Problem 1:

Let λ_i= 1 Å; Phonon E= 33 cm^{-1}
Find λ_f
Calculate Q, assuming the scattering angle = 90^0

Problem 2:

Monochromator Cu (111); assume a= 4 Å
Calculate the resolution dE_i/E_i for (a) E_i= 20 meV and (b) 80 meV
Analyser PG (002); assume c= 7 Å
Calculate the resolution dE_f/E_f for
(a) E_f= 20 meV and (b) 80 meV

Problem 3:

Calculate the structure factors for
(a) diffraction S(G) and (b) one-phonon scattering F(Q), for NaCl, assume b_{coh}(Na) = 2 fm, b_{coh}(Cl) = 1 fm; for LA, TA, LO, TO phonons at q= (0.01, 0, 0), and G= (2, 0, 0), (4,0, 0), (1, 1, 1), (2, 2, 2)

Hint: NaCl has face-centred cubic structure.

Problem 4:

Assume g(E) in the range E= 0 to 80 meV.
Calculate the typical range of Q. Assume $\langle u^2\rangle/3$ = 0.01 Å2 along one direction
Estimate relative contributions of one-phonon and multi-phonon intensity at the above calculated Q values.
Hint:one-phonon~$2W(Q) = Q^2\langle u^2\rangle/3$
two-phonon ~$(Q2\langle u^2\rangle/3)2/2!$ etc.

Problem 5:

Assume that the phonon frequency of hydrogen atom is 20 THz. Calculate the value of the wave-vector transfer Q for which the neutron inelastic scattering intensity for a polycrystalline sample will be the maximum at (a) 0 K, (b) 300 K, and (c) 1000 K.
Calculate the mean-squared displacement $\langle u^2\rangle/3 = (n+1/2)\hbar/(mw)$ along one direction.
Hint: Intensity is proportional to $Q^2\exp(-Q^2\langle u^2\rangle/3)$.

Problem 6:

Assume jump diffusion of atoms in a solid, with average jump length of 3 Å, and average residence time of 10 ps. Estimate the range of momentum transfer Q and energy transfer E for measurement of quasi-elastic neutron scattering. What is the typical energy resolution required for the experiment?
Hint: Use the expression for a jump-diffusion model.

Problem 7:

In a molecular dynamics simulation, assume the starting position of an oxygen atom at origin. Calculate its starting velocity, assuming its initial kinetic energy of 600 K. Assume the direction of the velocity to be along x-axis. Estimate a reasonable time-step, assuming a typical vibrational frequency of 10 THz.
Find the position at time-step 1 and 2. Assume a force $\mathbf{F} = -k\,\mathbf{u}$.
Hint: The vibrational frequency = $(k/m)^{1/2}$

Problem 8:

Assume jump diffusion of atoms in a solid, with average jump length of 3 Å, and average residence time of 10 ps at 600 K. Calculate the diffusion coefficient at 600 K.
Assume an activation energy for jumps of 0.5eV.
Calculate the diffusion coefficient at (a) 900 K, and (b) 1200 K.