4C3 – Advanced Functional Materials and Devices

Crib – v4

Q1 a) In terms of the crystal structure the behaviour of a material depends on the disposition of charges, and their symmetry. Briefly a piezo-electric material lacks a centre of symmetry so the application of strain causes a change in the charge separation, thus giving a polarisation. In addition to this pyro-electric materials exhibit an intrinsic dipole, and thus show a change in charge separation in response to a change in temperature.



A comprehensive answer will likely include a sketch to illustrate this:

b)i)

In contrast to the example of a pyroelectric camera there is no shutter involved, instead the various elements of the lens cause a modulation of the arriving infrared radiation as the heat source moves through the field of view. It is therefore the faceting of the lens on the sensor that generates the modulation.

If the office occupant is stationary no signal will be resolved and the office will appear empty even though it isn't. This is a common occurrence which can only really be resolved by going to finer lenses which are sensitive to the motion of body parts rather than just the whole individual (or encouraging people to get up from their desks more!).

ii) This is a relatively low frequency application. We can thus ignore the frequency response of the amplifier for the most part and operate in current mode. The behaviour of the system is thus dominated by the heat capacity of the element and the conductance to ground. The relevant time constant is therefore τ_t =H/G_T which has units of 1/s as required.

iii) Candidates should be able to derive

$$\frac{i_p}{W_0} = R_i = \frac{\eta p A \omega}{G_T \sqrt{1 + \omega^2 \tau_T^2}}$$

using their understanding and the information given. If the frequency is large with respect to the time constant this simplifies to:

$$R_i = \frac{\eta p A}{H} = \frac{\eta p}{cd}$$

Where c is the volume specific heat.

iv) No derivation is required here but need to think about the noise in the amplifier and sensor. The level of Johnson noise depends on the loss tangent of the material which is a materials property. The cost and ease of fabrication are probably more significant in this application. Candidates may remember that polymer pyro-electric materials are easily fabricated into large area sensors and are cheap.

The fact that a ferroelectric can be poled so the sensor element need not be an aligned single crystal means that in practice pyroelectric sensors are made from ferro-electrics although they need not strictly be so.

Assessor's comments:

1(b)(i) A good number of candidates did not refer to modulation of the arriving infrared radiation of a moving heat source. 1(b)(iv) answered quite poorly – not many candidates referred to noise or thoroughly examined choice of material.

Q2 a) i) Sketch for Type I should be slope -1 to Hc and then drops to 0. Sketch for unpinned Type-II should be as below:



Finally, students should remember that pinning adds hysteresis (as described by the Bean model) any sketch that shows a remnant magnetic moment is an acceptable answer as the M-H behaviour of practical Type-II superconductors can be very variable.

The three different behaviours arise from the different nature of Type-I and II materials. A type I material will exclude all field to Hc. This means it is a perfect diamagnet and the M-H plot should reflect this.

Type-II superconductors have an opposite sign of the free energy of the superconductor -normal interface. Consequently, it is energetically favourable above H_{c1} – rather than having flux excluded or suppressing superconductivity for the field to penetrate as individual flux vortices. Transitions from superconducting to normal state at H_{c2} .

ii)

The critical current for the wire for the case of a Type-I is going to be when the self field generated by the current flowing in the wire exceeds H_c in the wire. Consequently we need to be able to calculate the largest field in the wire. From Ampere's law (given in databook) we can see that around a current carrying wire H=I/2*pi*r. The condition for the critical current is when I is large enough such that H at the surface of the wire is at least H_c . Hence we have:

$$I_c = 2\pi r H_c$$

b)

i) At 4.2K traditional practical material for 15 T is Nb₃Sn. YBCO/MgB₂ have now reached these fields (as can be seen from plot) and can operate in persistent mode so allow and Bi-2212. NbTi is a good material but cannot work at 15T. Allow NbAl, which would in theory work, although it is uncommon in commercial magnets.

ii) For a solenoid $B=\mu_0 nl/L$ so number of turns per metre length is $B / \mu_0 l$. This is 15/ 1.25 x10⁻⁶ * 100 about 120000 turns per metre. J_c is I/A so A=I/J_c, min. cross sectional area is, as J_c of Nb₃Sn is around 1-2000 A/mm² at 15 T, area ~ 0.05-0.1 mm², diameter of 0.25-0.36 mm. This is slightly on the small side for commercial wire, but given a safety margin (this is *minimum* wire diameter) getting 120000 turns per metre length of wire this is reasonable, solenoid will be roughly 3 cm thick. [2000 wires by 60 wires] Other choices of material will give different numbers but method should be correct.

Assessor's comments:

2(a) M-H curves were generally sketched well, but physically understanding less so. Most candidates did not derive Ic from Hc well. 2(b) Generally answered well, but some candidates confused the bulk and wire forms of superconductor.

Q3 a) An electron-hole pair created when an electron leaves the valence band and enters the conduction band is called an exciton. The average distance between electron and hole is called the exciton Bohr radius a_B : $a_B = \frac{4\pi\epsilon\hbar^2}{m_0e^2} \left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)$ where $m_{e,h}^*$ are the respective effective masses. This is in analogy to the hydrogen Bohr radius. Quantum dots are nanomaterials where all dimensions are comparable to the exciton Bohr radius , i.e. generally have diameter D < 10 nm. The motion of electrons, holes and excitons are then spatially restricted, so called quantum confinement. [10%]

b) Electronic wavefunctions for 1D infinite potential well look like:



A standing wave pattern will be established, analogous to a vibrating string with fixed nodes. It follows that the well must contain an integral multiple of half electronic wavelengths: $a=n\times\lambda/2$.

Using the de Broglie wavelength of the electron $\lambda = \frac{h}{p}$, and taking the electron energy as E=p²/2m gives: $E = \frac{\hbar^2 \pi^2}{2ma^2} n^2$

Quantum dots are a realization of our ideal 1D potential well in 3D, and assuming the overall energy is simply the sum of the individual energies for each degree of freedom:

$$E = \frac{3\hbar^2\pi^2}{m^*m_0D^2}n^2$$

where m* is the respective effective mass.

[25%]

c) If the uncertainty in position is around D/2 in 1 dimension, then the uncertainty in the momentum is

$$\Delta p_x \ge \frac{\hbar}{D}$$

Giving a minimum energy

$$E = \frac{p^2}{2m} \sim \frac{\hbar^2}{2mD^2}$$

This can be multiplied by 3 to for each degree of freedom. This is lower than E1 above in (b), ie consistent as the momentum of the electron will always be above the minimum required by Heisenberg. Estimation for D=3nm: E= 12 meV [15%]

d) CdSe is example for material. Blue shift ie shift to smaller emission wavelengths can be achieved by making D smaller for the QD, as emission depends on separation of energy levels which increases with decreasing D. [10%]

e) In order to achieve high OLED efficiency, exciton should recombine radiatively, with minimum energy losses throughout the process. For a single layer structure, the active region can move towards electrodes, where emission is quenched and where electrons and holes recombine non-radiatively. Hence typically a heterostructure is employed to maximise electron and hole injection and to pose a barrier for carriers to reach electrodes.



OLED can be designed using filters with single emission layer for RGB. Operation with filters wont shift colour due to different aging of different polymer emitters.



[30%]

f) QDs superior to organic luminescent materials because of their inherent luminescent properties, including narrow spectral emission bandwidths, high photoluminescence quantum efficiency, good photostability and controllable bandgap.

Analogous to OLEDs typically a heterostructure is employed to maximise electron and hole injection and to pose a barrier for carriers to reach electrodes.



[10%]

Assessor's comments:

Electronic energy levels (3(b)) were generally well derived, while comparison to Heisenberg's Uncertainty Principle (3(c)) confused some candidates. 3(e) OLED operation was well explained, although band diagrams were not always drawn correctly. 3(f) Some candidates failed to sketch quantum dot emitter structure.

Q4 a) Graphene is a zero-band gap semiconductor. The E-k dispersion for graphene in the vicinity of the K-points (so called Dirac points) can be described by linear dispersion:

Its is symmetric (electrons and holes have same properties) and reminiscent to the linear dispersion for light. Standard semiconductors such as Si have parabolic dispersion. This implies that in graphene charge carriers can behave like zero rest-mass relativistic fermions. This gives rise to many unique electrical transport effects.

The structure of single-walled carbon nanotube (SWNT) can be thought of as a rolled up graphene sheet. The so called chiral vector (n,m) uniquely specifies their structure. Their Brillouin zone (BZ, reciprocal lattice) is given by a set of equidistant lines. If for a particular SWNT (n,m) the 1D BZ lines cross the graphene K, K' points (where the π and π^* bands touch), the SWNT is metallic. If the cutting lines do not pass through a K point then the SWNT will be semiconducting with a band gap. [15%]

b) FEDs can be thought of flat cathode-ray tubes. Electrons are emitted from the surface of a cathode material and are accelerated in vacuum towards an anode via an electric field. The electron energy excites a luminescent phosphor layer, which upon de-excitation, emits light.



Multi-walled carbon nanotubes (so there are metallic) have ideal properties for field emission, incl.

- highest current carrying capacity of any material, due to very high threshold for electromigration, due to its strong covalent bonds,
- small diameter, and very large aspect ratio, meaning high field enhancement around its tip
 High electrical and thermal conductivities.

CNT emitter arrays have also been developed for advanced X-ray and T-Hz sources, and microwave amplifiers.

[30%]

c) In a-Si, each Si still makes 4 bonds to neighbouring Si atoms. So considering the bonding model, with the bands depending on the presence of bonding and antibonding states, the overall band structure of a-Si is basically the same as for c-Si. But the band gap is no longer a totally forbidden gap. The valence and conduction band states tail into the original band gap. These tail states are now localised. They are not plane waves. The states in the conduction band and in the valence band are plane wave states like in a crystalline system. They are called extended states. A certain energy called the mobility edge separates the two types of state. The as-defined band gap for a-Si is 1.7eV, compared to 1.1 eV for c-Si. The continuous random network may also contain defects. These are coordination defects and dangling bonds (DBs) and give rise to defect states.

In practice, only the extended states conduct electricity well. These define the mobility, which is much lower for a-Si (of order of 0.5 cm2/Vs, compared to 1000 cm2/Vs for c-Si).



[20%]

d)



a-Si is used as processing over large are and low cost is required. Recently, it was found that oxides like amorphous InZnGaO4 (IGZO) are much better than a-Si:H. They have an electron mobility of 20-60 cm2/V.s, over 20 times that of a-Si:H, a considerable advance. They also have less instability, but this is still being studied. [20%]

e) Transparency is achieved by large bandgap (over 3eV for ITO, which is standard material for transparent electrodes), and conductivity is achieved via doping. CNT networks and graphene films present alternative transparent conductor systems. In contrast to conventional TCs, graphene can work as TC because it is so thin and at the same time its high mobility can give a very high conductivity. To compete with ITO, requires graphene with high mobility and doping. Same challenge for CNT networks. Doping thereby relies on charge transfer, rather than substitutional doping. Transparent conductor systems based on these new materials can be much thinner, and flexible, unlike brittle, thicker ITO. Graphene offers also transparencies over broad energy range. [15%]

Assessor's comments:

4(a) Band diagram of graphene was typically well explained but discussion of electronic structure of nanotubes was fairly scattered. 4(b) FED device structure well explained, but answer to other nanotube applications varied form very inventive to neglected. 4(c) A-Si structure very well explained, but mobility and band gap often not directly compared or mentioned. Answers to 4(e) varied from detailed, well structured and showing clear understanding, to very scattered and superficial.