IMPERIAL COLLEGE LONDON

DEPARTMENT OF ELECTRICAL AND ELECTRONIC ENGINEERING
EXAMINATIONS 2009

EEE PART I: MEng, BEng and ACGI

Corrected Copy Q4

ELECTRONIC MATERIALS

Monday, 1 June 10:00 am

Time allowed: 2:00 hours

There are FOUR questions on this paper.

Q1 is compulsory.
Answer Q1 and any two of questions 2-4.
Q1 carries 40% of the marks. Questions 2 to 4 carry equal marks (30% each).

Any special instructions for invigilators and information for candidates are on page 1.

Examiners responsible	First Marker(s) :	W.T. Pike, W.T. Pike
	Second Marker(s) :	T.J. Tate, T.J. Tate

Special instructions for students

Fundamental constants

Permittivity of free space, ε_0 = 8.85 x 10^{-12} F/m
Permeability of free space, μ_0 = 4π x 10^{-7} H/m
Planck's constant, h = 6.6 x 10^{-34} Js
Boltzmann's constant, k = 1.38 x 10^{-23} J/K
Electron charge, e = 1.6 x 10^{-19} C
Electron mass, m = 9.1 x 10^{-31} kg
Speed of light, c = 3.0 x 10^8 ms^{-1}

Schrödinger's equation

General form:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(\mathbf{r})\psi(\mathbf{r})=E\psi(\mathbf{r})$$

In one dimension:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

In radial coordinates:

$$\nabla^2=\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}$$

Free-electron theory

Density of states (3D):

$$g(E)=\frac{1}{\pi^2\hbar^3}(m)^{3/2}\sqrt{2E}$$

Fermi energy

$$E_f=\frac{\hbar^2\pi^2}{2m}\left(\frac{3n}{\pi}\right)^{2/3}$$

Fermi distribution

$$f(E)=\frac{1}{1+\exp\left(\frac{E-E_f}{kT}\right)}$$

Electrons in semiconductors

Effective mass:

$$m_e^*=\frac{\hbar^2}{d^2E(k)/dk^2}$$

Concentration of electrons in a semiconductor of bandgap E_g:

$$n = \frac{1}{\sqrt{2}h^3}\left(\frac{m_e^* kT}{\pi}\right)^{3/2} e^{-\frac{(E_g - E_f)}{kT}}$$
$$= N_c e^{-\frac{(E_g - E_f)}{kT}}$$

Concentration of holes

$$p = \frac{1}{\sqrt{2}h^3}\left(\frac{m_h^* kT}{\pi}\right)^{3/2} e^{-\frac{E_f}{kT}}$$
$$= N_v e^{-\frac{E_f}{kT}}$$

Polarization

Lorentz correction for local field:

$$\mathbb{E}_{loc} = \mathbb{E} + \frac{\mathbb{P}}{3\varepsilon_0}$$

Electronic polarization:

$$P_0 = \frac{\varepsilon_0 \omega_p^2 E_0}{\omega_m^2 - \omega^2 + j\omega\gamma}$$

where

$$\gamma = \frac{r}{m},$$
$$\omega_m^2 = \omega_0^2 - \frac{\omega_p^2}{3},$$
$$\omega_0^2 = k/m,$$
$$\omega_p^2 = \frac{ne^2}{m\varepsilon_0}.$$

Orientational Polarization:

Static:

$\mathrm{P} = n\mu\, \mathrm{L}(\mu E/kT)$ where $\mathrm{L}(x) = \coth(x) - 1/x$

Dynamic:

$$P_0 = \frac{P_s}{1 + \mathrm{j}\omega\tau},$$

Magnetism

Magnet dipole due to electron angular momentum:

$$\mathbf{\mu}_m = -\frac{e\mathbf{L}}{2m}$$

Magnet dipole due to electron spin:

$$\mathbf{\mu}_m = -\frac{e\mathbf{S}}{m}$$

Paramagnetism:

$$M = n\mu_m \mathrm{L}\left(\frac{\mu_m \mu_0 H}{kT}\right)$$

The Questions

1. [Compulsory]

a) If a material with a Young's modulus E has a negative Poisson's ratio ν, and experiences a compressive stress σ along one axis, what will be the resulting strain in direction perpendicular to the stress? [4]

b) Draw the shapes of the wavefunctions occupied by the four highest energy electrons in an atom of crystalline silicon. [4]

c) Heisenberg's uncertainty principle gives the relationship:

$$\Delta E \Delta t \geq \hbar/2$$

Show that for a photon whose wavepacket extends over 1 ns the range of frequencies in the wavepacket will be at least 80 MHz. [4]

d) The second moment of area for a rectangular beam is given by $\frac{1}{12}wt^3$ where w is the width and t the thickness of the beam and the neutral axis is as shown by the dashed line below. If $w = 2t$ what will be the ratio of deflections if the beam is loaded in the x or y directions?

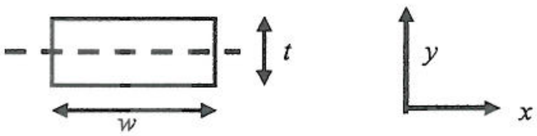


Fig. 1d: Cross section of a cantilever flat and edge on, with the direction of loading shown. [4]

e) Draw the free-body diagram for the pen you are holding as you mark a dot on the exam booklet. [4]

f) Draw two plots of the B-H diagram for a strong and weak magnet on the same set of axes. [4]

g) A block of a dielectric is placed in a uniform electric field. Explain how surface charges are formed on the dielectric. [4]

h) Why do holes have a positive mass and positive charge? [4]

i) Why is the occupancy of an electron state at the Fermi level independent of temperature? [4]

j) Why does increased scattering of electrons in a material lead to a drop in its conductivity? [4]

2.

a) Show that if the dielectric constant of the material used in a parallel plate capacitor is complex, $\varepsilon_r = \varepsilon_r' - j\varepsilon_r''$, the capacitor will behave as an ideal capacitor and resistor in parallel, with the leakage resistance given by $R = d/(\omega\varepsilon_0\varepsilon_r''A)$ where d is the spacing and A the area of the plates of the capacitor and ω is the angular frequency of the voltage across the capacitor. [12]

b) Hence show that the fractional power loss of the capacitor is given by $\varepsilon_r''/\varepsilon_r'$. [12]

c) Describe three mechanisms and their frequency ranges that can give rise to power loss in a capacitor. [6]

3.

a) The potential $V(r)$ between two atoms separated by a distance r can be modelled by

$$V(r) = \frac{A}{r^6} - \frac{B}{r}$$

Sketch the plot of the force, $F(r)$, between the atoms indicating on the plot the value of the equilibrium spacing r_0 and the spring constant, or bond strength, k. [6]

Derive an expression for r_0. [4]

b) Show that Young's modulus, E, along one of the axes of a cubic material is given by $E = k/r_0$. [8]

c) Show that the bond length for sodium chloride is 0.28 nm given that it has a relative density of 2.2, sodium has an atomic weight of 23, and chlorine 35.5. Avogadro's number is 6.0 x 10^{23}. [8]

Hence calculate a bond strength for a Young's modulus of 40 GPa [4]

4.

a) Explain why the radial form of Schroedinger's equation for the hydrogen atom can be written as:

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi(r)}{dr^2}+\frac{2}{r}\frac{d\psi(r)}{dr}\right)-\frac{e^2}{4\pi\varepsilon_0 r}\psi(r)=E\psi(r)$$

X → r

defining all the terms. [4]

Demonstrate that a possible solution is given by $\psi(r)=\psi_0 e^{-ar}$ and show that the energy of this state is -13.6 eV. [10]

b) Explain how the result for the hydrogen atom can be used to analyse the wavefunction of a donor electron in phophorous-doped silicon, and derive a value for the energy required to promote a donor electron into the conduction band. The relative dielectric constant of silicon is 11.8. [7]

c) Draw band-gap diagrams for n-type silicon indicating the distribution of electrons when it is in the following temperature regimes:

(i) intrinsic,

(ii) extrinsic,

(iii) freeze-out. [9]

E1.5 Electronic Materials

The Answers 2009

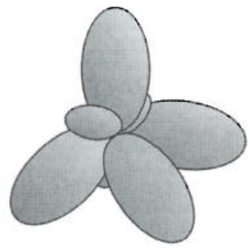
1. [Compulsory]

a) *If a material with a Young's modulus E has a negative Poisson's ratio ν, and experiences a compressive stress σ along one axis, what will be the resulting strain perpendicular to the stress?* [4]

The strain along the axis will be $-\sigma/E$ and so the strain along the perpendicular direction will be $-(-\nu) \times (-\sigma/E)$ so the strain will be $-\nu\sigma/E$, a contraction.

[new application of theory]

b) *Draw the shapes of the wavefunctions occupied by the four highest energy electrons in an atom of crystalline silicon.* [4]



[bookwork]

c) *Heisenberg's uncertainty principle gives the relationship:*

$$\Delta E \Delta t \geq \hbar/2$$

Show that for a photon whose wavepacket extends over 1 ns the range of frequencies in the wavepacket will be at least 80 MHz. [4]

As

$E = hf$,

$\Delta E = h\Delta f$.

Substituting into the uncertainty relationship:

$$\Delta E \geq \frac{\hbar}{2\Delta t}$$

$$h\Delta f \geq \frac{\hbar}{2\Delta t}$$

$$\Delta f \geq \frac{1}{4\pi\Delta t}$$

Hence if Δt = 1 ns, ΔF >/= 80 MHz [new application of theory]

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d) *The second moment of area for a rectangular beam is given by* $\frac{wt^3}{12}$ *where w is the width and t the thickness of the beam and the neutral axis is as shown below. If w = 2t what will be the ratio of deflections if the beam is loaded in the Y or X directions?*

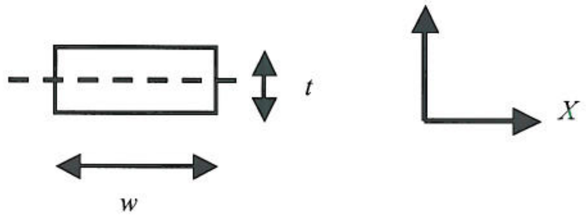


Fig. 1: Cross section of a cantilever beam with the neutral axis shown as a dotted line. [4]

The deflection is proportional to the second moment of area I,

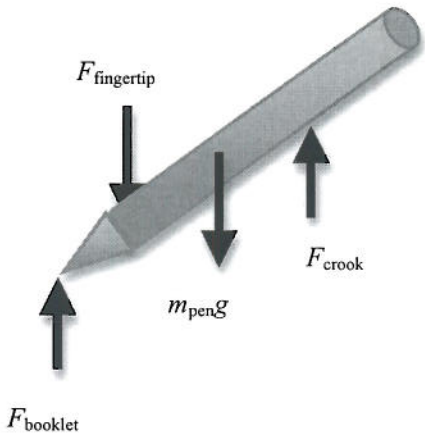
$$I_{flat} = \frac{wt^3}{12}$$

$$I_{edge} = \frac{tw^3}{12}$$

$$\frac{d_{flat}}{d_{edge}} = \frac{I_{flat}}{I_{edge}} = \frac{t^2}{w^2} = \frac{1}{4}$$

[new application of theory]

e) *Draw the free-body diagram for the pen you are holding as you mark a dot on the exam booklet.* *[4]*



[new application of theory]

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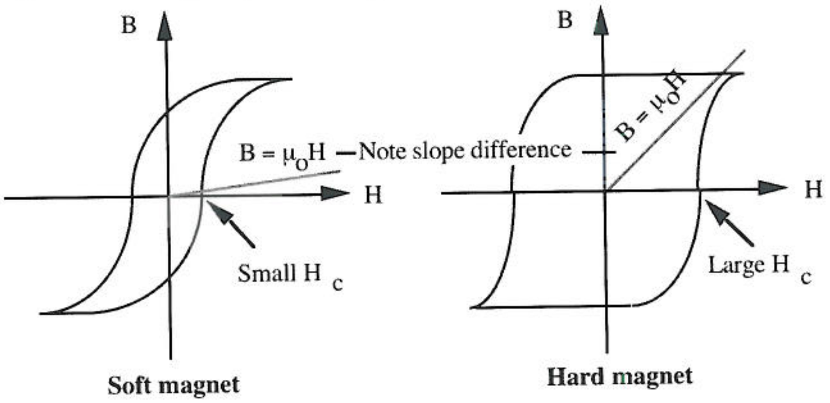
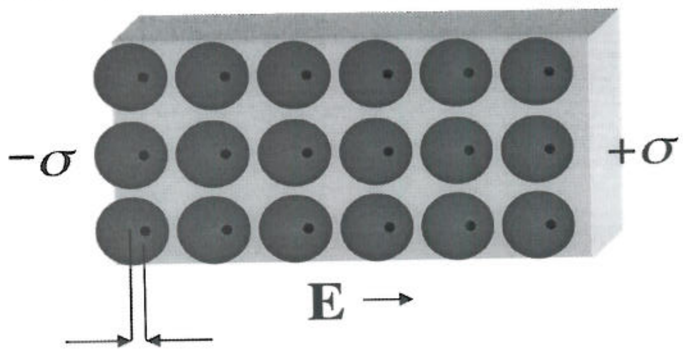
f) *Draw two plots of the B-H diagram for a strong and weak magnet.* [4]



[bookwork]

g) *A block of a dielectric is placed in a uniform electric field. Explain how surface charges are formed on the dielectric.* [4]



The electric field attracts the electrons, producing a displacement of their charge distribution and surface charge as shown. [bookwork]

h) *Why do holes have positive mass and positive charge?* [4]

Holes are produced by an unoccupied state at the top of the valence band of a semiconductor. As these stateshave a negative mass, if that negative mass is removed it leaves an unoccupied state with a positive charge and a positive mass.

i) *Why is the occupancy of an electron state at the Fermi level independent of temperature?*

The Fermi distribution is given by:

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_f}{kT}\right)}$$

When $E = E_f$, $f(E) = 0.5$ and is independent of temperature. [4]

j) *Why does increased scattering of electrons in a material lead to a drop in conductivity?*

Conduction is due to the movement of electrons under an electron field in a material. The electrons are accelerated by the field but repeatedly scatter due to collision with atoms of the material. Scattering resets an electron velocity back to an average of zero. Hence the more the scattering, the less time the electron has to accelerate under the field, and the

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lower the average velocity. As the current and conductivity are proportional to the average velocity, as the scattering increases, the conductivity drops.

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2.

a) *Show that if the dielectric constant of the material used in a parallel plate capacitor is complex, $\varepsilon_r = \varepsilon_r' - j\varepsilon_r''$, the capacitor will behave as a capacitor and resistor in parallel, with the leakage resistance given by $R = d/(\omega\varepsilon_0\varepsilon_r''A)$ where d is the spacing and A the area of the plates of the capacitor and ω is the angular frequency of the voltage across the capacitor.*

$$C = \frac{\varepsilon_0\varepsilon_r A}{d}$$
$$= \frac{\varepsilon_0(\varepsilon_r' - j\varepsilon_r'')A}{d}$$

[12]

The admittance is given by

$$Y = j\omega C$$
$$= \frac{j\omega\varepsilon_0\varepsilon_r'A + \omega\varepsilon_0\varepsilon_r''A}{d}$$
$$= Y_{Ceff} + Y_R; \quad C_{eff} = \frac{\varepsilon_0\varepsilon_r'A}{d}, \quad R = \frac{d}{\omega\varepsilon_0\varepsilon_r''A}$$

which is equivalent to a capacitor and resistor in parallel with the leakage resistance as required.

At DC the resistance will be infinite and the capacitor will behave as a pure capacitance.

b) *Hence show that the fractional power loss of the capacitor is given by $\varepsilon_r''/\varepsilon_r'$.* [12]

Both the effective resistor and capacitor will experience the same voltage though the current in the capacitor will be in quadrature with the current and hence power will be conserved while the current in the resistor will be in phase and hence dissipated. The ratio of power lost in the resistor to power conserved in the capacitor will therefore be:

$$\frac{V^2Y_R}{V^2\left|Y_{Ceff}\right|} = \frac{\omega\varepsilon_0\varepsilon_r''A}{\omega\varepsilon_0\varepsilon_r'A}$$
$$= \frac{\varepsilon_r''}{\varepsilon_r'}$$

[12]

[new application of theory]

c) *Describe three mechanisms and their frequency ranges that can give rise to power loss in a capacitor.*

At optical frequencies losses will be associated with damped oscillations of valence electrons. At infrared frequencies oscillations of atoms will absorb energy. At radio frequencies the flipping of dipoles, or orientational polarisation, is important. [6]

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3.

a) *The potential V(r) between two atoms separated by a distance r can be modelled by*

$$V(r) = \frac{A}{r^6} - \frac{B}{r}$$

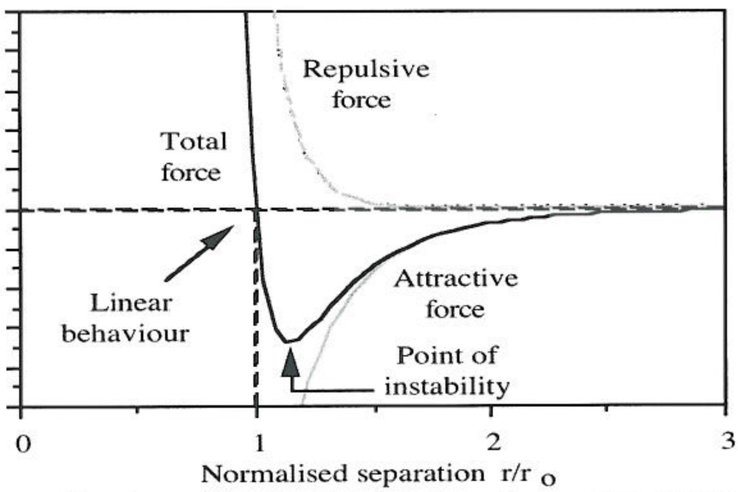
Derive and sketch the plot of the force, F(r), between the atoms indicating on the plot the value of the equilibrium spacing r_0 and the spring constant, or bond strength, k. [6]

Derive an expression for r_0. [4]

The force is given by:

$$F(r) = -\frac{dV(r)}{dr} = \frac{6A}{r^7} - \frac{B}{r^2}$$

which can be plotted as



The slope of the plot at r_0 gives the spring constant of the bond.

[bookwork]

r_0 is obtained from:

$$F(r_0) = 0 \Rightarrow$$

$$\frac{6A}{r^7} - \frac{B}{r^2} = 0$$

$$r^5 = \frac{6A}{B}$$

$$r_0 = \left(\frac{6A}{B}\right)^{1/5}$$

[new application of theory]

b) *Show that Young's modulus, E, along one of the axes of a cubic material is given by $E = k/r_0$.*
A elastic material can be modelled as a lattice of springs connecting the atoms. In a cubic material there will be one spring per area of unit cell. If an external tensile stress, σ, is applied along one of the axes, it will produce a force $F = \sigma r_0^2$ on each bond, which from F=kx will

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produce an increase in the bond length of $\sigma r_0^2/k$. This is a strain of $\varepsilon = \sigma r_0/k$ which will be felt in the material as a whole. As

$$\sigma = E\varepsilon,$$

$$E = \frac{\sigma}{\varepsilon}$$

$$= \frac{\sigma}{\sigma r_0 / k}$$

$$= \frac{k}{r_0}$$

[bookwork]

[8]

c) *Show that the bond length for sodium chloride is 0.28 nm given that it has a relative density of 2.2, sodium and chlorine have an atomic mass of 23 and 35.5 respectively. Avogadro's number is 6.0×10^{23}..* *[8]*

Hence calculate a bond strength for a Young's modulus of 40 GPa. [4]

To find the atomic spacing from the density and atomic masses, consider a unit cell of NaCl which is a cube of size $2r_o$. It contains 4 atoms of Na and 4 of Cl, and therefore has a mass of (4 x 23+4x35.5)X0.001/6.0x10^{23}g =39x10^{-23}g. Hence if the density of NaCl is 2.2 g/cm3, the volume of a unit cell will be 17.7 x 10^{-29} m from which r_o is given by (17.7 x $10^{-29})^{1/3}$/2= 0.28 nm.

[new calculation]

From the above,

$$k = Er_0$$

$$= 0.28 \times 10^{-9} \times 40 \times 10^{9}$$

$$= 11.2\, N/m$$

[new calculation]

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4. a) *Explain why the radial form of Schroedinger's equation for the hydrogen atom can be written as:*

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi(r)}{dx^2}+\frac{2}{r}\frac{d\psi(r)}{dx}\right)-\frac{e^2}{4\pi\varepsilon_0 r}\psi(x)=E\psi(x)$$

defining all the terms. Demonstrate that a possible solution is given by $\psi(r)=\psi_0 e^{-ax}$ *and show that the energy of this state is -13.6 eV.* [12]

In the general form of S.E.:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V(\mathbf{r})\psi(\mathbf{r})=E\psi(\mathbf{r})$$

where $\hbar$ is Planck's constant divided by 2π, m is the mass of the electron, ψ its wavefunction, $\mathbf{r}$ its position, V the potential and E its energy, substitute

$$\nabla^2=\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}$$

and

$$V(\mathbf{r})=\frac{-e^2}{4\pi\varepsilon_0 r}$$

for the coulomb potential of the proton, where e is the charge of the electron, and ε_0 the dielectric constant of vacuum. [4]

Substituting:

$$\psi(r)=\psi_0 e^{-ar}$$

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi(r)}{dx^2}+\frac{2}{r}\frac{d\psi(r)}{dx}\right)-\frac{e^2}{4\pi\varepsilon_0 r}\psi(x)=E\psi(x)$$

$$-\frac{\hbar^2}{2m}\left(a^2\psi_0 e^{-ar}-\frac{2a}{r}\psi_0 e^{-ar}\right)-\frac{e^2}{4\pi\varepsilon_0 r}\psi_0 e^{-ar}=E\psi_0 e^{-ar}$$

Solving for coefficients separately:

$$E=-\frac{\hbar^2}{2m}a^2$$

$$a=\frac{me^2}{4\hbar^2\pi\varepsilon_0}$$

From which

$$E=-\frac{me^4}{32\pi^2\varepsilon_o{}^2\hbar^2}=-13.6\text{eV}$$

[bookwork] [10]

b) *Explain how this result for the hydrogen atom can be used to analyse the wavefunction of a donor electron in phosphorus-doped silicon, and derive a value for the energy required to promote a donor* *electron into the conduction band. The relative dielectric constant of silicon is 11.8.* [7]

A phosphor donor atom has an additional proton and electron to the silicon atom it replaces. Hence it is possible to analyse the additional electron and proton as a hydrogen-like atom, but with the vacuum of the hydrogen atom replaced by bulk silicon. This is justified if the extent of the wavefunction is considerably greater than the spacing of the silicon atoms.

Modelling the donor electron in this fashion, the previous results need only have relative dielectric constant of silicon included in the formulae. Hence for the energy:

$$E = -\frac{me^4}{32\pi^2\varepsilon_o^2\varepsilon_r^2\hbar^2} = \frac{-13.6\text{eV}}{11.8^2} = -0.098\,eV$$

c) *Draw band-gap diagrams for n-type silicon indicating the distribution of electrons when it is in the following temperature regimes:*

(i) intrinsic,

(ii) extrinsic

(iii) freeze-out

[9]