respectively. The conduction band minimum is at $k = 1$ m^{-1} and valence band maximum is at $k = 0$ m^{-1}. The different k-values mean the band gap is indirect.

Calculating the E_c and E_v values at the turning points and taking the difference gives a band gap energy of $\underline{\underline{\text{1.3 eV}}}$.