# Slides
# Condensed Matter Physics
# Revision Lecture 1

# HOMEWORKS:

Go to my website for commentary

# Problem Set 1

Einstein, Debye, Drude, and Free Electron Models

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## 1.1. Einstein Solid

(a) **Classical Einstein Solid (or "Boltzmann" Solid):**
Consider a single harmonic oscillator in three dimensions with Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + \frac{k}{2}\mathbf{x}^2$$

▷ Calculate the classical partition function

$$Z = \int \frac{\mathbf{dp}}{(2\pi\hbar)^3} \int \mathbf{dx}\, e^{-\beta H(\mathbf{p},\mathbf{x})}$$

Note: in this problem $\mathbf{p}$ and $\mathbf{x}$ are three dimensional vectors (they should appear bold to indicate this unless your printer is defective).

▷ Using the partition function, calculate the heat capacity $3k_B$.

▷ Conclude that if you can consider a solid to consist of $N$ atoms all in harmonic wells, then the heat capacity should be $3Nk_B = 3R$, in agreement with the law of Dulong and Petit.

(b) **Quantum Einstein Solid:** Now consider the same Hamiltonian quantum mechanically.

▷ Calculate the quantum partition function

$$Z = \sum_j e^{-\beta E_j}$$

where the sum over $j$ is a sum over all Eigenstates.

the classical calculation has never been on the condensed matter exam (although it is examinable)

The quantum Einstein model could be on the exam (albeit rarely)

1.2. **Debye Theory:**

(a)‡ State the assumptions of the Debye model of heat capacity of a solid.

Debye Model is very frequently examined!

▷ Derive the Debye heat capacity as a function of temperature (you will have to leave the final result in terms of an integral that cannot be done analytically).

▷ From the final result, obtain the high and low temperature limits of the heat capacity analytically.

You may find the following integral to be useful
$\int_0^\infty dx \frac{x^3}{e^x-1} = \sum_{n=1}^\infty \int_0^\infty x^3 e^{-nx} = 6\sum_{n=1}^\infty \frac{1}{n^4} = \frac{\pi^4}{15}$
By integrating by parts this can also be written as $\int_0^\infty dx \frac{x^4 e^x}{(e^x-1)^2} = \frac{4\pi^4}{15}$

(b) The following table gives the heat capacity $C$ for KCl as a function of temperature.

▷ Discuss, with reference to the Debye theory, and make an estimate of the Debye temperature.

Drude theory does show up on exams -- particularly in the context of semiconductors!

### 1.3. Drude Theory of Transport in Metals

(a) Assume a scattering time $\tau$ and use Drude theory to derive an expression for the conductivity of a metal.

(b) Define the resistivity matrix $\underset{\sim}{\rho}$ as $\vec{E} = \underset{\sim}{\rho}\vec{j}$.

▷ Use Drude theory to derive an expression for the matrix $\underset{\sim}{\rho}$ for a metal in a magnetic field. (You might find it convenient to assume $\vec{B}$ parallel to the $\hat{z}$ axis. The under-tilde notation means that the quantity $\underset{\sim}{\rho}$ is a matrix.)

▷ Invert this matrix to obtain an expression for the conductivity matrix $\underset{\sim}{\sigma}$.

(c) Define the Hall coefficient.

▷ Estimate the magnitude of the Hall voltage for a specimen of sodium in the form of a rod of rectangular cross section 5mm by 5mm carrying a current of 1A in a magnetic field of 1T. The density of sodium atoms is roughly 1 gram/cm$^3$, and sodium has atomic mass of roughly 23. You may assume that there is one free electron per sodium atom (Sodium has *valence* one).

▷ What practical difficulties would there be in measuring the Hall voltage and resistivity of such a specimen (and how might these difficulties be addressed).

(d) What properties of metals does Drude theory not explain well?

AC Drude theory is probably too hard for an exam.

(e)* Consider now an applied AC field $\vec{E} \sim e^{i\omega t}$ which induces an AC current $\vec{j} \sim e^{i\omega t}$. Modify the above calculation (in the presence of a magnetic field) to obtain an expression for the complex AC conductivity matrix $\underset{\sim}{\sigma}(\omega)$. For simplicity in this case you may assume that the metal is very clean, meaning that $\tau \to \infty$, and you may assume that $\vec{E} \perp \vec{B}$. You might again find it convenient to assume $\vec{B}$ parallel to the $\hat{z}$ axis. (This problem might look hard,

ETC…. SEE MY WEBSITE

# PROBLEMS FROM PAST PAPERS

go to my website
for commentary on
papers from 1996-2010

B Paper 2010

Q1. On Syllabus. End of part d is tricky and was not really covered, but could be deduced by a perceptive student.

Q2. On Syllabus. The [7] point part is tricky

Q3. On Syllabus.

Q4. On Syllabus

Q5. On syllabus.

Q6. The first two parts are mostly on syllabus, although we covered them only very briefly. The final part about constructing a laser is certainly not. The students should be able to deduce the density of states of a 2d electron gas. Figuring out how the multiple states in a quantum well change this density of states would require some thinking and was not covered (but clever students might get it).

Q7,8 Not on syllabus

B Paper 2009.

Q1. On syllabus. This question is solved in great detail in my lecture notes (note also there is an error in the height of data point e of the plot. Discussed in my lecture notes page 136)

Q2. On syllabus.

Q3. On syllabus.

ETC !!!!
SEE MY WEBSITE!

STATISTICAL ANALYSIS
OF PAST PAPERS (2004-2011)

on my website

| Topic | Subtopic | Year = | 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | # of Times | | | | | | | | |
| **Something About Phonons** | | 8 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Define Phonon | | 1 | 1 | | | | | | | |
| Phonon Density of States | | 1 | | | | | | 1 | | |
| | In 2d | 1 | | | | | | 1 | | |
| | In 1d / diatomic | 1 | | | | 1 | | | | |
| How would you measure phonons (light/neutrons) | | 2 | | 1 | | 1 | | | | |
| Why is there a degeneracy of modes at... | | 2 | | 1 | | | | | 1 | |
| Debye Specific Heat | | 3 | | 1 | 1 | | | 1 | | |
| | Derivation in 3d | 1 | | | 1 | | | | | |
| | Derivation In 2d | 2 | | 1 | | | | 1 | | |
| | Derivation In 1d | 1 | | | 1 | | | | | |
| How many/ what kind of (acoustic/optical/transverse/longitudinal) phonon | | 4 | | | | 1 | 1 | 1 | 1 | |
| Describe Motion of acoustic/optical modes | | 4 | 1 | | | 1 | 1 | 1 | | |
| Some Sort of Harmonic Chain | | 6 | | 1 | 1 | 1 | 1 | | 1 | 1 |
| | Diatomic with Two Masses | 2 | | | | 1 | 1 | | | |
| | Monatomic | 2 | | | 1 | | | | | 1 |
| | Alternating Sprint Constants | 2 | | 1 | | | | | 1 | |
| | monatomic limit of diatomic | 2 | | 1 | | | 1 | | | |
| Sketch Dispersions / monotomic diatomic | | 2 | 1 | | | | | | | 1 |
| **Something about the Free Electron Gas** | | 5 | | 1 | | 1 | 1 | 1 | 1 | |
| Derive Specific Heat of Fermi Gas | | 2 | | 1 | | 1 | | | | |
| Define Fermi Energy / Fermi Surface | | 2 | | | | | 1 | | 1 | |
| Density of States of Free Electron Gas | | 3 | | 1 | | | 1 | | 1 | |
| | Definition of | 1 | | | | | 1 | | | |
| | Derivation In 3d | 1 | | | | | | | 1 | |
| | Derivation In 2d | 2 | | 1 | | | 0.5 | | 0.5 | |
| | Derivation In 1d | 0.5 | | | | | | 0.5 | | |
| Estimate a Fermi Energy / Relationship of N to Ef | | 3 | | 1 | | 1 | | 1 | | |

| Topic | Subtopic | # of Times | Year = 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|
| **Something about Band Structure/Semiconductor Physics** | | 8 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Nearly Free Electron Model (NFEM) | | 5 | | | 1 | | 1 | 1 | 1 | 1 |
| | Derive Gaps of NFEM at zone boundary | 3 | | | | | 1 | | 1 | 1 |
| | Draw Dispersion | 2 | | | | | | 1 | 1 | |
| | Describe Effective Mass | 2 | | | | | 1 | | 1 | |
| | Monovalent / Divalent - Metal/Insulator | 3 | | | | | 1 | 1 | 1 | |
| | Gaps open when doubling unit cell | 1 | | | | | | 1 | | |
| | Draw a fermi surface in 2d/3d for weak/strong potential | 2 | | | | | 1 | | | 1 |
| Tight Binding Band | | 1 | | | 1 | | | | | |
| | Describe Density of States | 1 | | | 1 | | | | | |
| | Describe opening of gap | 1 | | | 1 | | | | | |
| Define Effective Mass | | 3 | 1 | | | | 1 | 1 | | |
| Define Chemical Potential / Doping | | 1 | | | | | 1 | | | |
| Define Mobility | | 3 | 1 | | | | 1 | 1 | | |
| Define Conductivity | | 1 | | | | | | 1 | | |
| Define Hole | | 1 | | 1 | | | | | | |
| | Signs of velocity, energy, current, ... | 1 | | 1 | | | | | | |
| Law of Mass Action / formula for n(T,mu) | | 4 | | 1 | | 1 | 1 | | 1 | |
| | Derivation | 3 | | | | 1 | 1 | | 1 | |
| | Use to calculate some density/mu when doped | 3 | | 1 | | 1 | | | 1 | |
| Temperature dependence of semiconductors | | 2 | 1 | | | | 1 | | | |
| | Estimate band gap / doping from data | 1 | | | | | 1 | | | |
| | How this would be measured | 2 | 1 | | | | 1 | | | |
| How chemical potential changes with doping | | 1 | | 1 | | | | | | |
| Quantum Well | | 2.5 | | | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | |
| | Density of States in 2d | 1.5 | | | | 0.5 | 0.5 | | 0.5 | |
| | Density of States In 1d | 0.5 | | | | | | 0.5 | | |
| Optical Properties of Semiconductors | | 1 | | | | | | 1 | | |
| | Direct / Indirect Gap | 1 | | | | | | 1 | | |

| Topic | Subtopic | Year = | 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | # of Times | | | | | | | | |
| | States bound to donors | 1 | | | | | | 1 | | |
| Drude Theory | | 1 | | | | | | 1 | | |
| | Derive Hall Coefficient | 1 | | | | | | 1 | | |
| | Derive Conductivity/Mobility | 2 | | 1 | | | | 1 | | |
| | Extract mobility/density from experimental data | 1 | | | | | | 1 | | |

| Topic | Subtopic | Year = | 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | # of Times | | | | | | | | |
| **Something About Diffraction / Crystal Structure** | | 8 | | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Derive Structure Factor / Scattering Amplitude | | 5 | | 1 | 1 | | | 1 | | 1 | 1 |
| Calculate Interplanar distances | | 1 | | | 1 | | | | | | |
| Diffraction | | 5 | | 1 | | | | 1 | 1 | 1 | 1 |
| | Derive Systematic Absences | 2 | | | | | | | | 1 | 1 |
| | When two atoms scatter same; H not scattering | 2 | | | | 1 | | | | | 1 |
| | Analyze a Powder Diffraction Pattern | 3 | | 1 | | | 1 | | 1 | | |
| | Predict Diffraction Data | 2 | | | | 1 | | 1 | | | |
| | Write Down Structure Factor for X | 3 | | | | | | 1 | 1 | | 1 |
| | Identify a unit cell doubling | 2 | | 1 | 1 | | | | | | |
| Plan View | | 2 | | | | | | 1 | | 1 | |
| primitive vs conventional unit cell | | 4 | | | | 1 | | 1 | 1 | 1 | |
| Identify Lattice/Basis | | 2 | | | | 1 | | 1 | | | |
| Calculate Reciprocal Lattice | | 2 | | 1 | 1 | | | | | | |
| Wigner Seitz / Brillouin Zone Construction | | 2 | | 1 | | | | | | 1 | |
| Contrast neutron/xray | | 1 | | | | | | | 1 | | |
| Describe equipment for neutron/xray | | 2 | | 1 | 1 | | | | | | |

| Topic | Subtopic | Year = | 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | # of Times | | | | | | | | |
| **Something about magnetism** | | 7 | 1 | 1 | 1 | 1 | 1 | | 1 | 1 |
| | Define Para/Diamagnetism | 3 | | | 1 | | 1 | | 1 | |
| | Estimate Larmor Diamagnetism | 1 | | | 1 | | | | | |
| | Curie Law Derivation for Spin 1/2 | 3 | | | 1 | | 1 | | 1 | |
| | Derive Pauli Paramagnetism | 1 | | | | | 1 | | | |
| | Adiabatic Demagnetization | 1 | | | | | | | 1 | |
| | What is exchange J | 2 | 1 | | | 1 | | | | |
| | Molecular (mean) field | 5 | 1 | 1 | 1 | 1 | | | | 1 |
| | Relationship of J to Tc | 3 | | 1 | 1 | 1 | | | | |
| | What causes domains | 1 | 1 | | | | | | | |
| | Domain Relation to Hysteresis | 2 | 1 | | | 1 | | | | |
| | Derive Size of Bloch Wall | 1 | 1 | | | | | | | |

**3.** Explain what is meant by the following terms in relation to the electronic bandstructure: *Fermi energy, chemical potential, Fermi surface* and *effective mass.* [4]

Explain how a weak periodic potential in a (one-dimensional) crystal can lead to the formation of a *band gap*. Sketch and describe qualitatively how the band gap and effective masses close to the Brillouin zone boundaries change as the magnitude of the periodic potential is increased. [8]

A fictitious metal crystallises into a simple cubic lattice with lattice constant $a$ and one atom per lattice point. The potential in the crystal is weakly modulated with the periodicity of the lattice. Sketch the first Brillouin zone for this crystal. The metal is monovalent (that is, it has only one valence electron per unit cell). Describe the shape and dimensions of the Fermi surface if the modulation is extremely weak. What if it is somewhat weak (compared to the Fermi energy), but not extremely weak? A second metal has an identical unit cell, but is divalent (two valence electrons per unit cell). Give a qualitative description and sketch of the Fermi surface for this divalent metal. Discuss what happens in both the monovalent and divalent cases as the periodic potential becomes extremely strong. [8]

From 2008 Exam

From 2001 Exam

**5.** Explain briefly the origin of the electronic band gap in a typical electrical insulator. [6]

The periodic potential $V(x)$ experienced by an electron in a one-dimensional crystal may be given in the form

$$V(x) = V_0 + V_G\,\mathrm{e}^{-\mathrm{i}Gx} + V_{-G}\,\mathrm{e}^{+\mathrm{i}Gx},$$

where $G$ is the reciprocal lattice vector, and $|V_G| = |V_{-G}|$. Explain why a suitable wavefunction for an electron in such a potential may be written to a first approximation as

$$\psi(x) = A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{\mathrm{i}(k-G)x}. \qquad [3]$$

By substituting $\psi(x)$ into the Schrödinger equation and comparing coefficients in $\mathrm{e}^{\mathrm{i}kx}$ and $\mathrm{e}^{\mathrm{i}(k-G)x}$, show that the energy of an electron of mass $m$ and wavevector $k$ at the zone boundary is given by

$$E = V_0 + \frac{\hbar^2 k^2}{2m} \pm |V_G|\,.$$

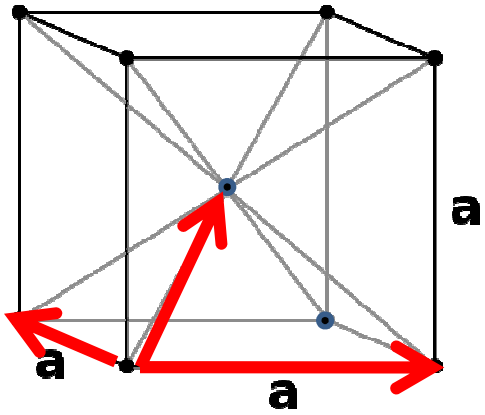
Discuss the significance of each of the three terms on the right-hand side of this equation in terms of band theory. [10]

Using this result explain why diamond is a good electrical insulator, whereas silicon and germanium, which have the same structure type as diamond, are semiconductors. (In the diamond structure there are two tetravalent atoms in the basis.) [6]

6.6. **Reciprocal Lattice**

Show that the reciprocal lattice of a FCC (face-centered-cubic) lattice is a BCC (body-centered-cubic) lattice. Correspondingly show that the reciprocal lattice of a BCC lattice is an FCC lattice. If an FCC lattice has conventional unit cell with lattice constant $a$, what is the lattice constant for the conventional unit cell of the reciprocal BCC lattice?

BCC



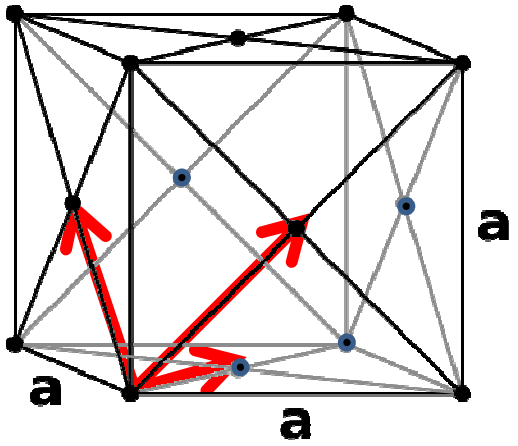

Primitive lattice vectors

$\mathbf{a}_1$=[1, 0,0] a

$\mathbf{a}_2$=[0, 1, 0] a

$\mathbf{a}_3$=[ ½, ½, ½] a

FCC

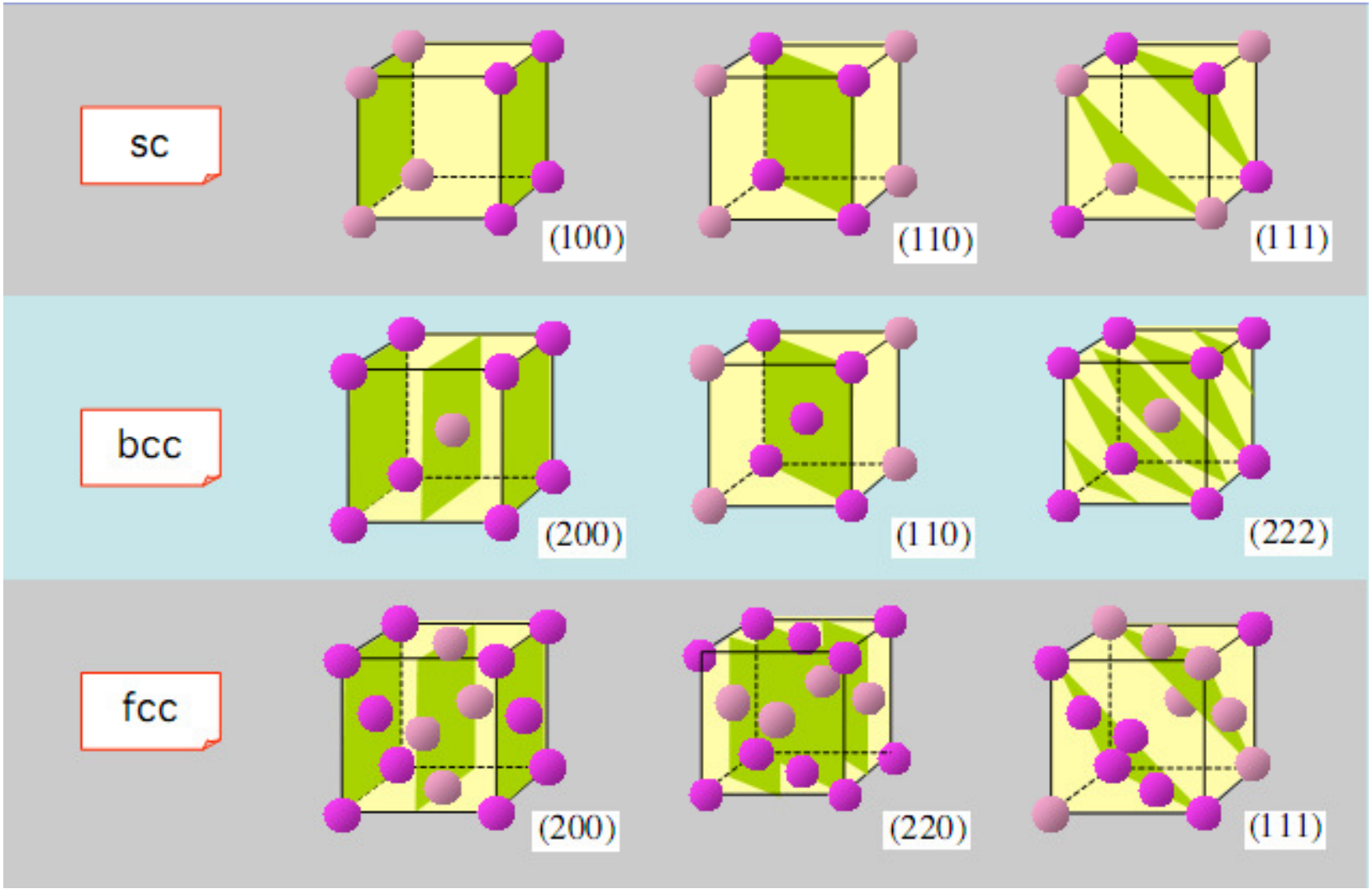



Primitive lattice vectors

$\mathbf{a}_1$=[½, ½, 0] a

$\mathbf{a}_2$=[0, ½, ½] a

$\mathbf{a}_3$=[½, 0, ½] a


sc
(100)
(110)
(111)
bcc
(200)
(110)
(222)
fcc
(200)
(220)
(111)

From Collection (2010 Exam)

**1.** Write down a formula for the structure factor $S(hkl)$, and find the condition for reflections to be missing in the diffraction pattern from *any* crystal whose lattice is all-face-centred. [5]

Silicon crystallises in a cubic structure whose lattice is face-centred with a basis [000] and $[\frac{1}{4}\frac{1}{4}\frac{1}{4}]$.

(a) Write out the fractional coordinates of *all* the atoms in the conventional unit cell of silicon.

(b) Sketch a plan diagram of the silicon structure viewed down the [001] axis. taking care to mark the axes and heights of the atoms within the unit cell.

(c) Write down the fractional coordinates of a centre of inversion symmetry in the structure.

(d) Show that reflections for which $h+k+l = 4n+2$ have zero intensity in a diffraction pattern. Careful measurements of the (222) reflection nevertheless do show a small amount of intensity: suggest a possible explanation for this. [11]

[Centre of inversion symmetry is when for every atom at $x, y, z$ there is an equivalent atom at $-x, -y, -z$.]

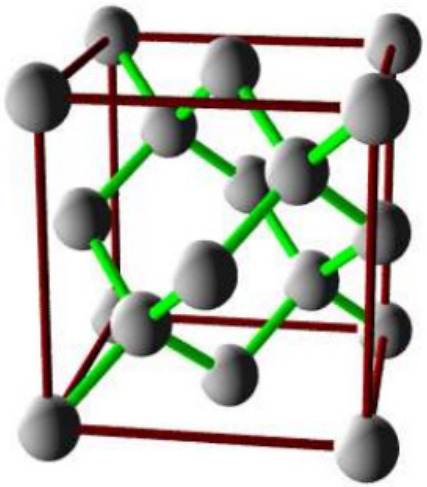
How many acoustic and optic branches are to be found in the phonon dispersion diagram of silicon? How many *distinct* branches would you expect along a (100) direction? [4]

# Diamond (C); also Si and Ge

Lattice = Cubic-F (fcc)

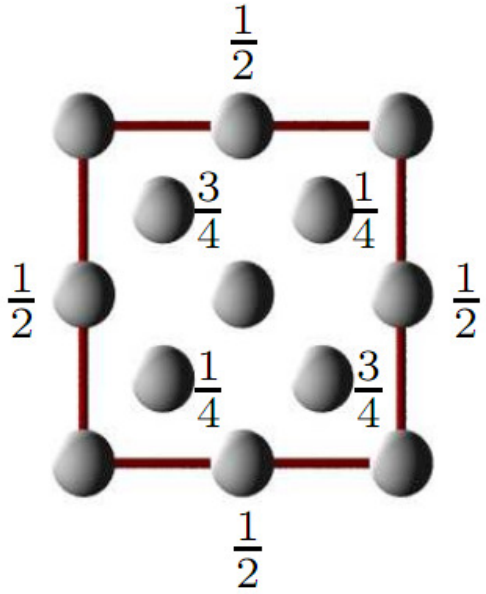
Basis = C at [000]

and C at $[\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4}]$



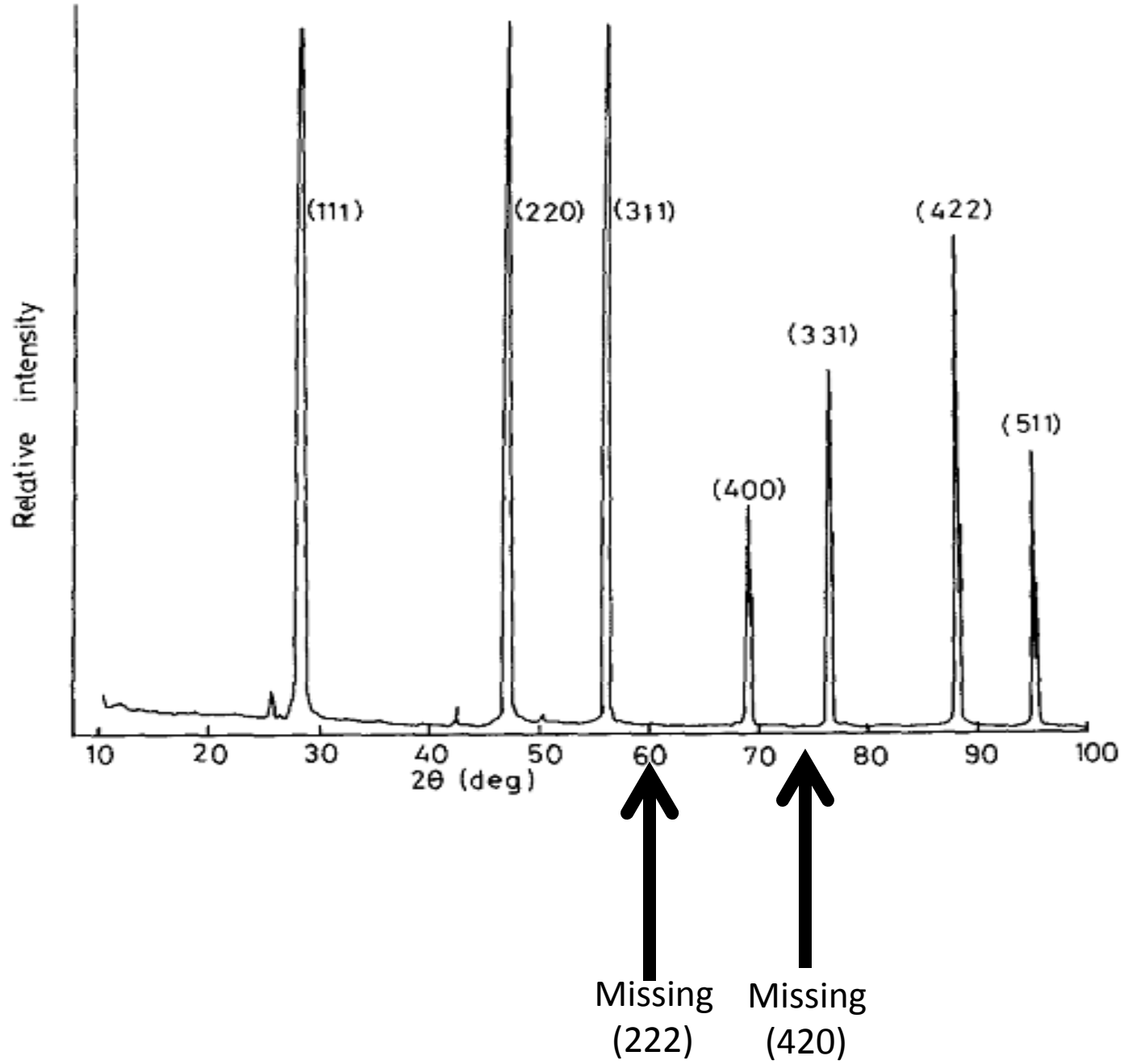
Plan View

unlabled points at $z = 0, 1$

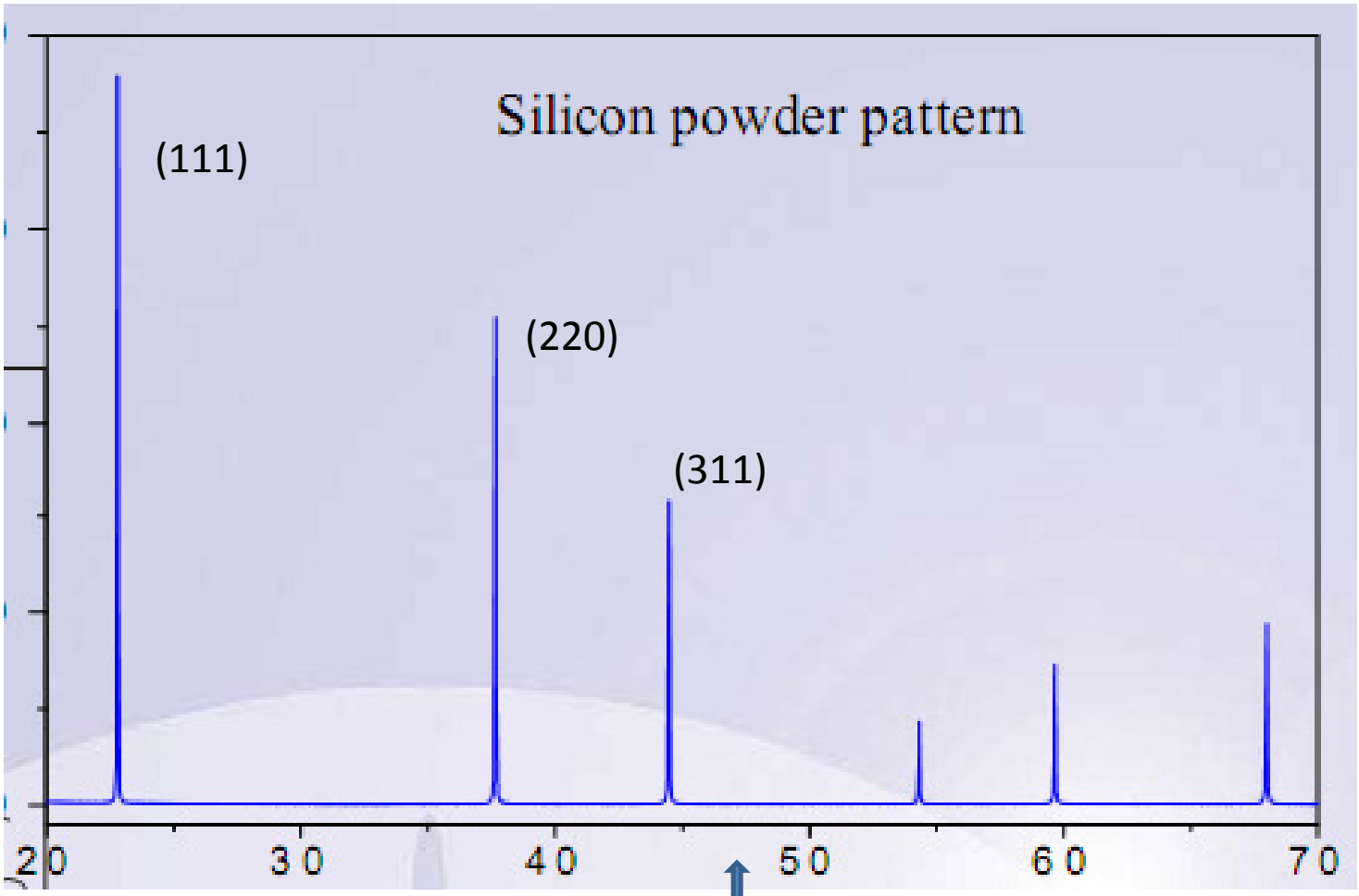


# X-ray scattering on dirty silicon

JOURNAL OF MATERIALS SCIENCE 23 (1988) 2379-2381



Clean Silicon (Data from Synchrotron)



PHYSICAL REVIEW LETTERS 49, 1438, 1982

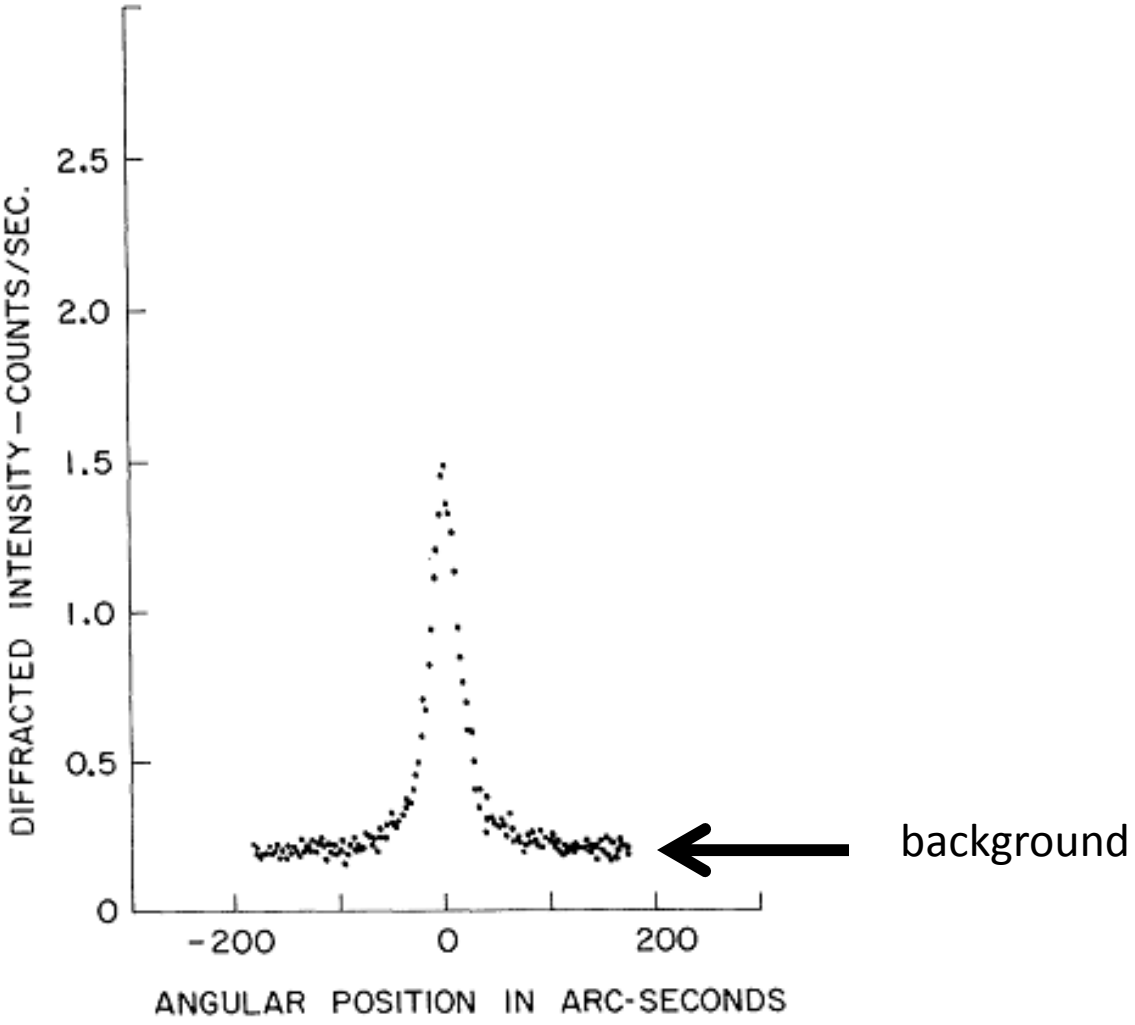
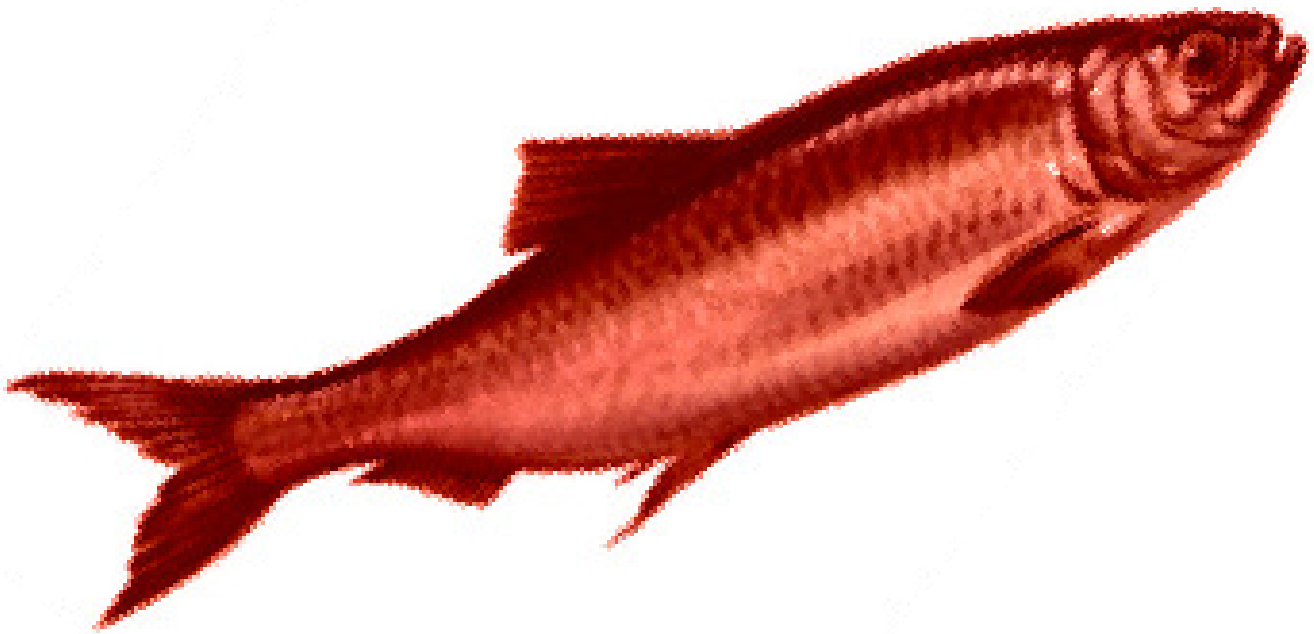



FIG. 1. Typical (222) diffraction profile from a Si crystal



***Red herring*** :

Something that diverts attention incorrectly. For example, in mystery fiction, an innocent party may be cast as highly suspicious so that attention is drawn away from the true guilty party.