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ENGINEERING TRIPOS PART IIB

Thursday 4th May 2006 2.30 to 4

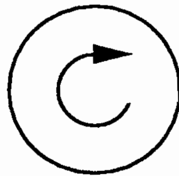
Module 4C3 : ELECTRICAL AND NANO MATERIALS SOLUTIONS

1(a) The basis of the Bean model for type II superconductors is that current density equal in magnitude to the critical current density, J_c, flows everywhere magnetic field penetrates the material. i.e.;

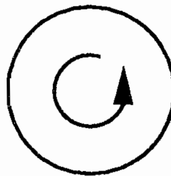
$J = J_c$ where field penetrates the sample

$J = 0$ where field = 0

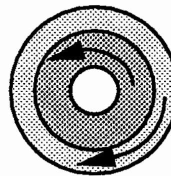
Application of a large magnetic field parallel to the axis of a long rod of bulk type II superconductor causes field to penetrate increasingly into the material as the field increases. Current flows where this field penetrates until the entire superconductor carries a current (providing the field is large enough to penetrate to the centre of the sample). The current reverses from the outside-in when the field is removed (since the sign of $d\phi/dt$ reverses). If the peak applied field, B_a, is significantly greater than the field required to fully penetrate the superconductor, B_p, then the induced current reverses completely when the field is removed. For a lower peak field amplitude the current loop only partially reverses, leaving nested current loops in opposite directions. In cross-section through the rod;



Fully penetrated



Fully reversed



Nested current lops for $B_a < 2\,B_p$

[20%]

(b) Slab geometry is particularly suitable for analysis by the Bean model since this simplifies the algebra significantly. The relationship between the flux density gradient and critical current density for a type II superconductor is derived from Maxwell's equation;

Curl $\mathbf{H} = \mathbf{J}$ or Curl $\mathbf{B} = \mu_0\,\mathbf{J_c}$

Therefore;

$$\text{Curl}\,\mathbf{B} = \Delta \wedge \mathbf{B} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ B_x & B_y & B_z \end{vmatrix} = \mu_0\,\mathbf{J_c}$$

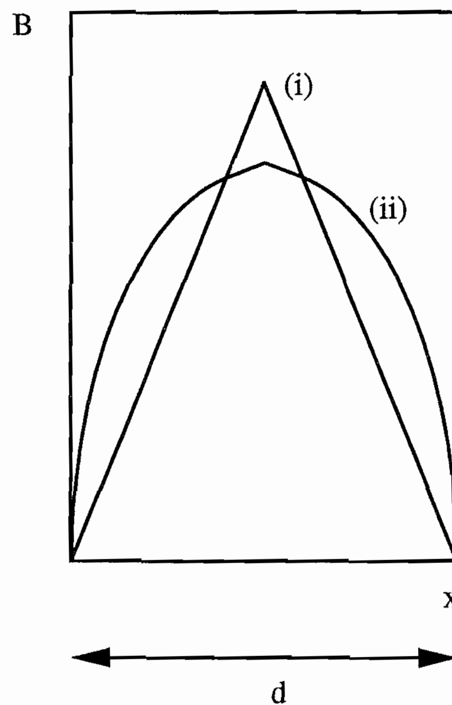
But $\mathbf{B}$ is constant for slab geometry for constant y and constant z. Hence $\frac{\partial}{\partial y} = \frac{\partial}{\partial z} = 0$.
Also $\mathbf{B_x} = \mathbf{B_y} = 0$.

Derivation of equation for slab geometry;

$$\text{Curl } \mathbf{B} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & 0 & 0 \\ 0 & 0 & B_z \end{vmatrix} = \mu_0 \mathbf{J_c} \qquad \text{i.e. } \frac{\partial \mathbf{B_z}}{\partial x}\mathbf{j} = \frac{\partial \mathbf{B}}{\partial x}\mathbf{j} = \mu_0 \mathbf{J_c}$$

i.e.; $\frac{\partial \mathbf{B}}{\partial x} = \mu_0 \mathbf{J_c}$ [30%]

(c) Variation of magnetic field through the slab thickness for (i) B is independent of J_c and (ii) $J_c = \frac{K}{B}$ is as follows;



A peak applied field of twice the magnitude required to fully penetrate the sample is required to fully magnetise the slab. [20%]

(d) A fully magnetised 1 cm thick slab of $YBa_2Cu_3O_{7-\delta}$ (YBCO) as shown in Fig. 1, carries a uniform, field independent critical current density of 40×10^4 Acm^{-2} throughout its volume. .

(c) For case (i), $\int_0^{B_{max}} dB = \mu_0 J_c \int_0^{d/2} dx$ i.e. $B_{max} = \frac{\mu_0 J_c d}{2}$

Therefore; $B_{max} = \frac{4\pi \times 10^{-7} \times 20 \times 10^{7} \times 5 \times 10^{-3}}{2} = \mathbf{0.63\ T}$

(not forgetting to convert Acm^{-2} to Am^{-2})

Nickel has an FCC crystal structure, which has 4 atoms, and hence $4 \times 0.6 = 2.4$ Bohr magnetons, per unit cell.

Unit cell volume = $(0.35 \times 10^{-9})^3 = 4.29 \times 10^{-29}\ m^3$

$$\text{Vol. magnetisation} = \frac{\text{number of Bohr magnetons per unit cell} \times \mu_B}{\text{unit cell volume}}$$

$$= \frac{2.4 \times 9.27 \times 10^{-24}}{(0.35 \times 10^{-9})^3} = \mathbf{5.19 \times 10^{5}\ A/m}$$

$B = \mu_0 M = 4\pi \times 5.19 \times 10^5 = \mathbf{0.65\ T}$

Nickel generates the greater magnetic field at the centre of the rod (the field is half this value at the end) . [30%]

2(a) Pyroelectric and piezoelectric materials are sub-classes of dielectrics, and are characterised by an asymmetry in their crystallographic structure, which leads to polar properties. Ferroelectrics are a sub-class of pyroelectrics. The crystal structure of piezoelectric materials is characterised by a lack of centre of symmetry (i.e. they exhibit point or axial asymmetry). As a result, 20 of the known 21 dielectric structures that exhibit such a lack of centre of symmetry are piezoelectric.

Pyroelectricity, on the other hand, occurs in polar dielectric materials whose structure contains at least one *axis* along which an electric dipole moment exists. Only 10 of the 21 dielectric structures, therefore, exhibit pyroelectric properties (orthorhombic, tetragonal and triclinic, for example). A pyroelectric material is necessarily piezoelectric, although the converse is not true.

Ferroelectrics are the most useful pyroelectric materials from an applications point of view although not all pyroelectrics are ferroelectric. Ferroelectrics are polar materials in which the direction of the spontaneous dipole moment can be changed by the application of an electric field. This property is due to the presence of a number of polar axes in the crystal structure which is a particular feature of the perovskite lattice. Some ferroelectrics undergo a structural phase transformation to a lower crystal symmetry at the Curie temperature, T_C. [25%]

(b)(i) Passive applications (E = 0) $P_i = d_{ijk}\, \sigma_{jk}$

(ii) Active applications ($\sigma = 0$) $S_i = d_{ijk}\, E_{jk}$

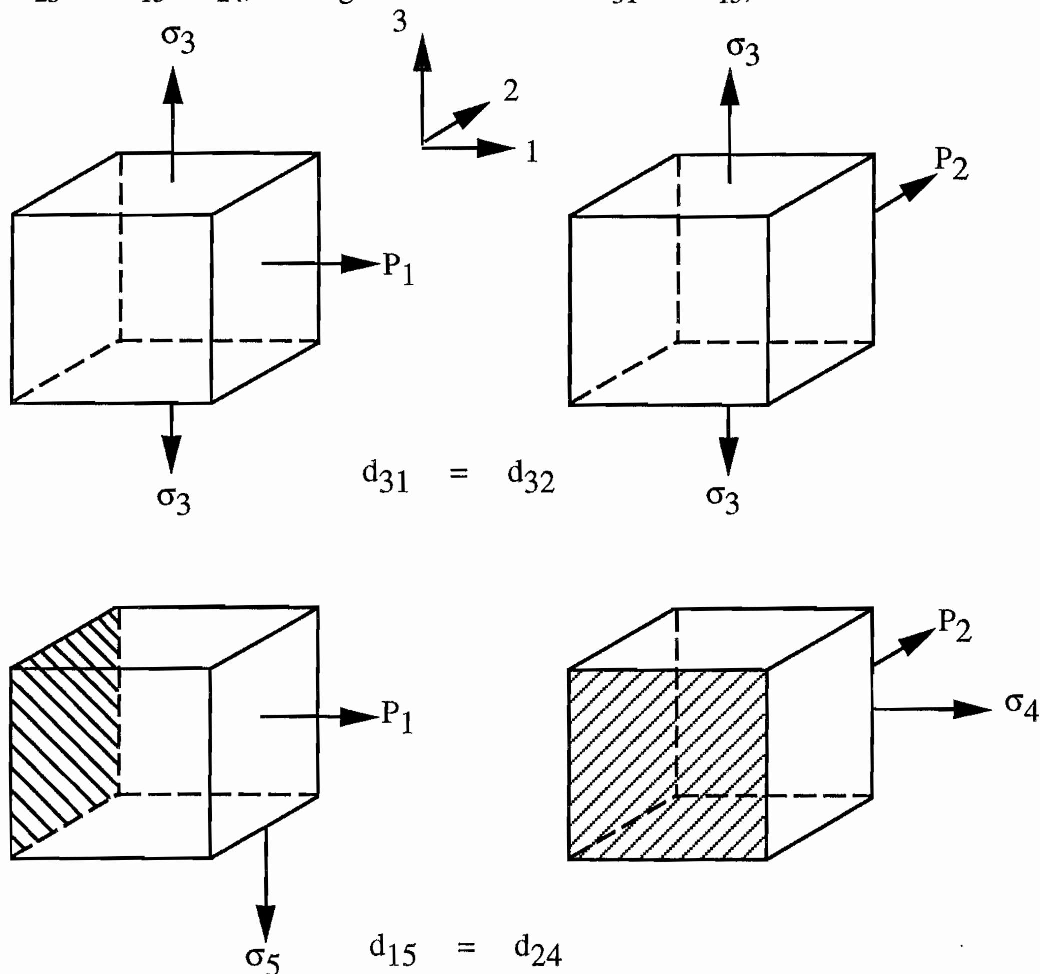
where S (strain), P (change in polarisation) E (electric field) and σ (applied stress) are all variable. d is the piezoelectric coefficient, which are both constant. i, j and k take the values of 1 to 3.

Therefore there are $3 \times 3 \times 3 = 27$ independent piezoelectric coefficients. These may be reduced to three as follows;

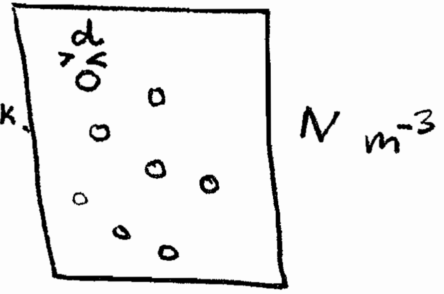
1. Indices i and j are interchangeable, so reduced suffix notation may be used (i.e. $d_{ijk} = d_{jik}$. As a result $d_{ijk} \rightarrow d_{ij}$ with i = 1 to 3 and j = 1 to 6. This reduces the number of independent stresses (fields) to 6, and the number of piezoelectric coefficients to $3 \times 6 = 18$.

Hence, for passive operation, $P_i = d_{ij}\, \sigma_j$

The number of modes is limited further by crystal structure and geometry for piezoelectric elements manufactured in the form of thin plates. As a result there are only 5 piezoelectric coefficients that are non-zero. These are d_{13}, d_{23}, d_{33}, d_{15} and d_{24}. Finally, by symmetry, $d_{13} = d_{23}$ and $d_{15} = d_{24}$, leaving three coefficients. d_{31} and d_{15};



(3) 4C3 a. Order of magnitude calculation of time to form a monolayer. DBm 1.1.200



First estimate velocity of a molecule at 300K from equipartition of energy

$$\frac{1}{2} m v^2 = \frac{3}{2} kT$$

$$V = \sqrt{\frac{3 \times 1.4\times10^{-23} \times 300}{16 \times 1.7\times10^{-27}}} = \sqrt{\frac{4.2 \times 300}{16 \times 1.7} \times 10^4} = 700\ ms^{-1}$$

The number of molecules arriving at the wall is $\frac{1}{4} N V$ per second per square metre

But the number required to form a complete monolayer is $\frac{1}{d^2}$ per square metre

Unity sticking coefficient

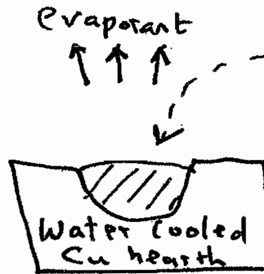
Hence time to deposit a monolayer $t = \dfrac{1/d^2}{\frac{1}{4}NV} = \dfrac{4}{700\, d^2 N} \approx \dfrac{1}{200\, d^2 N}$

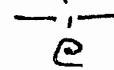
for example if a monolayer forms in 1 minute at $d = 10^{-9}$ m then $N = 10^{14}\ m^{-3}$ [30%]

b. (i) electron-beam evaporation

most refractory materials can be deposited (conductors)

eg. a 5 kV 1 amp beam heats the target to 3000 K



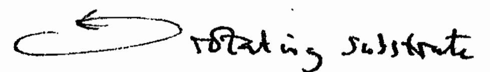


beam deflected in a circular orbit in a magnetic field.

electron filament e.g. at −5kV

the deposition is line-of-sight to the target hence a high vacuum is required with mean free path ~ 1 m.

the rate of deposition is high eg. 10 nm s^{-1}
no requirement for ultra high vacuum.



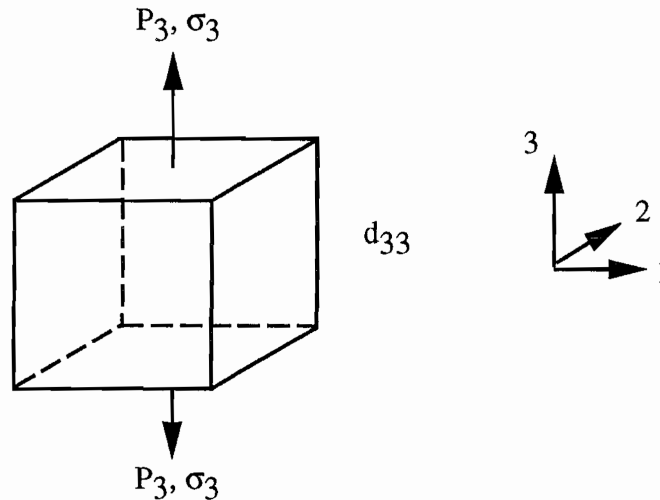
(ii) molecular beam epitaxy

the source material is heated with excellent temperature control to achieve a uniform stream of evaporated material which is line-of-sight incident upon the substrate.

the low deposition rate < 1 nm s^{-1} means that ultra high vacuum is required to reduce contamination.

Semiconductors such as GaAs can be deposited with good properties because the relative arrival rates of the components is well controlled and the materials arrive with low energy on a heated substrate allowing epitaxial growth conditions to be achieved.

d_{33};



[30%]

(c) Modes of operation of piezoelectric device for the given applications;
(i) Longitudinal mode operation for a microphone (couples via d_{31}). This amplifies the signal by the aspect ratio of the piezoelectric element.
(ii) Thickness mode operation for a spark igniter (couples via d_{33}). This give the biggest change in polarisation for an applied stress.
(iii) Shear mode operation for an accelerometer (couples via d_{15}).This is insensitive to pyroelectric effects which is necessary for low noise applications. [15%]

(d) $P = \chi E + d\sigma$ hence $\left(\frac{\partial P}{\partial \sigma}\right)_E = d$, $\Delta P = d\,\Delta\sigma$

$\Delta P = \Delta Q/A$, $\Delta\sigma = \Delta F/A$, $\Delta Q = C\,\Delta V$, $C = \frac{\varepsilon_0 \varepsilon A}{t}$

i.e. $\Delta P = \frac{\Delta Q}{A} = d\frac{\Delta F}{A}$ $\Delta Q = d\,\Delta F = C\,\Delta V$

$$\Delta V = \frac{d\,t\,\Delta F}{\varepsilon_0 \varepsilon A} = \frac{t\,\Delta F}{\varepsilon_0 A} \times \frac{d}{\varepsilon}$$

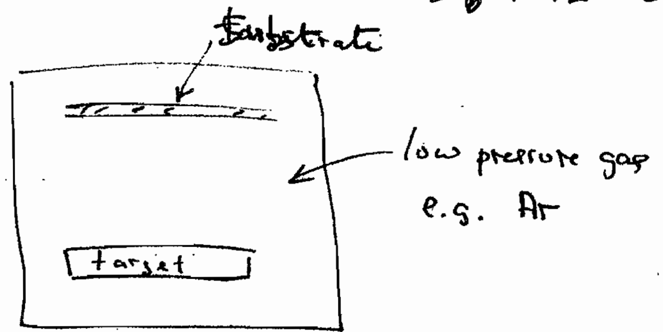
d/ε is the material figure of merit. In rank order for thickness mode operation;

Material	Density kg cm^{-3}	ε	d_{33} pC N^{-1}	d_{33}/ε pC N^{-1}
PT	7830	170	51	0.300
PZT-4	7750	1300	289	0.222
PZT-8	7600	1000	215	0.215
PZT-5	7500	3400	593	0.174
BT1	5700	1000	120	0.120

Note that the density is not required.

Other considerations include whether the piezoelectric is ‘hard’ or soft’ (soft materials are preferred for passive operation since they are easier to deform), whether the material can be fabricated in the appropriate geometry and cost of material. [30%]

electrons are accelerated by rf or dc applied voltage to form a gas discharge and ions e.g. Ar^+ knock atoms off the target, and diffusion results in coating of the substrate



a magnet field is used to confine the plasma and produce a more intense plasma.

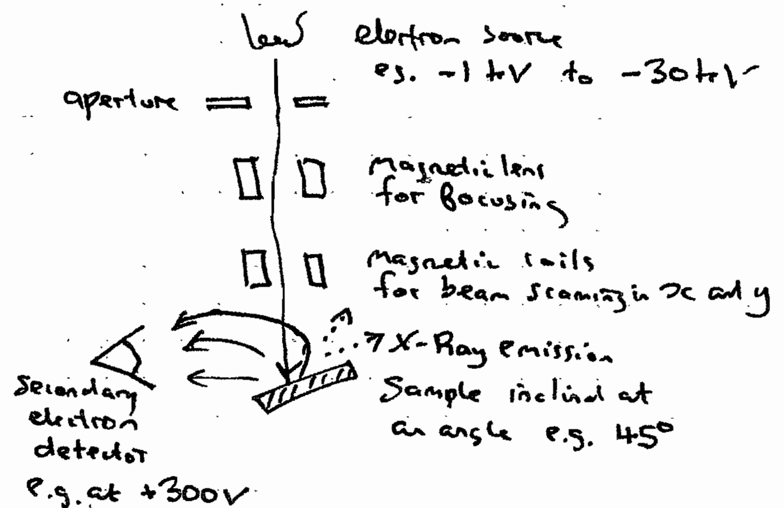
High rate deposition is achieved e.g. Al alloys at $> 10 \text{ nm s}^{-1}$

and there are only modest requirements on the quality of vacuum compared with MBE

In summary, MBE is high quality and high cost, sputter deposition can be low cost and generally is lower quality, and e-beam lies in between. [40%]

c Scanning electron microscopy

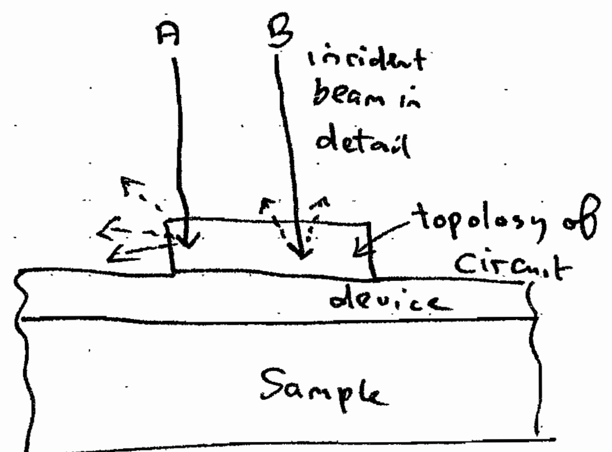
a high-vacuum enclosure is required to ensure an electron mean free path of order 1 m.



the sample is at zero potential and the incident electrons excite many secondary electrons at escape energies 0–50 eV which are attracted to the detector

as the primary beam is raster scanned the current of secondary electrons is monitored to build up a secondary electron image.

Enhanced signal at the edges of structures arises because in case A more of the secondary electrons can escape from the solid (at 10 kV the primary penetration into Si is about 1 µm)



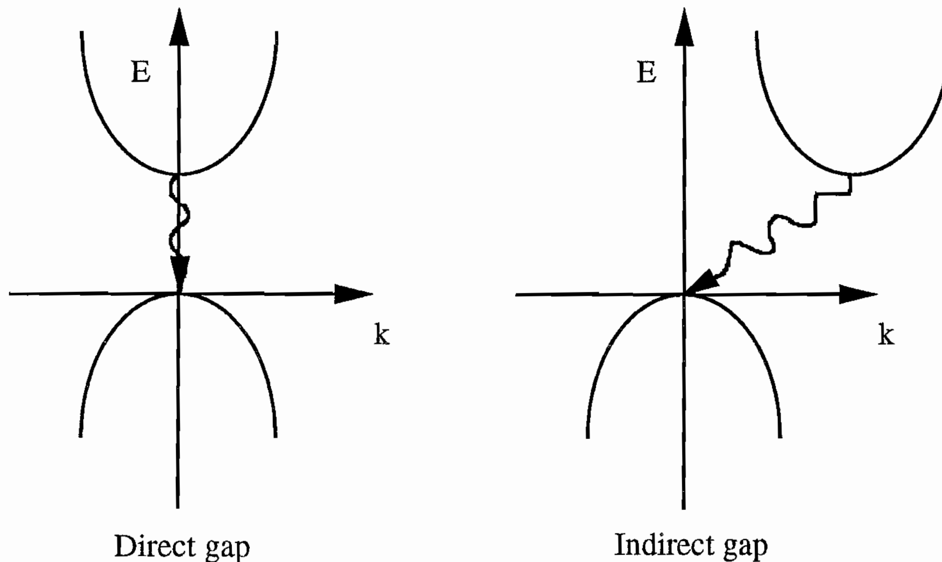
than in case B, resulting in very good topographical images from secondary electrons.

Signals from high energy backscattered electrons are noisier and give less topographical contrast but do give useful elemental contrast. [30%]

The two large features are bond pads to the circuit, centre to centre spacing of order 100 µm and the small features are wires in the input / output protection circuitry line width of order 3 µm in 1990.

4(a) Electronic transitions in a direct band gap material occur at constant k for the electron, or vertically in E-k diagrams. They have a high probability (i.e. they are fast with strong intensity).

Electronic transitions in an indirect band gap material are non-vertical and require phonons, to conserve momentum, and this strongly lowers their probability and speed of recombination(i.e. they are slow and weak).



Direct gap   Indirect gap

The most important property for optoelectronic devices is the conversion of electricity into light or photons. This occurs typically by the recombination of an electron and a hole in a semiconductor to give energy that is released as a photon. As in classical mechanics, this process must conserve both energy and momentum. i.e.;

E(photon) = E(electron) – E(hole)   and   k(photon) = k(electron) – k(hole)

Now, photons of a given energy have very small k vectors compared to electrons, because the speed of light is so large.

For photons; $k = \frac{\omega}{c} = \frac{E}{c\hbar}$.   For electrons; $k = \frac{\sqrt{2mE}}{\hbar}$

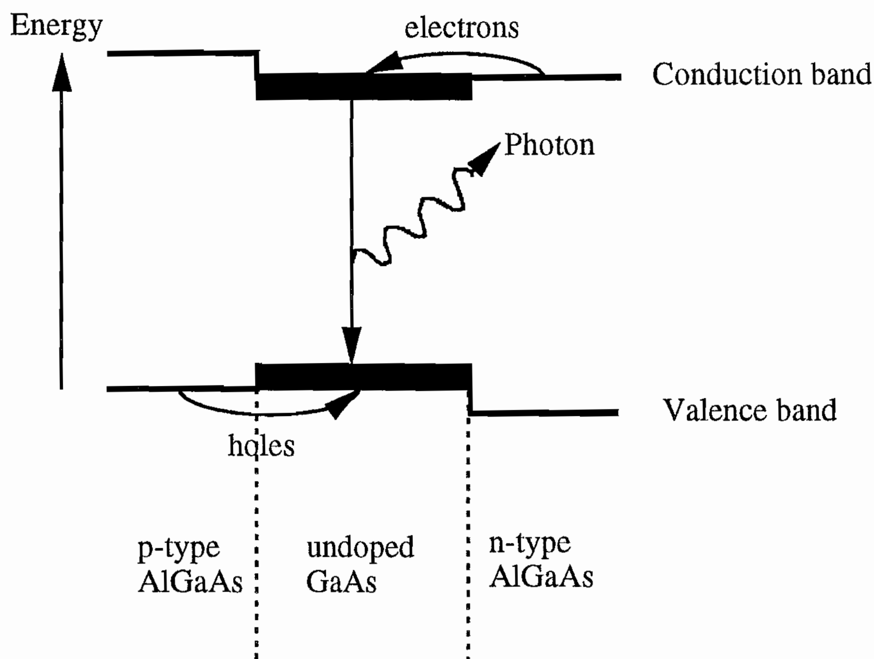
This means that the electron and hole that recombine must have essentially the same k vector. As a result, the bandgap of the semiconductor should be direct (i.e. vertical in k-space), which means generally that it should be at the centre of the Brillouin zone. Hence, a direct band gap is needed for an opto-electronic device, since $\Delta k=0$ is required for optical transitions. [20%]

(b) Direct; GaAs, GaAsP, InAsSb
Indirect; Si, GaP, GaAsP, Ge, AlAs [10%]

(c) Carrier confinement in light-emitting semiconductor heterostructures is achieved by 'band gap engineering'. This involves making heterostructures of alloys of different band

gaps so that band offsets in semiconductors of different band gaps confine both electrons and holes within the narrow gap. This increases the probability of recombination.

There are 3 layers in the band structure, as illustrated below;

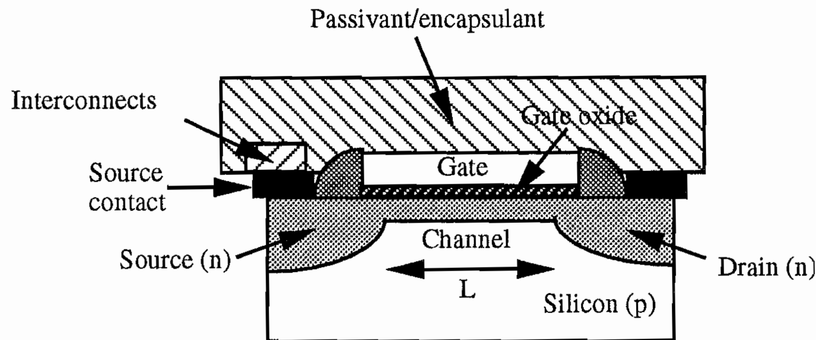


The AlGaAs layer on the right is doped n-type. However, its electrons can lower their energy by moving left into the GaAs layer, with the smaller band gap, and falling into its conduction band. The left hand AlGaAs layer is doped p-type. Holes are like bubbles; they gain (potential) energy by rising. As a result, the holes will move into the high valence band of the GaAs. In this case the GaAs layer will contain both holes and electrons, even though it was not doped itself. The carriers are confined to this layer by the potential barriers of the wider gap AlGaAs layers. The electrons and holes recombine to emit photons, which is the basis of the sample semiconductor laser. [30%]

(d) Band gap varies closely with bond length/lattice constant, so semiconductors with lattice matching tend to have the same (or very similar) band gap. The choice two semiconductors with different band gaps is very difficult.

Lattice matching is important between semiconductors of different band gaps (i.e. same lattice constant or bond length), otherwise interfacial defects result, which give rise to non-radiative recombination effects. Dislocations act as carrier recombination centres. [40%]

5 (a)



NMOS; channel = p-doped Si
Drain, source - n-doped Si
Gate = highly n-doped polycrystalline Si
metal contacts = silicides
Gate oxide = SiO_2
Passivant = SiO_2
Interconnect = Al, now Cu [20%]

(b) SiO_2 is used as a gate oxide, to be replaced by higher K oxide to stop gate leakage current.
SiO_2 used an inter-layer dielectric is to be replaced by low K dielectric to reduce RC time delays associated with excessive capacitance. [20%]

(c) The free surface of a semiconductor consists of dangling bonds. These give gap states, which act as recombination centres (i.e. limit the field effect). Coating the surface with SiO_2 converts dangling bonds into Si-O bonds, removing their gap states and enabling the FET to work. [10%]

(d) Interconnects conduct carriers between FETs. The current density is becoming too high in state of the art devices, so they fail by electromigration. This is a sort of self-electrolysis. Al is being replaced by Cu in interconnects. [15%]

(e)			
	IV, e.g. Si;	Group III as acceptors, group V as donors	
	III-V, e.g. GaAs;	Group II on Ga site or group IV on As site as acceptors	
		Group IV on Ga site and group VI on As site as donors	
	II-VI, e.g. ZnSe;	Group I on Zn site or group V on Se site as acceptors	
		Group III on Zn site or group VII on Se site as donors	[20%]

(f) Group 1 elements are used for interstitial doping. Interstitial dopants can move easily between atoms and so end-up in the SiO_2 and create fixed charge, compromising the operation of the FET. [15%]

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