EEE6212 exam

Model solutions for 2015/2016 exam (identical to 2014/2015 resit)

Q1a: The elements silicon (Si), phosphorus (P) and gallium (Ga) have numbers 14, 15 and 31 in the periodic table of the elements. The lattice parameters are very similar (a_{Si}=0.543nm, a_{GaP}=0.545nm). Explain the similarities and differences between the crystalline semiconductor materials Si and GaP qualitatively with respect to the following aspects:

  (i)   crystal structure;
  (ii) F_{002} structure factor;
  (iii) covalence bonding /ionicity;
  (iv)   size of bandgap;
  (v)   type of bandgap;
  (vi)   average atomic number;
  (vii) density.

   [7 points]

   Solution:
   Si has diamond structure, GaP has zinc blende (sphalerite) structure.
   As a consequence F_{002}=0 for Si (which is purely covalent) while it is large for GaP (which is ionic in bond character);
   Si has a small-medium indirect bandgap (1.12eV), GaP has a large indirect bandgap (2.26eV).
   The average atomic number of GaP is $\langle Z \rangle_{GaP}$=½(15+31)=23 > 14=Z_{Si}.
   and due to the larger $\langle Z \rangle$, at similar *a* value, GaP also has a slightly higher density.

Q1b: Sketch a three-dimensional view of the unit cell of a gallium phosphide crystal with all atoms in the cell. Label the origin and the directions of the basic unit cell vectors. Mark the [111] and the [$\bar{1}$11] directions. Calculate for a lattice parameter of *a*=0.545nm
  (i)   the atomic number density in units of atoms/nm^3,
  (ii) the atomic areal density of the (011) surface in atoms/nm^2,
  (iii) the spacings of the {111} lattice planes.

   [7 points]

   Solution:
   Sketch of a typical sphalerite unit cell with 8 atoms within the cubic unit cell (2 points). Correct axes labels with right-handedness <u>and</u> consistent markings of directions give another point each.
  (i) $n=8/a^3$= 49.4 nm^{-3}
  (ii) $N=(2+2)/(a \times \sqrt{2}\,a)=4/(a^2\sqrt{2}) = 9.52$ nm^{-2}
  (iii) $d_{111}=a/\sqrt{(1^2+1^2+1^2)}=a/\sqrt{3} \approx 0.31$nm

Q1c: Silicon carbide (SiC) exists in hundreds of different crystal modifications many of which are related in terms of stacking sequences and called polytypes. β-SiC (also called 3C-SiC) is cubic with

zinc blende structure and has a lattice constant of a_{cub}=0.436nm. α-SiC (also called 6H-SiC) is hexagonal with lattice parameters of a_{hex}=0.308nm and c_{hex}=1.512nm, where 3 wurtzite-type units are stacked on top of each other along the c-axis but rotated with respect to each other about the c- axis. Calculate and compare the Si-C bond lengths in α-SiC and β-SiC.

[*6 points*]

Solution:
cubic β-SiC (zinc blende or sphalerite):
4 bonds in a line make up the body diagonal of the cube, hence d_{bond}=¼ √3 a_{cub}=0.189nm.
hexagonal α-SiC:
In the wurtzite sub-unit the bond length along the (0001) direction is given by the displacement of the two hexagonal sub-lattices, i.e. 3/8 $c_{wutzite}$
In α-SiC three of these sub-units stacked on top, so $c_{wutzite}$ =c_{hex}/3.
Therefore the bond length is 1/8 c_{hex} = 0.189nm.
Both values are identical.

Q2a: Tetragonal crystals can be found as minerals in nature (e.g. rutile, anatase, zircon) and in strained semiconductor thin films. Name all possible symmetry elements of a tetragonal crystal (apart from the identity operation). For each, identify where they are and how many there are.

[*6 points*]

Solution:

1 tetrad (*4* or C_4) along [001] through (½½0), i.e. perpendicular to the square base faces,

4 diades (*2* or C_2) at height z=½ through the midpoints of opposite edges and at 45° to these, i.e. through the midpoint of the faces,

5 mirror planes (*m*): (200), (020), (110), (1-10) and (002)

Q2b: (i) Draw a three-dimensional sketch of the wurtzite lattice.

(ii) How many atoms are there effectively per unit cell?

(iii) State their relative coordinates.

(iv) In your sketch, indicate all tetragonal interstices commencing in the (*x,y*)-plane and pointing upwards (along *z*-direction). Which of them are occupied by atoms?

[*5 points*]

Solution:

1 point for a complete sketch of the unit cell with all 4 atoms in it. Their relative positions are: (0,0,0), (⅓,⅔,½), (0,0,⅜) and (⅓,⅔,⅞) (2 points in total for all four positions).

There are two tetrahedra formed by 3 atoms in the basal face, pointing upwards. One ends in point (⅓,⅔,½) where an atom sits and is occupied. The other ends in point (⅓,⅓,½) where no atom sits and is unoccupied (=empty).

Q2c: All possible unit cells can be divided into 7 crystal systems according to their shape, which comes from underlying point symmetry. These can be further divided into Bravais lattices and space groups. While most semiconductors are either cubic or hexagonal in bulk form, during epitaxy the unit cells can adopt different shapes of reduced symmetry.

(i) Define what a Bravais lattice is.
(ii) Explain the four types of space centering.
(iii) Explain why there are not 7×4=28 Bravais lattices, but only 14.
(iv) Why is there no tetragonal *C* lattice?

[4 points]

Solution:

Bravais lattice = lattice type classification due to combinations of point symmetry (7 lattice systems) with 4 space centerings (primitive P, base centred C, body centred I, face centred F) for all but the trigonal/rhombohedral system.

Space centering = gives spatial position of different, second atom within unit cell, if it exists

There are only 14 instead of 7*4=28 Bravais lattices because half of the combinations of crystal and centering can be represented by other combinations where the unit cell actually has a lower symmetry.

There is no tetragonal *C* lattice because this can also be described by a smaller tetragonal *P* lattice, rotated by 45° around the *c*-axis (this was explicitly considered in the tutorials).

Q2d: Dislocations are common extended defects in semiconductors. Define what the Burgers vector **_b_** and line direction **_u_** are. Sketch an edge dislocation and include **_b_** and **_u_** in your sketch. Using your sketch, explain how the scalar product **_b_**·**_g_** can be used in dark-field imaging with reciprocal lattice vector **_g_** to determine the Burgers vector direction.

[5 points]

Solution:

Define the line direction **_u_** as the line or lattice plane that defines the end of the row of atomic displacements and the Burgers vector **_b_** as vector that describes the closure fault when a complete circuit around the dislocation core is made.

In the case of an edge dislocation we get **_b_** ⊥ **_u_**, hence **_b_**·**_u_** =0.

In a dark-field image with **g,** **_b_**·**_g_** =0 means the dislocation will be invisible, so from 3 different (non co-planar) **_g_**-vectors, the direction (but not the magnitude) of **_b_** can be determined.

Q3a: Give an example of and provide a suitable sketch for types of lattice defects in zero, one, two and three dimensions of space.

[8 points]

Solution:
Naming and sketch each yield 1 point.

0-dimensional defects: vacancy, dopant, interstitial, Schottky defect, Frenkel-pair, colour centre
1-dimensional defects: edge or screw dislocations, mixed dislocation, partial dislocation
2-dimensional defects: stacking fault, special grain boundary (APB, IDB, low index GB)
3-dimensional defects: pores, precipitates, clusters, general phase boundaries between domains

Q3b: The electron density in a heavily p-doped semiconductor at low temperature may be written as

$$p=\sqrt{\tfrac{1}{2}N_v N_a} \exp[-(E_a-E_v)/(2k_B T)] \qquad \text{(equation 1)}$$

Describe how you can extract the magnitude of the energy of the acceptor level relative to the valence band edge using a series of conductivity measurements.

[5 points]

Solution:

In general, conductivity is $\sigma=e(n\mu_n+p\mu_p)$ where for p-doping only the 2nd term counts, i.e. $\sigma\approx ep\mu_p$. As the elementary charge e and the mobility μ are constants for a given material, σ has the same temperature dependence as given in the expression for the electron density, so

$\sigma \propto \exp[-(E_a-E_v)/(2k_B T)]$,

Hence, $\ln \sigma \propto -(E_a-E_v)/(2k_B T)$,

i.e. a plot of $\ln \sigma$ vs. $1/T$ should have a slope of $-(E_a-E_v)/(2k_B)$.

NB: In a decadic plot, where $\ln \sigma= 2.3 \log \sigma$, the slope of $\log \sigma$ vs. $1/T$ is 2.3 times lower, i.e. given by $-(E_a-E_v)/(4.6k_B)$.

Q3c: Provide a sketch of the cross-section through a p-channel MOSFET device used for high-speed switching or high-frequency amplification.

   (i)   Name all terminals.
   (ii) Indicate the sign and strength of doping levels in all relevant regions.
   (iii) Explain the role of channel length and width and gate oxide type and thickness.
   (iv) Explain the difference between enhancement and depletion mode and give an application example of each.

[7 points]

Solution:

The cross-sectional sketch gives 1 point. Correct identification of source, gate and drain contacts gives 1 point. Correct doping levels (substrate: n, source: p^+, drain: p) gives 1 point. Critical device dimensions are (full answer gives 2 points):

1. channel length (-> speed and ultimately transition frequency),
2. channel width (-> current),
3. gate oxide dielectric constant & thickness (-> capacitance and break-through voltage)

more elaborate alternative solutions for the second half would involve the width/length aspect ratio but are not necessary.

Enhancement-mode MOSFETs are normally OFF at zero gate–source voltage and need to be turned on by pulling the gate voltage either higher than the source voltage, for NMOS, or lower than the source voltage, for PMOS. They are commonly used as switching elements. Depletion-mode MOSFET are normally ON at zero gate–source voltage and need to be turned off by applying a gate voltage. Such devices are used as load resistors in logic circuits (full answer gives 2 points).

Q4a: Consider the force on an electron by the electric field in a crystal and from this derive an expression for its drift velocity. Define mobility and describe how the mobility of a semiconductor may be increased by the choice of material and synthesis methods.

[5 points]

Solution:

$v_d = a \times t = F/m^* \tau = -eE\tau/m^*$

where a is the acceleration, $t=\tau$ the time between two scattering events, F the force, m^* the effective mass, E the electric field strength and e the electron charge.

The mobility is defined as the ratio

$\mu = \| v_d/E \| = e\tau/m^*$

From this follows that for high mobility materials with low m^* should be used.

Also, τ should be maximised by using high purity crystalline material and/or spatially separating electrons and holes by forming 2-dimensional electron or hole gases (2DEG/2DHG) at doped hetero-interfaces.

Q4b: Write down Shockley's equation for the current of a diode, defining all parameters used. Sketch a typical diode characteristic and name its three important regions.

[6 points]

Solution:

$I_d = I_S [\exp (eV_d/(kT) - 1]$ is known as Shockley's diode equation.

I_d is the diode current, I_S the saturation current, e the electron charge, V_d the voltage, k Boltzmann's constant and T absolute temperature. The characteristic curves should look like this:
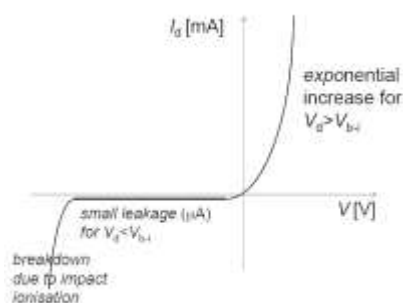
Q4c: With the help of a suitable sketch, explain the difference between a type-I and a type-II band alignment between two semiconductors. Which is better for application as light-emitting device, and why?

[4 points]

Solution:

In a type-I alignment, conduction and valence band offsets are anti-correlated, in a type-II alignment they are correlated (2 points for proper sketches). As a result, in type-I band alignment electrons and holes are both located in the same material, namely that with the smaller bandgap, while in type-II the electrons are located in one and the holes in the other material. In result, radiative recombination in type-II semiconductors is much less likely, so the optical output is reduced. Type-I alignment is thus preferred for optoelectronic devices.

Q4d: The relationship between the lifetime τ of an excited electron state and electron density n is often modelled as

$$1/\tau = A + Bn + Cn^2 \qquad \text{(equation 2)}$$

Explain the physical meaning of the term what the parameters A,B and C describe. Which of the terms describes optical emission?

[5 points]

Solution:

$1/\tau$ is the decay probability of the excited electron state.

A describes non-radiative contributions due to defects, e.g. dislocations.
B describes radiative recombinations of electrons and holes across band-gap, producing light (or X-rays).
C describes non-radiative Auger recombination (a 3 electron process), producing free electrons.

So the correct answer is the middle term, Bn.

Q5a: Identify both physical principles that the function of every LASER system relies on. Describe one possible technical implementation of each. Explain why you need more than just two energy levels to make a LASER.

[6 points]

Solution:

Pumping (optically, electrically or by HF coupling) creates a *population inversion* in a system with at least three energy levels where the topmost is long-lived, which is necessary for stimulated, coherent emission.

Then a cavity with mirrors (one partially transparent or with a small hole to couple out a fraction of the light) acts as a resonator which provides optical *feedback* to amplify the radiation.

In order to get population inversion, you need to get more electrons into an upper energy level than there are in a lower energy level. Due to excitation and de-excitation being proportional to the number of initial states, if one starts with more electrons in the lower level, the harder one pumps the more electrons will reach the upper level, until excitation and de-excitation rates match in equilibrium. Then the maximum occupancy in the upper level is the same as in the lower level, i.e. there can never be more electrons in the excited than in the ground state with just transitions between two levels. So at least a third level will be needed to pump to from the ground state. From this upper third level the electrons quickly then go to a slightly lower, long-lived level from where they can return to the ground state.

Q5b: Using schematic diagrams describe absorption, spontaneous and stimulated emission processes in a semiconductor, and define their rates.

[6 points]

Solution:

This is pure bookwork. One point each for a proper sketch showing valence and conduction bands and the corresponding electron before and after the transition for the three processes.

One point each for writing down rate equations with correct Einstein coefficients for transitions between upper levels of density N_2 and lower levels of density N_1 and spectral density s

absorption 1>2: $dN_2/dt = B_{12} \times s \times N_1$

spontaneous emission 2>1: $dN_2/dt = -A_{21} \times N_2$

stimulated emission 2>1: $dN_2/dt = -B_{21} \times s \times N_2$

Q5c: Define the external quantum efficiency of a photo detector as function of photocurrent, incident power P_{opt} and detector area A. Define all parameters you use. Consider that the incident light intensity falls off exponentially within the detector with distance z from its surface and that the generation rate for electron-hole pairs is given by the expression

$$g(z) = (1-R)P_{opt}/(Ahf) \exp(-\alpha z) \qquad \text{(equation 3)}$$

where R is the reflectivity of the surface and α the absorption coefficient.

From this, calculate the photocurrent by depth integration over the depletion region width d.

Insert this into your expression for the external quantum efficiency.

Interpret the results in terms of optimal choice of material reflectivity and thickness.

[8 points]

Solution:
$\eta =$ # electrons produced / # photons incident $= (I_{photo}/e) / [P_{opt}/(hf)] = I_{photo} \, hf / (eP_{opt})$ (2 points)
where I_{photo} is measured photocurrent and P_{opt} the incident optical power. The photon energy is hf. The detector area is not relevant! (1 point)
$I_{photo} \quad = eA \int_0^d g(z) \, dz$
$\qquad = e(1-R) P_{opt}/(hf) \int_0^d \exp(-\alpha z)$
$\qquad = e(1-R) P_{opt}/(hf) [1 - \exp(-\alpha d)]$ (3 points)

Insertion into the first equation yields
$\eta = (1-R)[1 - \exp(-\alpha d)]$ (1 point)
This shows that one wants a material with low reflectivity and sufficient thickness so ideally the expression $\exp(-\alpha d) \longrightarrow 0$ and all light is absorbed. (1 point)

Q6a: Explain what is meant by Density of States (DOS). Sketch and compare the DOS for a bulk semiconductor and for a quantum dot. Which is more suitable for applications in optoelectronics? Give reasons for your decision, taking into account both the form of the DOS and commenting on the absolute number of carriers available.

   [5 points]

Solution:

The DOS describes the number of allowed electronic states per unit interval of energy.

The DOS of bulk material has the form of a square root function, similar to the $k=2\pi\sqrt{(2m^*E)}/h$ relationship for a free electron.

The DOS of a quantum dot is a series of spikes (δ-functions).

The DOS of a quantum dot has the advantage that more states of the same energy are available, so lines in emission or absorption spectra will be sharper (closer to mono-energetic, corresponding to a specific colour).

Bulk of course has more absolute volume, so can provide more absolute carriers. This may be compensated partially by repeated growth of layers of quantum dots in vertical stacks.

Q6b: Sketch the amplitudes of the electron wavefunctions for the four lowest energies of an electron confined in an infinitely deep quantum well (QW).
Derive an explicit expression for the energy levels, starting from the model that considers bound particles as standing waves.
Calculate and compare the ground level ($n=1$) confinement energies in meV of electrons and holes in GaAs quantum wells of width $l=10$nm and $l=3$nm, assuming the following constants:
Planck's constant: $h=6.6261 \times 10^{-34}$ Js,
$\hbar=h/(2\pi)$,
elementary charge: $e=1.6022 \times 10^{-19}$ As,
electron rest mass: $m_0=9.1095 \times 10^{-31}$ kg,
effective electron mass: $m_e^*= 0.063m_0$,
effective heavy hole mass: $m_{hh}^*=0.51m_0$,
effective light hole mass: $m_{lh}^*= 0.082m_0$,

   [7 points]

Solution:
The sketch should show wavefunctions of the form of sine or cosine functions, with nodes at the quantum well begin and end, where $n=1,2,3,4$ would depict $n/2$ full wavelengths. (1 point)

If one considers the electron as a wave with wavelength λ, then the QW width is $l=n\ \lambda/2$. (1 point)

If one starts with the classical $E=p^2/(2m^*)$ and inserts $p=\hbar k=hk/(2\pi)$ and the above, one obtains
$E= \hbar^2k^2/(2m^*) = (\hbar\pi n)^2/(2m^*\ l^2)$ (1 point)

Inserting numbers for the 10nm quantum well yields: $E_{1,e}=60$meV, $E_{1,hh}=7$meV, $E_{1,lh}=46$meV
Inserting numbers for the 3nm quantum well yields: $E_{1,e}=663$meV, $E_{1,hh}=82$meV, $E_{1,lh}=510$meV
(3 points, ½ for each correct number)

The confinement energies for electron and light hole are quite similar, because their masses are similar. The confinement energy for the heavy hole is negligible in the wide QW.
Narrowing the quantum well from 10nm to 3nm, i.e. by 30%, increases the confinement energies by more than on order (factor $1/0.3^2=11.1$). (1 point)

Q6c: Define what an exciton is.
Sketch an excitonic transition in a direct-gap semiconductor and write down an equation for the line energy observed in a photoluminescence experiment that includes the bandgap, the ground level energies of electron and hole and the exciton binding energy.
Calculate and compare the excitonic binding energies for the ground states ($n=1$) in the two following semiconductors, using the Rydberg constant of $R_y=13.6$eV:
   GaAs with $m_e^*=0.063m_0$, $m_{hh}^*=0.51m_0$, relative permittivity: $\varepsilon_r=14.4$;
   Si with $m_e^*=0.98m0$, $m_{hh}^*=0.49m_0$, relative permittivity: $\varepsilon_r=11.7$.
Assume a phonon energy is given by $E_{phonon}=k_BT$ where $k_B=1.38$ x 10^{-23} J/K is the Boltzmann constant and $e=1.6022 \times 10^{-19}$ As the elementary charge.
Decide whether the excitons will be stable at room temperature.

   [8 points]

Solution:

An exciton is a bound electron-hole complex, held together by electrostatic attraction of their opposite charges. This is called a quasi-particle. (1 point)

The sketch would show, bottom to top, the energy levels of E_h, E_v, E_c, E_e, where $E_g=E_c-E_v$ (1 point)

The line energy in PL is: $E_{PL}=E_g +E_e + E_h - \|E_X\|$, where $E_g=E_c-E_v$ is the bandgap and E_X the (negative) binding energy of the exciton complex. (1 point)

$E_X = -M/m_0 R_y / (\varepsilon_r^2 n^2)$ where $M=(1/m_{e*} + 1/m_{h*})^{-1}$ is the effective mass of the exciton (1 point) (reduced mass in system of common centre-of-mass system). The exciton mass to electron rest mass ratio is given as

$M/m_0= 0.056$ (for GaAs) and 0.327 (for Si). (1 point)

Insertion into above equation gives

$E_X \approx 4$meV (for GaAs) and ≈ 32meV (for GaAs) (1 point)

The phonon energy near room temperature ($T=300$K) is $E_{phonon}=k_BT=26$ meV. (1 point)

Excitons with a binding energy below that value (i.e. here: GaAs) are unstable, the exciton in Si will be <u>just</u> stable. (1 point)