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Structure and Properties of Functional Materials

Homework Set 4

Due Wednesday, 6 February, 2013 by 4 p.m.

Problem 1: Terms and definitions (8 marks)

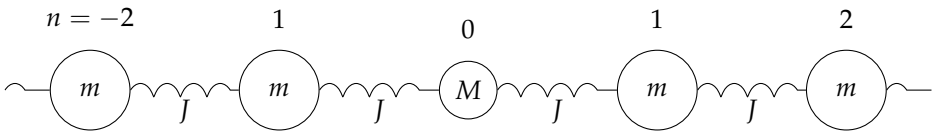
Explain the following terms or concepts, giving an example of their significance in condensed matter physics:

(a) Phase problem (4)

(b) Longitudinal mode (4)

Problem 2: Substitutional defects (16 marks)

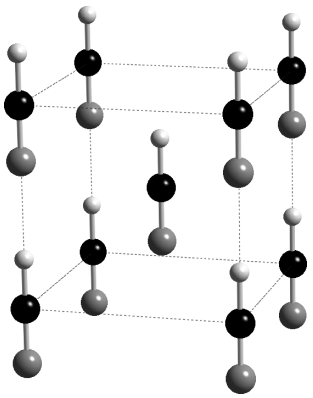
Defects in a crystal lattice can sometimes produce localised vibrational modes. As a model of this phenomenon, consider an infinite 1D chain of atoms, all of mass m except for a single atom of mass M at position $n = 0$. Each atom is connected to its neighbours by a spring of force constant J.



Under certain circumstances, this system can undergo oscillations that are localised in the sense that their amplitude decreases exponentially with distance from the defect, so that the displacement of each atom takes the form $u_n = \tilde{u}(-1)^n \exp(-\kappa|n| - i\omega t)$. Find the angular frequency ω and decay constant κ of these oscillations. For what range of M are such oscillations possible? Check that your answer makes sense in the limit as $M \to m$.

Problem 3: Lattice dynamics of a ferroelastic molecular material (16 marks)

The crystal structure of HCN is body-centred tetragonal ($a = b = 4.63\,\text{Å}$, $c = 4.34\,\text{Å}$), with one molecule, oriented along [001], on each lattice point:



(In this diagram H atoms are shown in white, C in black, N in grey; the c axis is vertical.)

Consider only nearest-neighbour interactions: for instance, the central molecule in the figure interacts only with the four other molecules shown. Assume that these can be modelled by a single spring constant J.

Show:

(a) that the longitudinal and transverse (displacements along y) modes along [100] are degenerate (have the same energy); (5)

(b) that the frequency of the longitudinal mode along [110] has the same maximum value as the modes in (a); and (5)

(c) that the transverse (displacements along $x - y$) mode for all wavevectors along [110] has zero frequency in this approximation. (6)

(This final result causes mechanical instability, giving a ferroelastic phase transition in this material at 170 K.)