

(a)(i) – generally well answered, occasional misreading of the graph, and some lack of explanation for direct transition. (a)(ii) – generally well answered, some confusion between electrons and holes. (a)(iii) – generally well answered, some focused on properties not relevant to optoelectronics. (a)(iv) – Generally well answered, occasional mix up of colours. (b)(i) – Sometimes lack of detailed description of density of states, or lack of clarity on length scales. (b)(ii) – Typically well answered, but occasionally the total emission energy was used as the confinement energy, rather than the difference between the bandgap and the emission energy. (c) – Occasional mix up between decrease and increase in bandgap with temperature, implications to telecoms generally understood. (Mean 13.96/20)

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jaa59

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Question 1

(a) (i) [15%]

- Top of the valence band is at 0 eV. Conduction band minimum is at ~ 1.8 eV. Bandgap ≈ 1.8 eV.
- Direct Bandgap. Top of the valence band and bottom of the conduction band occur at the same k-value, the gamma point.

(a) (ii) [15%]

- **Effective mass:** Curvature (second derivative) close to the conduction band minimum is greater than valence band curvature ($m^* \propto 1/\text{curvature}$). Electron mass is lighter than the hole mass.
- **Mobility:** In the Drude model $\mu \propto 1/m^*$, (from $\mu = e\tau/m^*$). Electron mobility is higher.

(a) (iii) [10%]

- **Efficiency:** Direct bandgap allows efficient radiative recombination. Si is indirect semiconductor, radiative recombination requires phonon scattering to provide the momentum mismatch.
- **Applications:** 1.8 eV corresponds to visible light, enabling display applications. Si is a near IR emitter.

(a) (iv) [10%]

$\lambda = hc/E$ or alternatively noted during the lectures

$$\lambda = 1240 \text{ nm} \frac{1 \text{ eV}}{E [\text{eV}]} = 1240 \text{ nm} \frac{1 \text{ eV}}{1.8 \text{ eV}} \approx 689 \text{ nm}$$

Colour: Red.

(b) (i) [15%]

- Confinement of a particle in dimensions comparable the wavelength of the particle, i.e. the de Broglie wavelength (or alternatively the exciton Bohr radius for excitons), leads to quantisation of energy levels ($E \propto 1/D^2$). Only certain half integer numbers of full oscillations of the wavefunction are allowed due to boundary conditions.
- Continuous parabolic DOS of bulk material becomes discrete $E-k$ values, for given values of n (or n_x, n_y , and n_z).

(b) (ii) [20%]

Shift in emission from 1.8 eV to 2.0 eV is required.

$$E = E_g + \Delta E_{\text{confinement}} - E_{\text{Coulomb}}$$

Assumption: Confinement energy scales with $1/D^2$, while Coulomb energy scales with $1/D$, so for small dots Coulomb energy is neglected. Confinement energy $\Delta E = 2.0 - 1.8 = 0.2$ eV.

Need to use $n_x = n_y = n_z = 1$ to calculate the lowest energy confined state i.e. closest to the bandgap energy.

Can calculate separate electron and hole contributions using the given equation and their respective effective masses. Assumption: It is required to estimate the effective mass of the holes. This could be that m_h is larger than the electron mass, as with answer to aii above. Assuming equal electron and hole mass is acceptable for simplification.

$$\Delta E = \frac{3h^2}{8D^2m_e^*} + \frac{3h^2}{8D^2m_h^*} = \frac{3h^2}{8D^2m_{eff}^*}$$

Where m_{eff}^* is the reduced effective mass.

Convert 0.2 eV to Joules: $0.2 \times 1.6 \times 10^{-19} = 3.2 \times 10^{-20}$ J.

$$D = \sqrt{\frac{3h^2}{8m_{eff}^*\Delta E}}$$

For large hole mass assumption (e.g. $m_h^* = 0.5 m_0$)

$$D \approx \mathbf{8.5 \text{ nm}}$$

For equal hole mass assumption (e.g. $m_h^* = 0.1 m_0$)

$$D \approx \mathbf{10.6 \text{ nm}}$$

Alternatively they can state the assumption that the hole effective mass $m_h^* \gg m_e^*$, which means that the majority of the confinement energy is due to the electron since $\Delta E \propto 1/m$, leading to:

$$\Delta E \approx \frac{3h^2}{8D^2m_e^*}$$

$$D = \sqrt{\frac{3h^2}{8m_e^* \Delta E}} = \sqrt{\frac{3(6.63 \times 10^{-34})^2}{8(0.1 \times 9.11 \times 10^{-31})(3.2 \times 10^{-20})}}$$

$$D \approx \sqrt{56.5 \times 10^{-18} \text{ m}} \approx \mathbf{7.5 \text{ nm}}$$

(c) [15%]

- As the lattice constant of a crystalline semiconductor increases the bandgap E_g typically decreases. As T increases the average separation between atoms increases leading to a decrease in bandgap.
- Laser wavelength λ therefore increases (red-shifts) with increasing temperature. Such temperature changes could be present due to electronic power dissipation in a device or system, or environmental temperature variations.
- In telecommunications, this causes crosstalk between channels if multiple wavelengths are used to encode different data streams (wavelength multiplexing).

(a)(i) – generally well answered, sometimes the comparison to $k_B T$ was missed. (a)(ii) – generally well answered, occasionally no explanation to choice of dopant. (b)(i) – Definition typically well answered, sometimes lack of clarity on implications to spectrum of light. (b)(ii) – Generally well answered, particularly if (a)(i) was answered correctly. (c) – Sometimes focused on high-k dielectrics alone rather than including discussion of channel/gate geometry e.g. finFET, or GAA structures. (d) – Often well attempted, mostly mix ups with different (non-2D) materials, occasional confusion between 2D material properties semiconductor/insulator/conductor etc. (Mean 13.11/20)

Question 2

(a) (i) [20%]

The ionization energy E_D for a shallow donor is estimated using the hydrogenic model:

$$E_D = 13.6 \text{ eV} \times \frac{m_e^*}{m_0} \times \frac{1}{\epsilon_r^2}$$

For ZnO:

Using $\epsilon_r = 7$ and $m_e^* = 0.24m_0$:

$$E_D = 13.6 \times \frac{0.24}{7^2} = \mathbf{67 \text{ meV}}$$

For InAs:

Using $\epsilon_r = 15.0$ and $m_e^* = 0.023m_0$:

$$E_D = 13.6 \times \frac{0.023}{15.0^2} = \mathbf{1.4 \text{ meV}}$$

Thermal energy ($k_B T$) at room temperature $\approx 26 \text{ meV}$.

- In **InAs**, $E_D \ll k_B T$, so dopants are fully ionized at room temperature (easy to dope).
- In **ZnO**, $E_D > 2k_B T$. Ideally, dopants should have $E_D \approx k_B T$ or lower for full activation. With $E_D = 67 \text{ meV}$, a significant proportion of the donors will not be ionized at room temperature.

ZnO is more difficult to dope n-type efficiently at room temperature due to the deeper donor level.

(a) (ii) [15%]

InAs consists of Indium (Group III) and Arsenic (Group V). To create an n-type semiconductor by substituting on the Indium (Group III) site, we need a donor element with one more valence electron.

- The substituent must come from Group IV.
- e.g. C, Si, Ge, or Sn.
- When replacing In (Group III), Group IV atoms provide one extra electron from the outer shell which becomes a free carrier when excited from the donor level (e.g. by thermal excitation at room temperature).
- (Note that substituting a Group V for the In site would technically be n-type doping but would lead to deep level donor states due to larger charge difference. This would not be efficient doping.)

(b) (i) [15%]

- An exciton is an electron-hole pair, bound by an attractive Coulomb force. It is electrically neutral and can move through the lattice. Its typical size is known as the exciton Bohr radius and ranges from the order of the lattice constant to 10's of nm.
- If binding energy E_b is large ($E_b > k_B T$), excitons are stable. Radiative recombination yields an emission peak slightly below the bandgap energy ($E_{\text{photon}} = E_g - E_b$). There may be additional peaks at higher energy associated with higher order excitons ($n = 2, 3, \dots$). Emission spectrum may be narrow due to a long exciton lifetime.
- If E_b is small ($E_b < k_B T$), thermal energy is large enough to break excitons. Emission in this case will be due to conventional band-to-band recombination with a photon energy equal to the bandgap energy.

(b) (ii) [20%]

Need to know that an exciton can be treated with the hydrogenic model but with a combined (“reduced”) effective mass incorporating both electron and hole mass. First, calculate reduced mass m_{eff} : $m_{\text{eff}} = \frac{m_e^* m_h^*}{m_e^* + m_h^*}$

For ZnO:

$$m_{\text{eff}} = \frac{0.24 \times 0.59}{0.24 + 0.59} \approx 0.17 m_0$$

$$E_b = 13.6 \text{ eV} \times \frac{0.17}{7^2} \approx 47 \text{ meV}$$

For InAs:

$$m_{\text{eff}} = \frac{0.023 \times 0.41}{0.023 + 0.41} \approx 0.022 m_0$$

$$E_b = 13.6 \text{ eV} \times \frac{0.022}{15.0^2} \approx 1.3 \text{ meV}$$

Conclusion: At 300 K, $k_B T \approx 26 \text{ meV}$. InAs ($1.3 \text{ meV} \ll 26 \text{ meV}$) dissociates; ZnO ($47 \text{ meV} > 26 \text{ meV}$) remains stable. Excitonic effects are relevant for ZnO.

(c) [15%]

- **(i) Physical Structure:** Shift from planar FETs to FinFET (or Gate-All-Around) for nodes below 20 nm. Channel is etched into either tall fins (FinFET) or narrow sheets (GAA). The 3D gate structure wraps around the channel, increasing electrostatic control due to the larger surface area of the capacitor relative to the channel cross-sectional area.
- **(ii) Gate Dielectric:** Quantum mechanical tunnelling is inescapable for atomically thin dielectric barriers (gate dielectrics). This caused a shift

from SiO_2 to high-k dielectrics (e.g., HfO_2 , ZnO_2 , Al_2O_3). Capacitance scales with dielectric constant (k or ϵ). This allows for a physically thicker layer to achieve the same capacitance while preventing quantum mechanical tunnelling.

(d) [15%]

- **Channel:** Examples include several materials from the transition metal dichalcogenides (TMD or TMDC) (e.g., MoS_2 , WSe_2). These are semiconductors with a bandgap of around $1 - 3$ eV. Bandgap essential for switching. Other examples could be black phosphorous, but TMDs often more stable under ambient conditions.
- **Gate Insulator:** e.g. Hexagonal boron nitride (h-BN). Wide bangap $\approx 4 - 6$ eV, so it is an insulating material. Atomically flat surface with no dangling bonds.
- **Source-drain contacts and gate electrode.** Main example would be graphene, although there are some metallic TMDs for example. High conductivity, which can be increased by increasing the number of layers, or by doping. Another benefit of graphene is the tunable work function by doping which can therefore be aligned with respect to the semiconductor.

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3) a) In a crystalline material the piezo- and pyro- electric properties are intrinsically linked to the symmetry of the lattice. If, on application of stress, the centres of the positive and negative ions do not change then there is no change in charge and a material does not exhibit piezo-electricity. The asymmetry giving rise to the piezo-electric effect can be intrinsic or generated by an external electric field.

Consequently it is only the 21 crystal structures that do not exhibit a centre of symmetry that can be piezo-electric. Of these 20 exhibit piezo-electric effects with one structure not being piezo-electric for geometric reasons beyond the scope of the course.

Of the 20 piezo-electric structures, 10 further exhibit pyroelectricity because they have an intrinsic dipole, in addition to lacking a centre of symmetry. There are two contributions to the pyro-electric. The first (dominant) is due to thermal disorder competing with polarization at increasing temperature while the second arises from the change in lattice parameters with temperature.

[20 %]

b)

i) The force is being applied perpendicularly to both polarisation and the electric field. This is, therefore, longitudinal mode where the relevant piezoelectric coupling coefficient is d_{31}

[10 %]

ii) From the basic piezoelectric equation of state $P_3 = d_{31} \sigma_1$ [basic relation expected to be able to recall or work out from memory]. This implies in the geometry shown that $Q/A = d_{31} F/a$.

From this we can write that $Q = d_{31} F A / a$.

[15 %]

iii) For numbers given we have $F = 0.02 \text{ N}$ $d_{31} = -274 \times 10^{-12} \text{ C/N}$ $A = 4 \times 10^{-4}$ and $a = 1 \times 10^{-5}$. Consequently, charge release is $2.19 \times 10^{-10} \text{ C}$

From Capacitor eqn $Q = CV$ so $V = Q/C$. In this case $C = \epsilon \epsilon_r A / t$ so $V = t Q / \epsilon \epsilon_r A$

This is $5 \times 10^{-4} \times 2.19 \times 10^{-10} / 8.85 \times 10^{-12} \times 3400 \times 4 \times 10^{-4}$ which gives a potential difference of 9.1 mV. This magnitude of signal is eminently reasonable for further amplification.

[20 %]

c) i) So this is a question of using the equations derived earlier with different values. Easier if we rewrite to $V = d_{31} F t / \epsilon \epsilon_r a$

which gives: $-25 \times 10^{-12} \times 0.02 \times 5 \times 10^{-4} / 8.85 \times 10^{-12} \times 14 \times 1 \times 10^{-5}$

which is 200 mV .

[15 %]

ii) The smaller piezoelectric constant in PVDF is more than compensated for by the smaller relative permittivity. The overall voltage responsivity of the device is therefore improved. It must be remembered, however, that the charge released is less due to the smaller piezoelectric co-efficient and thus with a real amplifier the realised performance will not be as good.

PZT contains lead which poses health and environmental concerns, especially given limits on the lead content of consumer facing devices. It is a hard ceramic which can be difficult to process, whereas PVDF can be easily produced as a thin film using polymer processing techniques which means there is scope for reducing thickness and thus “ a ” which would further increase the amount of charge released for a particular applied force. Alternatively, the PVDF element could be used with a small diaphragm to make a more compact microphone.

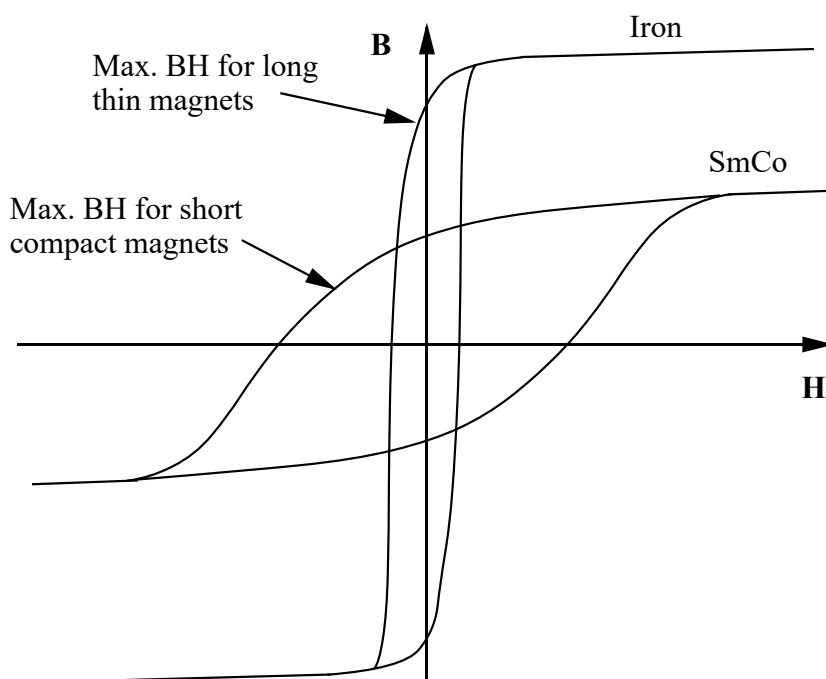
PVDF is also cheaper to make and to process than PZT-5.

[20 %]

4) (a) The magnetisation of a ferromagnet arises from alignment of spin in the atoms in the material. As the maximum number of Bohr magnetons available per volume to be aligned is a property of a material there is a limit to the magnetisation which is independent of sample size.

In a superconductor however, the magnetisation depends on a current loop and thus depends on the size of the sample as well as the maximum critical current available.

b) i) From the notes :



This question was very well answered on the whole with only a small number of attempts scoring less than 14. Most difficulty was experienced by candidates in providing a brief account of the origin of the demagnetisation field, some invoked the principle of continuity of the normal component of the B field at the surface of the magnet. While this is valid it does not, in and of itself, account for the existence of the demagnetisation field. (Mean 15.6/20)

A hard material has a larger coercive field which means it will robustly retain magnetic alignment after magnetisation.

[15 %]

ii) Important properties include the saturation magnetisation which is the field at which all the spins in the material are aligned (this isn't different between soft and hard materials) and the coercive field which is the field required to de-magnetise a magnetic material (large in a hard material and small in a soft material). Further properties include the Curie temperature above which magnetic ordering disappears (not a signature of a soft or hard material) and $(BH)_{\max}$ which is the maximum energy density in the magnetic field achievable when a permanent magnet is fabricated from a particular material (aim to maximise for a hard material and must not be large in a soft material as this would lead to excessive losses).

[10 %]

iii) In an electric motor the magnetic circuit would be made from a soft magnetic material with a large permeability so as to maximise the field in the gap. A hard magnetic material would be used in place of a stator coil or rotor coil in a permanent magnet motor. Modern high-performance motors often use a permanent magnet rotor so as to eliminate the need for brushes coupled with a variable frequency drive for the stator coils.

[10 %]

c) i)

The magnitude of the demagnetising field is given by $-NM$ where N is the shape factor of the magnet. For an infinite rod no field returns through the material so N is 0 for a flat plate all field returns so it is 1.

[10 %]

ii) Magnetisation leads to a magnetic field in the magnetic material that acts on the material itself to oppose the magnetisation – hence the term demagnetisation. Another way to think about this is that creating a magnetic field “costs” energy and demagnetisation tends to reduce the energy of the system.

[10 %]

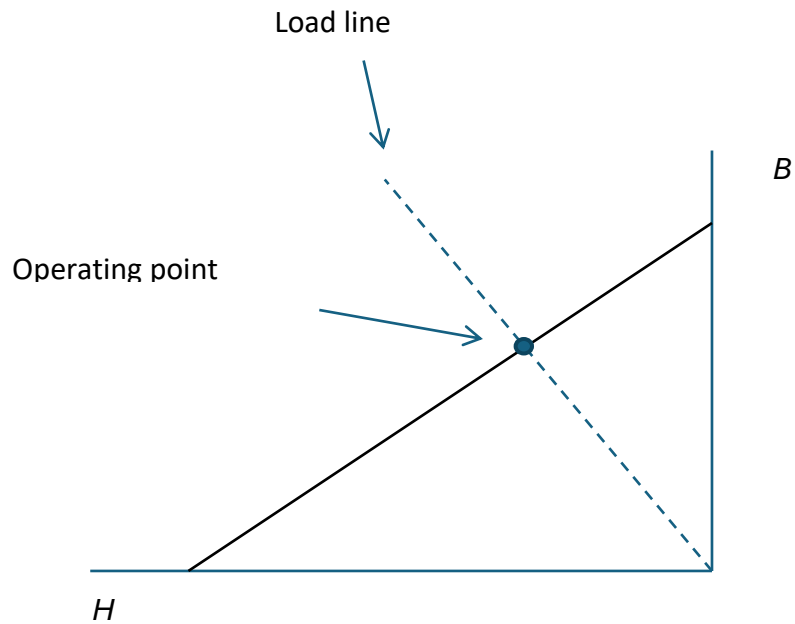
iii) From $\mathbf{B} = \mu_0(\mathbf{M} + \mathbf{H}_0)$ we can then write that $\mathbf{B}_{op} = \mu_0(\mathbf{M} - \mathbf{M}N)$ or $\mathbf{B} = \mu_0\mathbf{M}(1 - N)$. However $\mathbf{M} = \mathbf{H}/-N$ so we obtain the required result $\mathbf{B} = \mu_0(1 - N)/N$

This is a line on a BH plot through the origin with gradient:

$$\frac{B_{op}}{H_m} = \mu_0 \frac{M - NM}{-NM}$$

Rearranging we obtain the required result. If this is plotted on the BH characteristic for the magnetic material in question the intersection defines the operating point of the magnet. At that point the values of B and H give the energy product.

[20 %]



iv) It can be shown straightforwardly that the BH product is maximised (assuming H_c is large enough to permit this) when the shape factor is $\frac{1}{2}$. A squat disc with $h=r$ has roughly this shape factor. From observation we can see that this is a common format in which magnets are made.

[10 %]