

We can rewrite $E_0(x) = xE_{g,AB} + (1-x)E_{g,CD} - bx(1-x)$ (Eqn. 1)

as $E_{g,(AB)_x(CD)_{1-x}} = xE_{g,AB} + (1-x)E_{g,CD} - bx(1-x)$. (Eqn. 1b)

1. Substituting $x=0.5$ into Eqn.1,

$$E_0(x=0.5) = 0.5E_{g,AB} + (1-0.5)E_{g,CD} - b \times 0.5 \times (1-0.5) = 0.5E_{g,AB} + 0.5E_{g,CD} - 0.25b$$

$$\therefore b = 4 \left[\frac{E_{g,AB} + E_{g,CD}}{2} - E_0(x=0.5) \right] \quad (3 \text{ pts}) \quad (\text{Eqn. 2})$$

2. $\text{Al}_x\text{Ga}_{1-x}\text{N}$ can be expressed as $(\text{AlN})_x (\text{GaN})_{1-x}$. From Eqn. 1b, the energy gap of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ can be expressed as

$$E_g(x) = xE_{g,\text{AlN}} + (1-x)E_{g,\text{GaN}} - bx(1-x). \quad (3 \text{ pts}) \quad (\text{Eqn. 3})$$

3. As quaternary alloy $\text{A}_{1-x}\text{B}_x\text{C}_{1-y}\text{D}_y$ can be expressed by $\text{A}_{1-x}\text{B}_xC$ and $\text{AC}_{1-y}\text{D}_y$, we will consider ternary alloy $\text{A}_xB_{1-x}C$ only. If there is no crystallographic phase change with composition, the lattice constant of the alloy is a function of its composition,

$$a_{\text{A}_xB_{1-x}C} = g(x). \quad (\text{Eqn. 4})$$

For instance, it can be expressed by the Vegard's law,

$$a_{\text{A}_xB_{1-x}C} = xa_{AC} + (1-x)a_{BC} := g(x) \quad (\text{Eqn. 4b})$$

Moreover, the band gap for $\text{A}_xB_{1-x}C$ is a function of its lattice parameter a ,

$$E_g = f(a), \quad (\text{Eqn. 5})$$

$$\therefore E_g = f(a) = f[g(x)] := E(x). \quad (6 \text{ pts}) \quad (\text{Eqn. 6})$$

4. For III-V ternary alloys, Vegard's law doesn't always hold. The linear relation is invalid. Instead, we have

$$a_{\text{A}_xB_{1-x}C} = xa_{AC} + (1-x)a_{BC} - b'x(1-x) \quad (\text{Eqn. 7})$$

Figure Sol6-4 shows the lattice parameter-composition relation of a ternary alloy.

Generally, there are similar equations for other properties T, i.e.

$$T_{(AB)_x(CD)_{1-x}} = xT_{AB} + (1-x)T_{CD} - bx(1-x) \quad (+5 \text{ pts}) \quad (\text{Eqn. 8})$$

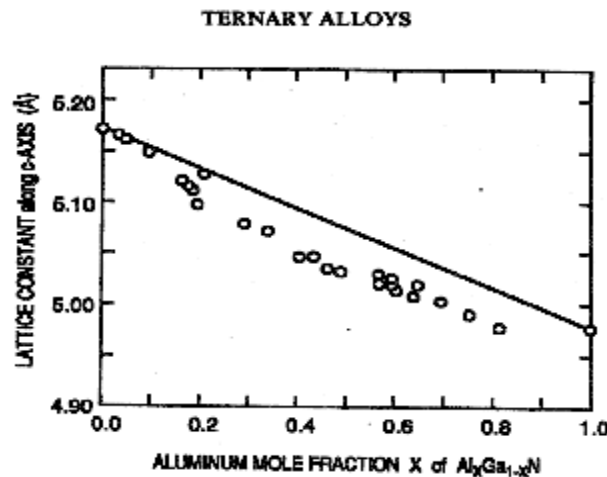


Figure Sol6-4 The lattice parameter-composition relation of a ternary alloy.

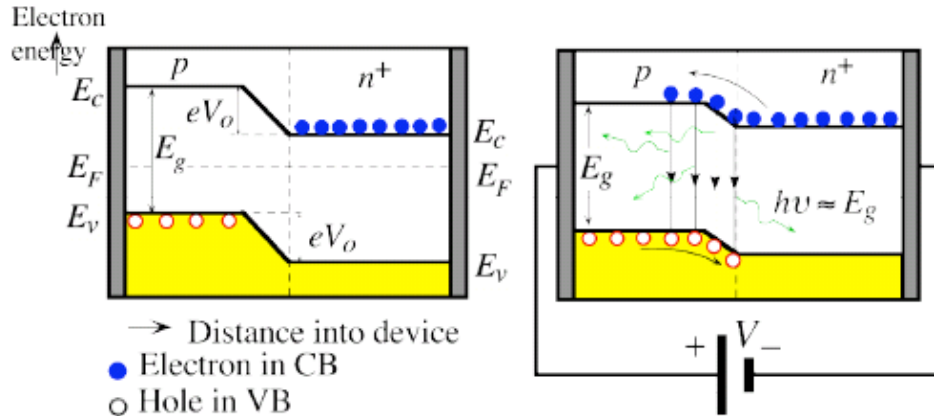


Fig. Sol6-5 A typical energy band diagram for pn junction LED.

5. An LED is basically a *pn* junction diode, in which the electron-hole pair (EHP) recombination results in the emission of a photon. A typical energy band diagram is shown in Figure *Sol6-5*. Further considerations can be found in the textbook (Section 6.9). **(6 pts)**

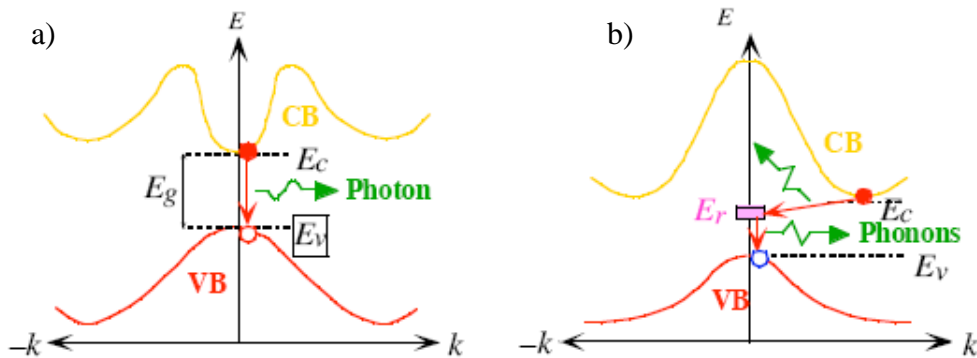
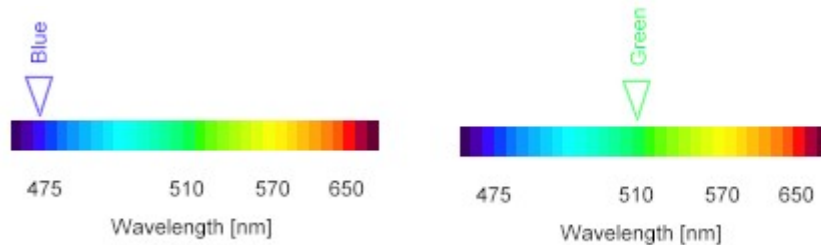


Fig. Sol6-6 Recombination in a) direct bandgap & b) indirect bandgap semiconductors.

6. For an indirect bandgap semiconductor, EHP recombination processes occur through recombination centers and involve lattice vibration (phonon emission) rather than photon emission, which is the case for a direct bandgap semiconductor. Hence, direct bandgap semiconductors are preferred. (Refer to Figure *Sol6-6* and Kasap §5.4.1, 5.7, 5.8 and 5.11 for details). **(6 pts)**



(Photo after: http://eosweb.larc.nasa.gov/EDDOCS/Wavelengths_for_Colors.html)

7. From Figures HW6-3, we can find that (at room temperature)

III-V alloy	AlN	GaN	InN
$E_g(eV)$	6.2	3.4	2.0

The wavelength and energy of blue and green lights are $\lambda=424.0-491.2\text{ nm}$, $h\nu = hc/\lambda = 2.925-2.385\text{ eV}$ and $491.2-575.0\text{ nm}$, $2.385-2.157\text{ eV}$, respectively.

(Data after: *CRC Handbook of Chemistry and Physics*) (2 pts)

(1) From Eqn. 3, $E_g(\text{Al}_x\text{Ga}_{1-x}\text{N}) = 6.2x + 3.4(1-x) - x(1-x) = x^2 + 1.8x + 3.4$

As the band gap is between 3.4eV and 6.2eV, which corresponds photons with wavelength between 364.7 nm and 200.0nm. It can't emit blue and green lights. (6 pts)

(2) Similarly, $E_g(\text{In}_x\text{Ga}_{1-x}\text{N}) = xE_{g,\text{InN}} + (1-x)E_{g,\text{GaN}} - bx(1-x) = x^2 - 2.4x + 3.4$

i) In the case of blue LED, $2.925\text{ eV} \geq h\nu \geq 2.385\text{ eV}$. In other words, we have

$$\left. \begin{array}{l} x^2 - 2.4x + 3.4 \geq 2.385 \\ x^2 - 2.4x + 3.4 \leq 2.925 \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} x^2 - 2.4x + 1.015 \geq 0 \\ x^2 - 2.4x + 0.475 \leq 0 \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} 0 \leq x \leq 0.548 \\ 0.218 \leq x \leq 1 \end{array} \right.$$

Hence, $\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys with composition $0.218 \leq x \leq 0.548$ will emit blue light.

ii) In the case of green LED, $2.385\text{ eV} \geq h\nu \geq 2.157\text{ eV}$. In other words, we can solve

$$\left\{ \begin{array}{l} x^2 - 2.4x + 3.4 \geq 2.157 \\ x^2 - 2.4x + 3.4 \leq 2.385 \end{array} \right. \Rightarrow \left\{ \begin{array}{l} x^2 - 2.4x + 1.243 \geq 0 \\ x^2 - 2.4x + 1.015 \leq 0 \end{array} \right. \Rightarrow \left\{ \begin{array}{l} 0 \leq x \leq 0.756 \\ 0.548 \leq x \leq 1 \end{array} \right.$$

$\text{In}_x\text{Ga}_{1-x}\text{N}$ alloys with composition $0.548 \leq x \leq 0.756$ will emit green light. (12 pts)

To solve these inequalities, such as $h(x) := x^2 - 2.4x + 1.015 \leq 0$, please keep in mind that $0 \leq x \leq 1$. The solutions to corresponding equation $h(x) = 0$ are

$$x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{2.4 \pm \sqrt{(-2.4)^2 - 4 \times 1 \times 1.015}}{2 \times 1} = 1.852, 0.548.$$

The solution to $h(x) \leq 0$ is then $0.548 \leq x \leq 1$, as shown in Figure Sol6-7.

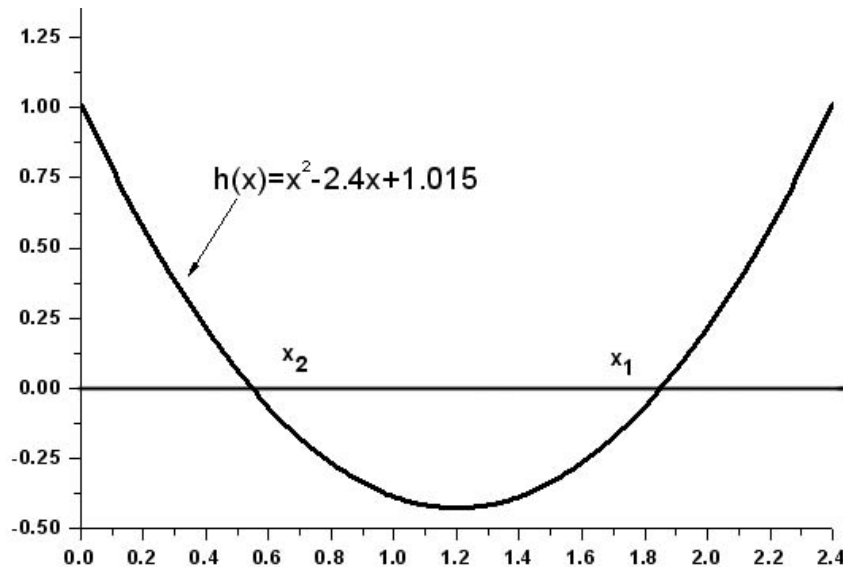


Fig. Sol6-7 Sketch of how to solve the inequality $h(x) := x^2 - 2.4x + 1.015 \leq 0$.

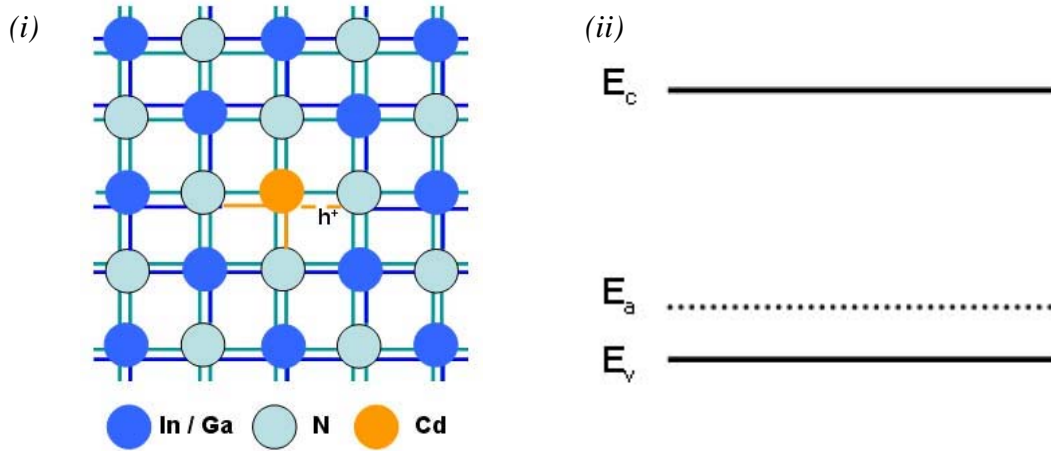


Fig. Sol6-8 (i) Cd-doped $\text{In}_x\text{Ga}_{1-x}\text{N}$ and (ii) its energy band diagram.

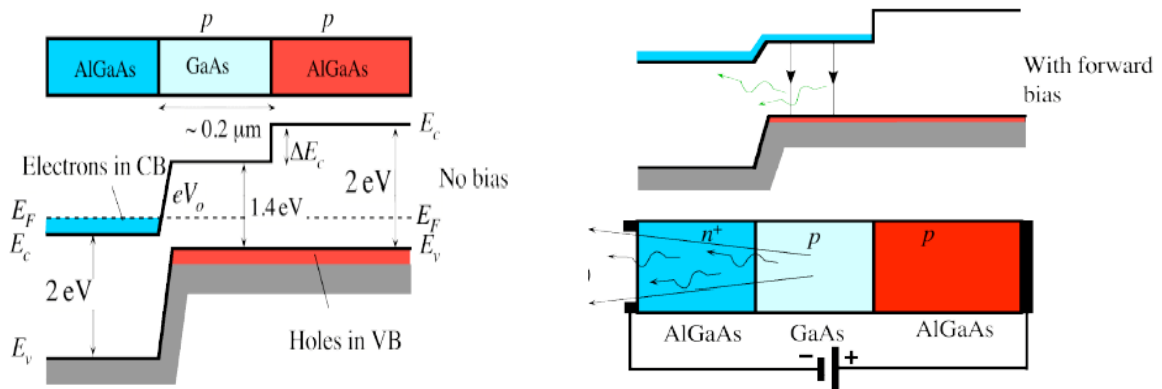
8. (i) From the electron configurations:

${}^7\text{N}$: $[\text{He}]2s^2 2p^3$; ${}^{31}\text{Ga}$: $[\text{Ar}]3d^{10} 4s^2 4p^1$; ${}^{49}\text{In}$: $[\text{Kr}]4d^{10} 5s^2 5p^1$; ${}^{48}\text{Cd}$: $[\text{Kr}]4d^{10} 5s^2$,

we can construct the bonding mode Cd-doped $\text{In}_x\text{Ga}_{1-x}\text{N}$ as shown in Figure Sol6-8(i). Cd contributes only 2 electrons bonding with its near neighbor N. Around each Cd atom, there is one bond with an electron missing and therefore a hole. Hence, it belongs to *p*-type. **(2 pts)**

(ii) Curve (a) in Figure HW6-4 is the calculated band gap using Eqn. 3, while the other one is the emission energy level of this material. Consider the band diagram of a *p*-type semiconductor, one can argue that it is possible for

$h\nu = E_c - E_a = E_g - (E_a - E_v) := E_g - \Delta E_{av}$. For instance, $E_a - E_v = 0.550\text{eV}$ as in Cd-doped GaN. **(4 pts)**



9. Refer to Kasap §6.9.2. **(+5 pts)**