Series - Electronic and optical semiconductor devices

Series 2 - Basic notions of semiconductor physics - two level system

Exercise 1

① Silicon (Si)

Number of atoms / conventional cubic cell (diamond structure):

$$N_{Si\,at./cell} = 8 \times 1/8 + 6 \times 1/2 + 4 \times 1 = 8$$

(corner of cubic cell; center of the faces; internal to the cell)

Cube edge of length a (lattice parameter) $\Rightarrow V = a^3$

$$N_{at.} = 8/a^3 \sim 5.00 \times 10^{22}\ cm^{-3}$$

Density $\rho_{Si} = N_{at.} \times \frac{\text{atomic weight}}{N_A} = \frac{5 \times 10^{22} \times 28.09}{6.022 \times 10^{23}} \sim 2.33\ g.cm^{-3}$

② Gallium arsenide (GaAs)

$$N_{GaAs\,at./cell} = \underbrace{8 \times 1/8 + 6 \times 1/2}_{Ga\ (or\ As)} + \underbrace{4}_{As\ (or\ Ga)} = 8$$ (zincblende structure)

This system is made of two interpenetrating face-centered cubic (fcc) Bravais lattices (one for each type of atoms) with one of them displaced along the body diagonal of the cubic cell by one quarter of the length of the diagonal. Each atom has four atoms of the opposite kind as nearest neighbors which form the vertices of a regular tetrahedron. This structure is an example of a lattice with a basis, which must be so described both because of the geometrical position of the atoms and because two types of atoms occur.

$N_{at.} = 8/a^3 \sim 4.43 \times 10^{22}\ cm^{-3}$ (one half of Ga and one half of As)

$$\rho_{GaAs} = \frac{4.43 \times 10^{22} \times 144.64}{\textcircled{2} \times 6.022 \times 10^{23}} \sim 5.32\ g.cm^{-3}$$

② → cf. remark

Remark: the "2" at the denominator results from the fact that one mole of GaAs is made of 6.022×10^{23} atoms of Ga and 6.022×10^{23} atoms of As!

③ Gallium nitride (GaN)

Wurtzite structure (hexagonal cell) → two lattice constants

$$N_{GaN\,at./cell} = \underbrace{12 \times 1/6 + 2 \times 1/2 + 3 \times 1}_{Ga\ (or\ N)} + \underbrace{4 \times 1 + 6 \times 1/3}_{N\ (or\ Ga)} = 12$$

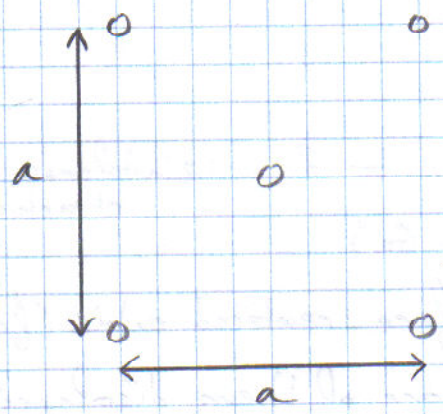
Volume of the hexagonal prism: $V = \frac{3\sqrt{3}}{2} a^2 c$

$$N_{at} \sim 8.76 \times 10^{22}\ cm^{-3} \qquad \rho_{GaN} = \frac{8.76 \times 10^{22} \times 83.73}{2 \times 6.022 \times 10^{23}} \sim 6.09\ g.cm^{-3}$$

Exercise 2

(100) plane of GaAs

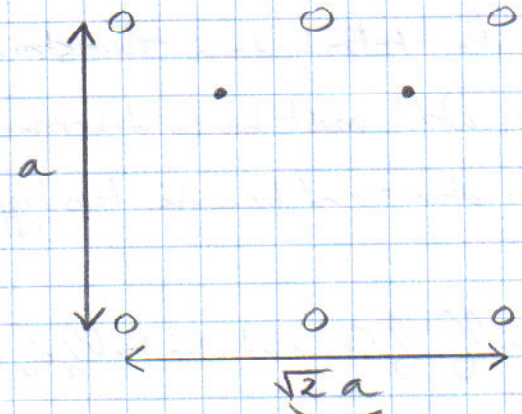
Notations: ○ Ga • As



$$N_{at./face} = 1 + 4 \times 1/4 = 2$$

$$N_{at.} = 2/a^2 \sim 6.26 \times 10^{14}\ cm^{-2}$$

(110) plane of GaAs

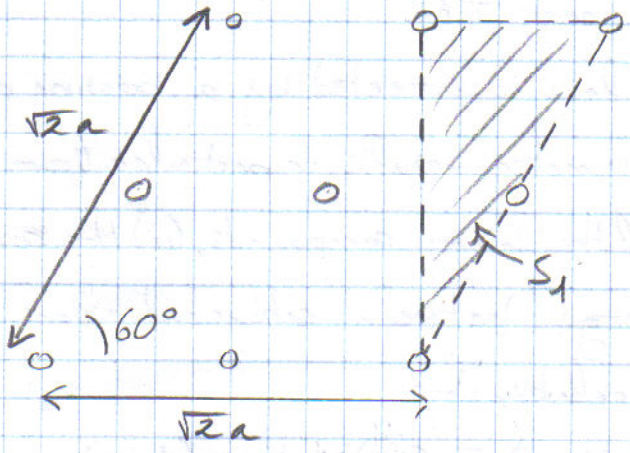


$$N_{at./face} = \underbrace{2}_{As} + \underbrace{2 \times 1/2 + 4 \times 1/4}_{Ga} = 4$$

$$N_{at.} = 4/(\sqrt{2} a^2) \sim 8.91 \times 10^{14}\ cm^{-2}$$

→ diagonal of one of the faces of the cube

(111) plane of GaAs

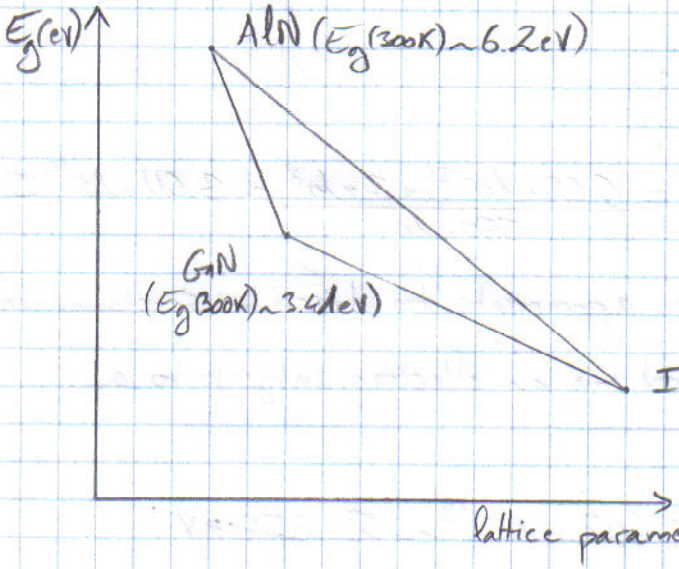


$N_{at./face} = 1 + 4 \times 1/4 + 4 \times 1/2 = 4$

$N_{at} = 4/(4S_1) = 1/S_1$

$S_1 = \frac{\sqrt{3}}{4} a^2 \Rightarrow N_{at} \sim 7.23 \times 10^{14}\ cm^{-2}$

Exercise 3



Ternary compounds allow to transit gradually from one binary compound to the other by varying the atoms of the column III (for III-V semiconductors here!)

⇓

We could also imagine keeping atoms of column III and change only those of column V (GaN → GaAsN → GaAs)

The $In_xGa_{1-x}N$ alloy makes thus the link between InN and GaN ($x \in [0,1]$). Vegard's law accounts for the transition between the two binary compounds of interest assuming a linear interpolation. (This would be also true if switching from Si to Ge by considering the binary compound SiGe).

We will thus get: $E_{In_xGa_{1-x}N} = x E_g(InN) + (1-x) E_g(GaN)$

For $x = 0.3 \Rightarrow E_{In_{0.3}Ga_{0.7}N} = 0.3 \times 0.65 + 0.7 \times 3.41 = 2.582$ eV

$x = 0.65 \Rightarrow E_{In_{0.65}Ga_{0.35}N} = 1.616$ eV

The ternary compound InGaN theoretically allows covering an energy range from the near UV down to the near IR.

In most cases however, Vegard's law is corrected by a bowing parameter which is phenomenological. This parameter results in particular from (i) the differences in the lattice parameters of the binary compounds, (ii) the conduction band offset, (iii) the binding energy between cations and anions.

In this latter case, we get the relationship:

$$E_{In_xGa_{1-x}N} = x E_g(InN) + (1-x) E_g(GaN) + b x(1-x)$$

b can be $>$ or <0.

Exercise 4

$\lambda = 550\,nm$, $E = h\nu = \frac{hc}{\lambda}$ $\qquad E = \frac{6.62\times10^{-34}\times 3\times10^{8}}{550\times10^{-9}} \sim 3.611\times10^{-19}\,J$

The electron-volt is a unit much more appropriate to describe semiconductors.

$1\,eV = 1.602\times10^{-19}\,J$ (energy acquired by an electron subject to a potential of 1V)

$E(eV, \lambda = 550\,nm) = 3.611\times10^{-19}/1.602\times10^{-19} \sim 2.254\,eV$

$1\,nm = 10^{-7}\,cm$

$\lambda = 550\,nm \Rightarrow (550\times10^{-7})^{-1}\,cm^{-1} = 18181.81\,cm^{-1}$

$\Rightarrow 1\,eV \leftrightarrow 8067.5\,cm^{-1}$

Wavenumbers are usually expressed in cm^{-1} and are commonly used to describe energy transitions in the infrared (vibrational spectroscopy) and to define energy shifts in Raman spectroscopy (separation of a mode from the laser line → case of optical phonons (acoustic phonons ≡ Brillouin spectroscopy).

Exercise 5: Determination of the eigenenergies of a two-level system

Preliminary note: W being a hermitic matrix, it implies that W_{11} and W_{22} are real (general case). In addition, we have $W_{12} = W_{21}^*$.

In the absence of any coupling, E_1 and E_2 are the eigenenergies of the system and $|\psi_1\rangle$ and $|\psi_2\rangle$ are stationary eigenstates. The problem will consist in quantifying the modifications resulting from the introduction of the coupling term W.

Consequences arising from the coupling

1) When measuring the energy of the system, one can only get one of the eigenvalues E_+ or E_- of H which generally differ from E_1 and E_2. The first step thus consists in calculating E_+ and E_- as a function of E_1 and E_2 and of the matrix elements W_{ij} of W.

2) $|\psi_1\rangle$ and $|\psi_2\rangle$, being not in most cases eigenstates of H, are not stationary states anymore. If, for example, the system is at $t=0$ in the $|\psi_1\rangle$ state, there is a given probability $\mathcal{P}_{12}(t)$ to find it at time t in the $|\psi_2\rangle$ state. W induces then transitions between the two unperturbed states, hence the name of coupling term (between $|\psi_1\rangle$ and $|\psi_2\rangle$) given to W. In the following, we will only consider the static aspect of the coupling. Note that the dynamical aspect gives rise to Rabi oscillations (Isidor Rabi (USA) got the Nobel Prize in Physics in 1944: "for his resonance method for recording the magnetic properties of atomic nuclei".

1- In the $\{|\psi_1\rangle, |\psi_2\rangle\}$ basis, the matrix H can be written:

$$(H) = \begin{pmatrix} E_1 + W_{11} & W_{12} \\ W_{21} & E_1 + W_{22} \end{pmatrix} \quad \text{(General case)}$$

The eigenvalues of the system are obtained by solving the characteristic

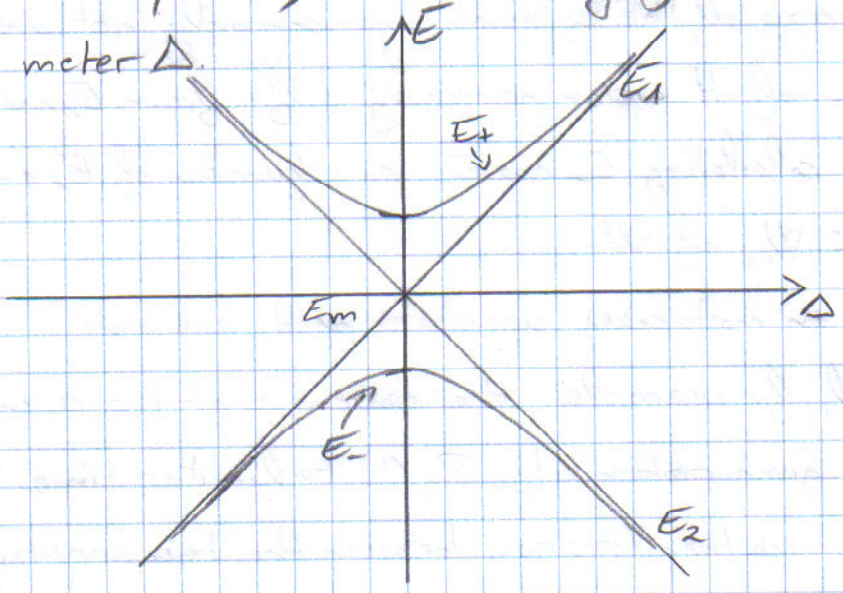
equation $\det[(H)-\lambda I] = 0$

We then get: $E_\pm = \frac{1}{2}(E_1 + W_{11} + E_2 + W_{22}) \pm \frac{1}{2}\sqrt{(E_1+W_{11}-E_2-W_{22})^2 + 4|W_{12}|^2}$

which simplifies in the case of a purely diagonal matrix into:

$E_\pm = \frac{1}{2}(E_1 + E_2) \pm \frac{1}{2}\sqrt{(E_1-E_2)^2 + 4|W_{12}|^2}$ i.e. $E_\pm = E_m \pm \sqrt{\Delta^2 + |W_{12}|^2}$

2- It is immediately seen from the previous equation that the dependence of E_+ and E_- on E_m is extremely simple. A change in E_m simply corresponds to change the origin of the energy axis. As a consequence, we will only focus on to the influence of the parameter Δ.



When Δ varies, E_+ and E_- follow the two branches of a symmetrical hyperbola with respect to the coordinate axes. The two straight lines ascribed to unperturbed levels are the asymptotes of the hyperbola.

The points nearest to E_m are split by an energy equal to $2|W_{12}|$, the so-called "Rabi splitting"

In the absence of any coupling, the levels will cross at the origin.

When the coupling term is "on", the unperturbed levels repel each other and we get an anticrossing.

This anticrossing behavior is often met in semiconductor physics and gives rise to new eigenstates corresponding to composite-particles or quasi-particles. We can cite among others: polarons resulting from the coupling between electron and optical phonons (≡ lattice distortion), optical polaritons (≡ optical phonon-photon coupling), exciton polaritons (exciton-photon coupling