PROF D CARDWELL

Thursday 3rd May 2012 2.30 to 4

Module 4C3: ELECTRICAL AND NANO MATERIALS SOLUTIONS

1 (a) The Bean model describes the flow of current and penetration of magnetic field into a bulk type II superconductor. It assumes that there are no local magnetic dipoles (i.e. unpaired spins) present in the material so the currents can be treated as in the free space case (i.e. $B = \mu_0 H$) and that the current flowing is either $+J_c$ or $-J_c$ where the field penetrates the material. J_c is zero elsewhere.

A bulk superconductor of slab geometry is magnetized by first cooling below its superconducting transition temperature, followed by the application and removal of a magnetic field (the zero field cooling magnetization process). It is necessary to apply approximately twice the penetration field to completely magnetise a bulk superconductor of slab geometry when the applied field is removed to achieve complete reversal of the induced current.



It is necessary to apply approximately twice the penetration field to completely magnetise a bulk superconductor of this geometry when the applied field is removed to achieve complete reversal of the induced current. [30%]

(b) (i) Generally, Curl
$$\mathbf{H} = \mathbf{J} + \frac{d\mathbf{D}}{dt}$$
 (Maxwell)

For a thin superconducting slab with a d.c. field (i.e. $\frac{d\mathbf{D}}{dt} = 0$) applied parallel to the slab surface with the assumption of the Bean model (i.e. $\mathbf{B} = \mu_0 \mathbf{H}$ and $\mathbf{J} = \mathbf{J}_c$):

Curl
$$\mathbf{B} = \mu_0 \mathbf{J_c}$$

Curl **B** =
$$\Delta \wedge \mathbf{B} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} \frac{\partial}{\partial y} \frac{\partial}{\partial z} \\ B_x B_y B_z \end{vmatrix} = \mu_0 \mathbf{J}_0$$

Assumptions;

1. **B** is constant in the slab for constant y and constant z. Hence $\frac{\partial}{\partial y} = \frac{\partial}{\partial z} = 0$. 2. **B**_x = **B**_y = 0.

Therefore : Curl **B** =
$$\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & 0 & 0 \\ 0 & 0 & B_z \end{vmatrix} = \mu_0 \mathbf{J_c}$$
 i.e. $\frac{\partial \mathbf{B_z}}{\partial x} \mathbf{j} = \frac{\partial \mathbf{B}}{\partial x} \mathbf{j} = \mu_0 \mathbf{J_c}$
 $\frac{\partial \mathbf{B}}{\partial x} = \mu_0 \mathbf{J_c}$ where $\mathbf{J_c}$ is parallel to y. [25%]

(ii) Distribution of J_c and B through the cross section of the slab when J_c varies as 1/B for complete sample penetration;



[15%]

(c) By integrating the above equation, derive an expression for a thin superconducting slab which relates the average flux density to slab width and J_c . Calculate the field trapped by a superconducting slab of width 1cm that can carry a critical current density of 5 x 10⁴ Acm⁻₂.

$$\int_0^{\mathbf{B}} d\mathbf{B} = \int_0^{d/2} \mu_0 \, \mathbf{J}_c \, d\mathbf{x} \quad \text{i.e.} \quad \mathbf{B} = \frac{\mu_0 \, \mathbf{J}_c \, d}{2}$$

where B is the average (trapped) flux density in the slab.

The field trapped by a superconducting slab of width 1 cm carrying a critical current density of 5 x 10^4 Acm⁻² (i.e. 5 x 10^8 Am⁻²) is:

$$B = \frac{4\pi \times 10^{-7} \times 5 \times 10^{8} \times 10^{-2}}{2} = 3.14 \text{ T}$$

The maximum field produced by a fully magnetized iron rod is approximately 1.7 T, which is half the field of the slab, and approximately 4 times the energy density. [3]

[30%]

2(a) The following explanation is very full. Full marks could be obtained for bullet point descriptions of these effects. Pyroelectric materials are sub-classes of dielectrics, and are characterised by an asymmetry in their crystallographic structure, which leads to polar properties. Pyroelectricity occurs in polar dielectrics whose structure contains at least one *axis* along which an electric dipole moment exists (in contrast to piezoelectrics, which are characterised by point symmetry). 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 versatile form of pyroelectric materials for the manufacture of pyroelectric devices, 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 due to the presence of a number of polar axes in the crystal structure (which is a particular feature of the perovskite lattice). As a result, ferroelectrics may be processed in the form of ceramics (polycrystalline materials), and polarised using an applied electric field. This is cheaper and easier than using non-ferroelectrics such as LiTiO₃, which has only one polar axis and, therefore, has to be processed in the form of a single crystal. This is both complex and expensive (although single crystals tend to have higher pyroelectric coefficients than polycrystalline materials).

Finally, some ferroelectrics undergo a structural phase transformation to a lower crystal symmetry at the Curie temperature, T_c , which limits their pyroelectric response. [25%]

Incident radiation, sinusoidally modulated Vs Absorbing V_0 0 electrode, Area A d C_{A} RG RL 1_p C_E Pyroelectric element Thermal conductance

(b) The following circuit is used in a pyroelectric device;

Incoming infra-red radiation is modulated and focused onto the pyroelectric element (which has been coated in a radiation-absorbing surface, such as platinum-black). This causes the temperature of the element to rise, and for its intrinsic polarisation to decrease. This, in turn, causes charge to be released from the element (which is effectively the dielectric filling in a capacitor), with the amount of charge being directly proportional to the temperature change. The signal is then amplified using a FET, which has high input impedance to take the signal from a high impedance source.

For a good response, a pyroelectric element should:

- 1. Absorb and retain as much heat as possible during charge release monitoring;
- 2. Have a low thermal capacity (for max. temperature rise for given heat input);
- 3. Retain the charge long enough for it to be amplified (long enough electrical time constant required).

The detector will operate under (i) current mode at low frequencies (~10 Hz - current has time to flow) and (ii) voltage mode at high frequencies (~kHz - current does not have time to flow).

(c) Definition of
$$R_V$$
; $R_V = \frac{i_p}{Y W_0}$ also $\Delta T = \frac{\eta W_0 e^{i\omega t}}{G_T + i\omega H}$ (given)

Substitute Y = $\frac{1}{R_G}$ + i ω C (C = C_E + C_A) and H = τ_T G_T;

[30%]

$$i_{p} = A p \frac{dT}{dt} = \frac{\eta p A i \omega W_{0} e^{i\omega t}}{G_{T} + i \omega H}$$
$$R_{V} = \frac{i_{p}}{Y W_{0}} = \frac{\eta p A i \omega e^{i\omega t}}{G_{T} (1 + i \omega \tau_{T}) (\frac{1}{R_{G}} + i \omega C)}$$

But $C = \tau_E / R_G$ hence;

$$R_{V} = \frac{\eta R_{G} p A i \omega e^{i\omega t}}{G_{T} (1+i \omega \tau_{T}) (1+i \omega \tau_{E})} = \frac{\eta R_{G} p A i \omega e^{i\omega t} (1-i \omega \tau_{T}) (1-i \omega \tau_{E})}{G_{T} (1+\omega^{2} \tau_{T}^{2}) (1+\omega^{2} \tau_{E}^{2})}$$

$$R_{V} = \frac{\eta p A R_{G} \omega e^{i\omega t} (i+\omega \tau_{T}) (i+\omega \tau_{E})}{G_{T} (1+\omega^{2} \tau_{E}^{2})} |R_{V}| = \frac{R_{G} \eta p A \omega}{G_{T} \sqrt{1+\omega^{2} \tau_{T}^{2}} \sqrt{1+\omega^{2} \tau_{E}^{2}}}$$
[25%]

(d) F_D is the figure of merit used to describe the optimum signal to noise ratio of the pyroelectric material. This is derived from the materials term in the expression for the detectivity of the device (this represents the responsivity to Johnson noise ratio) i.e.

$$D = \frac{R_V}{\Delta V_J} = \frac{p}{c \sqrt{\epsilon_r \epsilon_0 \tan \delta}} \times \sqrt{\frac{\eta}{4kT d A}} \times \sqrt{\frac{1}{\omega}}$$

Materials Design
term term

The full equation is not required!

Therefore $F_D = \frac{p}{c\sqrt{\epsilon_r\epsilon_0 \tan \delta}}$, which needs to be evaluated for each material.

Material	Tc	р	٤r	tan ð	с	FD
	°C	μ Cm ⁻² K ⁻¹		∞10 ⁻³	MJm ⁻³ K ⁻¹	∞10-6/√Pa
PZFNTU	230	380	290	10	2.5	30
SBN - 50	121	550	400	3	2.3	73
PVDF	80	27	12	15	2.6	8
PGO	178	110	40	0.5	2.0	131

Order of potential is PGO, SBN, PZFNTU and PVDF.

3 (a) Schematic of CVD process (see lecture notes):

(1) Bulk gas transport of reactants/precursors;

(2) Diffusive transport of reactants across boundary layer;

(3) Adsorption of reactants on substrate;

(4) Surface processes incl. chemical decomposition, reaction, and surface migration;

(5) Desorption of by-products;

(6) Diffusive transport of by-products across boundary layer;

(7) Bulk gas transport of by-products.

(b) $h_g = 10 \text{ cm sec}^{-1}$ $k_s = 10^7 \times \exp(-1.9 \text{eV/kT}) \text{ cm sec}^{-1}$, for 900°C=1173K: kT=0.101eV hence $k_s = 0.068$ cm sec⁻¹

Therefore $k_s \ll h_g$ which means that at these conditions the CVD process is surface reaction controlled. For this regime, process control is highly dependent on temperature, but less restrictive on gas flow and substrate placement. Thus option (b) hot-walled, stacked wafer type CVD reactor is the best choice.

(c) At 10⁻⁶ mbar impingement flux is given $b\dot{y}_{O_2} = n_{O_2} v_{O_2} / 4$

In Ar at 1bar $j_{Ar-O_2} = f n_{Ar} \overline{v}_{Ar} / 4$

Ar (40u) and O₂(32u) molecules have similar mass, hence $\overline{v}_{Ar} \approx \overline{v}_{O_2}$

Hence

$$f = \frac{10^{-6} mbar}{10^3 mbar} = 10^{-9}$$

ie very pure Ar required (only $1 O_2$ in 10^9 Ar).

(d) Ellipsometry would be a suitable choice to measure film thickness. The change in light polarisation upon reflection from film/interface is thereby detected. Given optical transparency and known optical properties, the film thickness can be calculated (see lecture notes).

(e) (i) In XPS, the sample is irradiated with (relatively low energy) X-rays and the absorption of these photons results in the ejection of electrons via the photoelectric effect. The kinetic energy of the emitted photoelectrons is given by $E_{kin} = \frac{hc}{\lambda} - E_b$ where E_{kin} , hc/λ and E_b are energies for the ejected e-, incident photon and involved bound electron state, respectively. Since values of the binding energy are element specific, atomic identification and characterisation of elemental composition is possible through measurement of photoelectron energies and number of photoelectrons. E_b also depends on electron density of atom (screening of core electrons) and narrow XPS linewidths allow these so called chemical shifts to be resolved. Hence a determination of the chemical state/bonding environment of detected elements is possible (see lecture notes). Typical

[20%]

[10%]

[15%]

XPS detection limits are 0.1 at%, which is not sufficient to resolve Si doping concentrations in the ppm level.

(ii) Increasing the X-ray excitation energy leads to higher kinetic energies of the photoelectrons (see above). Since the escape depth of photoelectrons depends on their energy via the so-called universal curve (given in lecture notes, e- mean free path increases for increasing energies (>50 eV)), depth resolved XPS can be achieved by measuring the same core-level signature for different X-ray excitation energies (the higher the X-ray excitation energies (the higher the X-ray excitation energy the higher the information depth). XPS is highly surface-sensitive. The universal curve shows that electron mean free paths are sub-1nm for electron energies from 50-500 eV, hence information depth is sub-5 nm (i.e. 95% of all detected electrons originate from 3λ , where λ is the electron mean free path).



The display is split into a series of pixels which make up the total image. Light from back light source passes through a polariser. It then passes through the liquid crystal that can rotate the plane of polarisation, depending on the voltage across it. The light then passes through a crossed polariser. Only if light is rotated does light come through. Hence this behaves as a voltage controlled light valve. There is one for each colour.

(b)

4(a)



[20%]

[15%]

TFT = gate electrode a bottom, gate insulator (silicon nitride not SiO_2), conductive a-Si layer (instead of c-Si), followed by source and drain electrodes (Cr).

The TFT operates like a standard FET. The a-Si:H is undoped and the FET operates in enhancement mode, with electrons are the majority carrier. A positive voltage on the gate induces excess electrons in the channel, some of which are mobile electrons in extended states. These flow from source to drain under the influence of the s-d voltage. The electrons must cross over from top (source) to bottom (gate side) and back to top (drain) of the channel to flow all the way down the channel, which adds excess resistance. The FET is on for positive gate voltages and off for negative gate voltages.

The TFT operates just as a standard MOSFET, except that its materials are thin films, that it is back gate, not top gate, and that it uses Si nitride not Si oxide as gate insulator.



The density of states of a-Si is based on that of c-Si, with a valence band and conduction band in the same energy ranges. There is still a band gap in a-Si. The disorder causes broadening of CB and VB states into the gap – the band tails. There are also defect states in the middle of the gap.

The main band states are extended, and can conduct electricity at 0 K. Those in gap and the defect states are localised, and do not conduct electricity, except under high fields or above 0 K.

Mobility of a-Si $\sim 1 \text{ cm}^2/\text{Vs}$

(d) (i) The defect is the Si dangling bond, which appears in the band structure as follows;

[25%]



(ii) Role of hydrogen. H is used to passivate the defects – remove the gap states in a-Si. The midgap states are due to dangling bonds, and the H makes Si-H bonds, thereby removing them. The H also sits in weak Si-Si bonds, thereby sharpening up the band tails. This reduces defect density from 1E20 to 1E16 cm-3 and improves mobility.

(e) Carbon nanotubes can be placed as a mat or assembly, for example by dispersing in a liquid and then depositing on an insulating layer (eg glass). CNTs on average are a mixture of metallic and semiconducting tubes. It is necessary to remove the metallic tubes, otherwise you cannot turn the transistor off. This can be done by some sort of chemical sorting process, or by making the transistor and burning out the metallic tubes by passing a high current through them.

5(a)



[20%]

(b) Interconnects were recently Al, changed to Cu for higher conductivity, will change ultimately to carbon nanotubes. Need for higher conductivity

Gate oxide will change from SiO_2 to a high dielectric constant (K) oxide such as HfO_2 this year. Need for higher K so that oxide can be thicker to stop gate leakage.

Channel semiconductor will be changed to a higher mobility substrate like strained Si, or SiGe alloy. Need for high mobility to get higher channel current for a given gate voltage.

Interconnect dielectric. SiO2 is replaced by a low K dielectric such as SiOx-CHx alloy. [20%]

(c)(i)



As defect states (dangling bonds) are not forming a bond, their states form energy levels which lie at the energy of the unbonded state. These lie between bonding and antibonding levels. Hence they lie in the middle of the band gap.

Some times defects are created in response to doping. Sometimes, by ion implantation. Sometimes by lattice mismatch. [20%]

(ii) Defects are undesirable because they allow carriers to recombine. This lowers the photoefficiency of lasers and photo-diodes. It also reduces the gain of transistors.



It also reduces the doping efficiency because donor electrons fall down into the defect levels.



[20%]

(d) Defect states due to dangling bonds are monovalent. They are passivated by monovalent elements like hydrogen or F. They form Si-H bonds, whose states lie well outside the band gap.

Surface states come from the dangling/broken bonds on the surface. They are usually passivated by oxidation. This turns the DBs into Si-O bonds. The states of the Si-O bonds lie well away from the band gap, so it passivates them. [20%]



Grammer's comments:

Quession 1

A popular question. The description of the Bean model in (a) was generally briet, although the process to magnetise a bulk superconductor was understood well. Most candidates were able to derive the equation in (b), although few were able to sketch the field and current distribution for an inverse field dependence for J. The calculation in part (c) was generally done well.

Question 2

A popular and straightforward question, answered very well by most candidates. A common source of lost marks in (a) was for lack of detail in describing the properties of ferroelectrics. Parts (b) and (c) were generally answered well, although details of the calculation were frequently omitted in (c), even though the correct rank order was determined.



This was a question about thin film transistors (TFTs) and the properties of amorphous silicon that goes into them. The question was generally answered well, with relatively few mistakes. The candidates generally lost marks because of lack of detail. Few students were able to answer the final part of the question on large area TFTs made from carbon nanotubes. Some candidates assumed that it was a question about CNTs for another application.

question 5:

This was a question about the materials used in CMOS, and scaling, and was a popular question. Candidates answered the first part about the MOSFET well, and the replacement of the different materials. Candidates were less good at describing the nature of defects and their limitation in the second half of the question, giving rather simple answers, especially for the role of SiO_2 in surface passivation where no one was able to give the correct diagram.