Figure 1: The atoms and bonds within a piece of single-layer graphene (purple balls and grey lines). The black vertical lines indicate the propagation of electromagnetic waves through the crystal (the direction is indicated by the black arrow). The grey shaded areas in the background are to indicate the areas where there are many atoms, whereas the areas with a white background indicate "channels" between the atoms. The red square indicates an area at the edge of the sample which is shown as a zoom-in region in figure 2
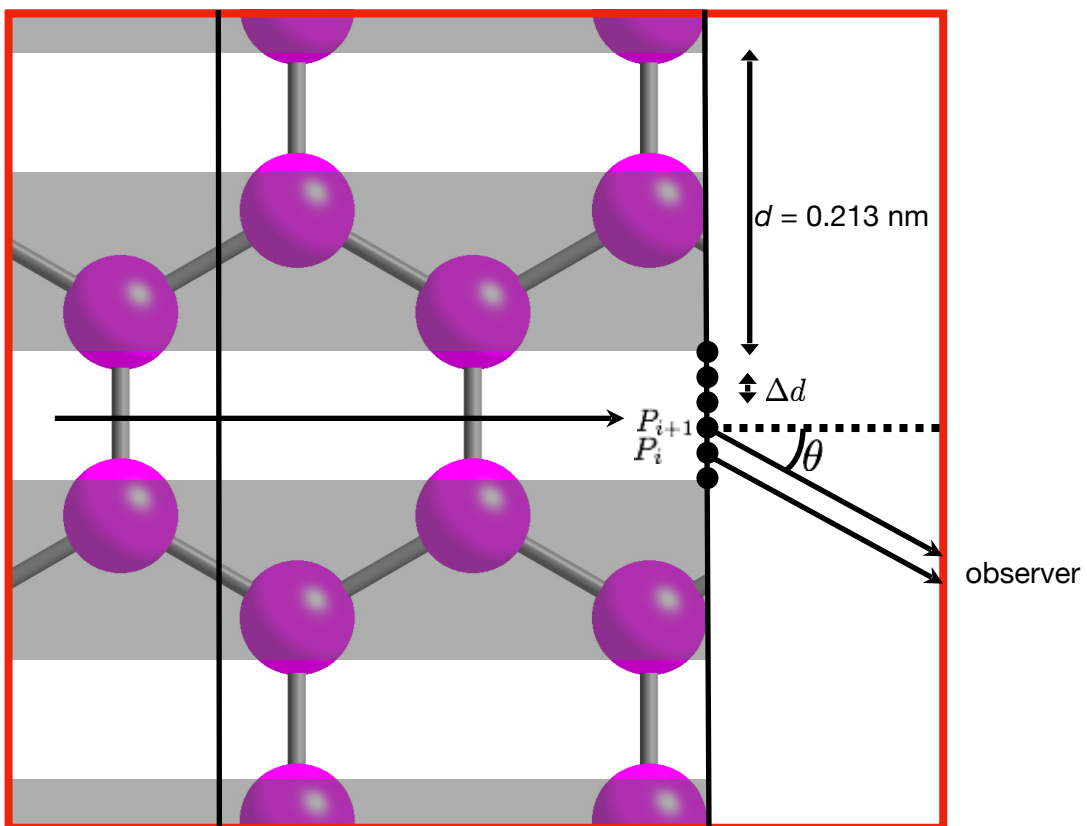
Figure 2: zoom in of the previous figure. The wavefront leaving the crystal is divided into *N* points (indicated as small black circle, and labelled P_i and P_{i+1}) with a separation Δd. The wavefronts are show as solid black lines, and the position of the observer is indicated.
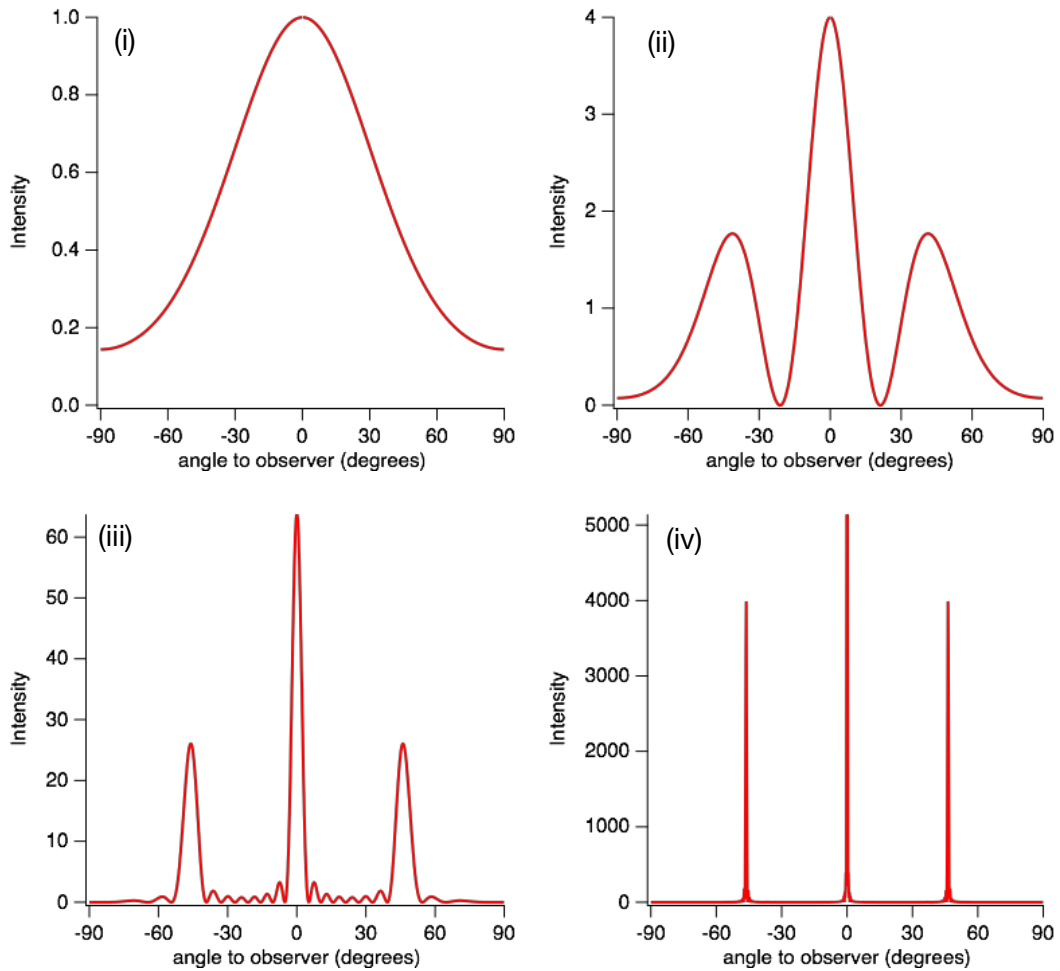
Figure 3: Some possible diffraction patterns from the sample geometry in figures 1 and 2. To simulate each pattern, a different number of slits has been included
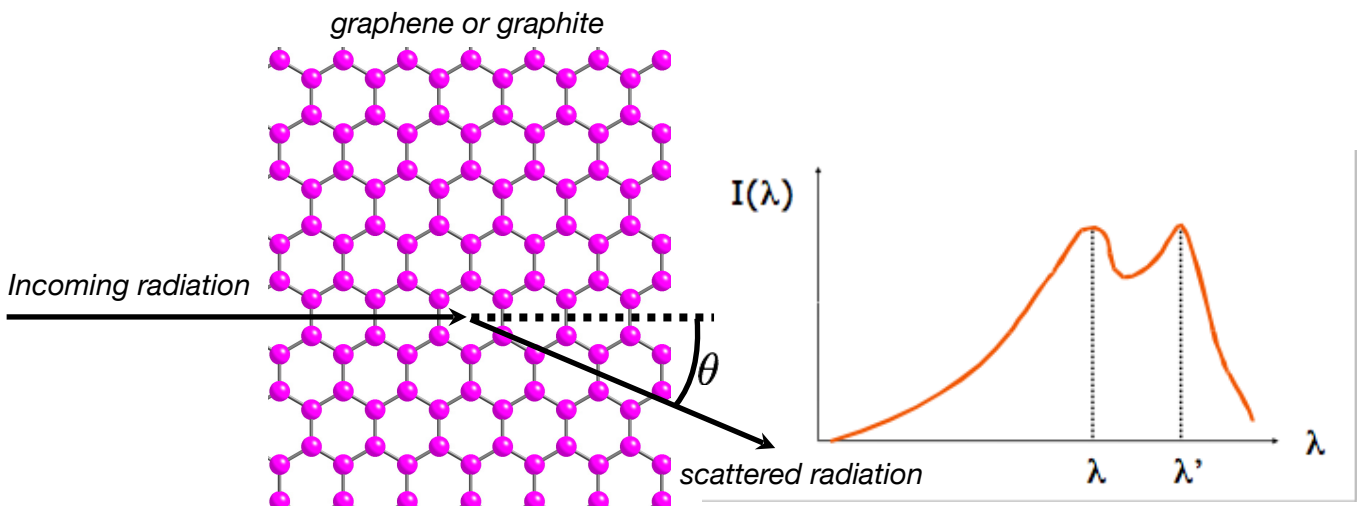

Figure 4: The Compton scattering experiment. Electromagnetic radiation of a particular wavelength (λ) enters the graphene or graphite sample. The radiation is scattered, and an observer at an angle θ sees a spectrum which contains more than one wavelength.

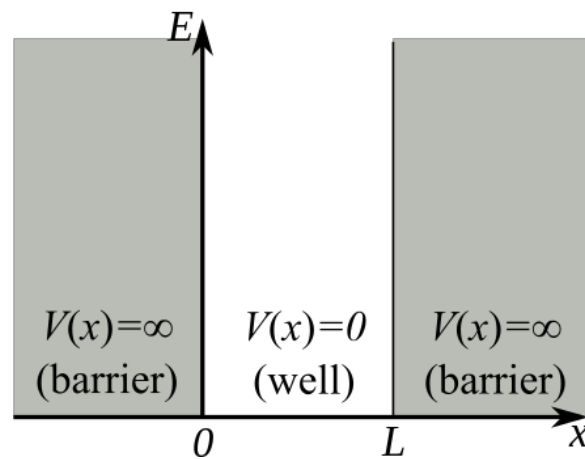| element	photon energy
Aluminium	1.48 keV
Copper	8.04 keV
Silver	22.16 keV
Molybdenum	17.48 keV

Figure 5: The 1D square well; the potential is defined as zero inside the well and infinite outside of it. In this example, the well is defined as existing between $x=0$ and $x=L$.
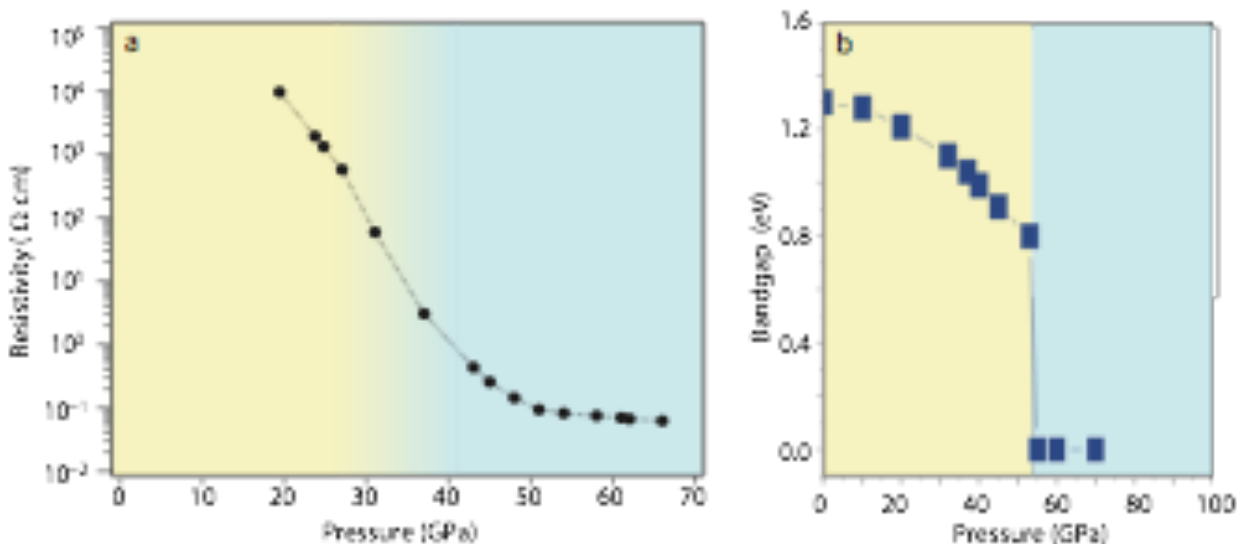

Figure 6: The resistivity and bandgap of $SrFeO_2$ as a function of pressure. Note that the resistivity is plotted on a logarithmic scale which spans many orders of magnitude. The yellow background indicates insulating behaviour and the blue background indicates metallic behaviour. This figure is adapted from a recent article in *Nature Chemistry* (www.nature.com/articles/nchem.289)

Note: Throughout this exam, the aim is to provide useful estimates, not to calculate precise values.

Question 1: Diffraction in a crystal.
Look at figure 1. It shows wavefronts electromagnetic waves propagating through a single layer of graphene.

a) What kind of radiation is this?
    (i) X-ray, (ii) Ultraviolet, (iii) Visible, (iv) Infra-red, (v) radio waves, (vi) Something else?

In this question we will assume that every point on a wavefront can be considered to be the source of a new wave. Is this assumption reasonable/common?
Take a look at figure 2 (which is a zoom-in of figure 1). We have now divided the wavefront into N discrete points, separated by a distance Δd. In particular, consider two neighbouring points (labelled P_i and P_{i+1}), and consider that they behave as two point sources. An observer standing at a distance x_i from the source P_i observes a wave of amplitude A_i (due to source P_i), where A_i is given by:

$$A_i = \frac{A_0}{N} \exp i(\omega t - k x_i)$$

b) Write an expression (in terms of x_i and x_{i+1}) for the total amplitude seen by the observer due to the two point sources, i.e. $A_i + A_{i+1}$

c) Unless $\theta = 0$, the observer will not see A_i and A_{i+1} to have the same phase. Write an expression for the phase difference ϕ as a function of angle (θ), i.e.:

$$\phi = k(x_i - x_{i+1}) = \ ?$$

d) Since we define Δd to be small (relative to the wavelength of the radiation), ϕ will also be relatively small. Construct an *Argand diagram* in which A_i and A_{i+1} are shown. (Reminder: an Argand diagram has a "real" and an "imaginary" axis, and allows complex amplitudes to be plotted as vectors)

The total amplitude due to all N points along the wavefront can be written as.

$$A_{singleslit} = \sum_{i=1}^{N} A_i$$

e) Draw a new Argand diagram to graphically represent this summation, and use your diagram to demonstrate that

$$A_{singleslit} = A_0 \frac{\sin \alpha}{\alpha}$$

f) What is α? i.e. Derive an expression for α in terms of the geometry of the observer and the slit/channel width.

Hints: It may help to start by considering the phase difference between P_i and P_N.
You may assume that the grey "blocked" areas and the white "channels" are both $d/2$ wide.

g) Look at the diffraction patterns below. Which pattern is the *intensity* seen by the observer for a single slit and which is the pattern due to many (approx 100) slits? [Note: these patterns are calculated for the specific example used in figures 1 and 2.]

h) In order to simulate the single-slit and many-slit diffraction patterns correctly, it is necessary to know the wavelength (or energy) of the propagating waves. This wavelength (and energy) depends on the material used in the radiation source. Look at table 1: which element has been used for the above simulations?

Question 2: Compton scattering.
The experiment is very similar to the one used in question 1, however now we will consider the wavelength of the scattered electromagnetic radiation.

Look at figure 4. The incoming radiation has wavelength λ. Some of the scattered radiation has changed wavelength (λ'), and a typical spectrum is shown in the figure. We also find out that the change is wavelength has a particular angle dependence:

$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

Briefly describe what is happening. Your answer should include:

a) What is causing the scattering? i.e. what is the underlying mechanism?

b) Why does the wavelength change have this angle dependence (you don't need to derive the formula, just try to explain in words why λ'-λ is larger at larger angles).

c) How can we explain that some of the radiation scatters without changing wavelength?

d) Why was the understanding of Compton scattering an important step for the development of quantum mechanics and `modern physics'?

(hint: It could be helpful to refer back to your answers to Q1 in which only the wave nature of the electromagnetic radiation was considered)

Question 3: Quantum mechanics and an introduction to solid state physics.
In this question, we will use the 1D square well approximation to understand some basic properties of elements and solid matter. We will start by considering the coulomb potential around a carbon nucleus to be a square and infinite well (as in Figure 5).

Carbon has 6 electrons (and 6 protons in the nucleus). The atomic radius is approximately $r = 1$ Å (i.e. 0.1nm). Let us approximate this as an infinitely deep well with width $2r$
a) draw a figure to illustrate the $n=1$ to $n=4$ wavefunctions.

b) At $T=0$ K, which of these levels are occupied and which are unoccupied?

c) What is the difference in energy (in eV) between the highest occupied state and lowest unoccupied state? Note: The energy of the nth level is

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

We will now assemble many C atoms to form a diamond crystal (the crystal is a cube with side length = 1 mm). In a diamond crystal, the separation between two atoms is 0.252 nm.

d) Consider a 1D chain of atoms in a diamond. Each atom has a square potential well (as we used in Q3(a-c)). Do you think that this chain of atoms will be electrically conducting? Will your answer be different at $T \approx 0$ K and room temperature? (hint: At room temperature, $kT \approx 0.025$ eV)

e) A real diamond crystal is not a 1D chain, but a 3D solid. How to think that this will impact on your answer above (note: you don't need to calculate anything, just comment on *degeneracy* and the magnitude of the *bandgap).*

f) Carbon atoms can form other crystal structures; for example graphite, graphene, bucky-balls, etc. In graphene, the atomic separation is 0.142 nm. Estimate the value of n_F (i.e the value of n at the Fermi level) for a 1 mm piece of graphene. (note: it is sufficient to use the same 1D chain approximation which you used in Q1d) [*This "hint" caused some confusion during the exam. I mean that you should use the same general idea, but not exactly the same numerical values*].

g) Estimate the energy difference between states at the Fermi level i.e. $E(n_{F+1})-E(n_F) = ?$

h) Do you think that graphene will be electrically conducting at low temperature ($T \approx 4$ K) and at room temperature?

i) Look at figure 6. It is adapted from a recent article in *Nature Chemistry* and shows that a solid sample of $SrFeO_2$ becomes very much more conductive under high pressure, and that the bandgap reduces to almost zero for $P > 50$ GPa. Comment on this: why do you think it is conductive under pressure? and why is the transition so sudden?