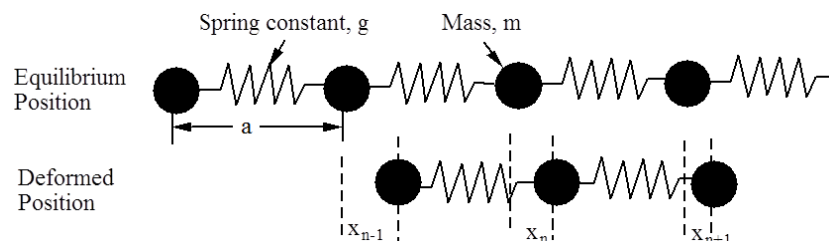


Module II

Practical assignments:

1. Consider vibrations in an infinite 1D-lattice having one atom in the basis as shown in Fig.1 below



- (a) Derive the dispersion relation for a wave propagating in this crystal;
 - (b) Make a graph and explain why it is sufficient knowing the dispersion relation within the 1st Brillouin zone (BZ) only;
 - (c) Analyze the group velocity, specifically at the center and at the edges of the 1st BZ;
 - (d) Assume the schematics in Fig.1 to model a longitudinal wave propagating in [100] direction in Na crystal, estimate the maximum amplitude of the vibrations.
2. Derive/analyze the phonon density of states (DOS) in 1D containing N atoms; e.g. use the following scenario:
 - (a) Introduce periodic boundary conditions, derive DOS in the k -space, and plot $DOS(k)$;
 - (b) Use the 1-D dispersion relation as obtained solving problem 1, i.e. $\omega = \omega_0 \sin(ka/2)$, find DOS as a function of ω , and plot $DOS(\omega)$.
 - (c) Pay attention to a relative "simplicity" of $DOS(k)$ and significantly bigger "complexity" of $DOS(\omega)$, providing an argument for calculating DOS in k -space.
 3. Evaluate progress/limitations of Dulong-Petit, Einstein, and Debye models for explaining temperature dependence of the lattice heat capacity - $C_v(T)$. (Suggestion: instead of deriving formalisms in full, consider making a qualitative comparison of "oscillator models" assumed to be responsible for the corresponding $C_v(T)$ dependences.
 4. A two-dimensional finite hexagonal lattice has a spacing of $a = 3 \text{ \AA}$. Assuming the sound velocity in this material to be $c = 10^3 \text{ m}\cdot\text{s}^{-1}$, what is the Debye frequency ω_D ?

5. Provide a qualitative explanation of the T^3 -Debye law comparing the fraction of phonon modes occupied at a given temperature T versus all modes within the Debye cut-off wavevector K_D . Estimate K_D and θ_D for Na crystal.
6. The thermal conductivity coefficient κ is given by $\kappa = \frac{1}{3} C_V \Lambda$, where C_V is the heat capacity and Λ is the phonon mean free path. Consider temperature dependences for C_V (account for the lattice related heat capacitance only), Λ , and κ at low/high temperature limits and fill Table I. Make a plot illustrating temperature dependence of κ and elaborate on “normal” versus “umklapp” processes.

Table I

	C_V	Λ	κ
low T			
high T			