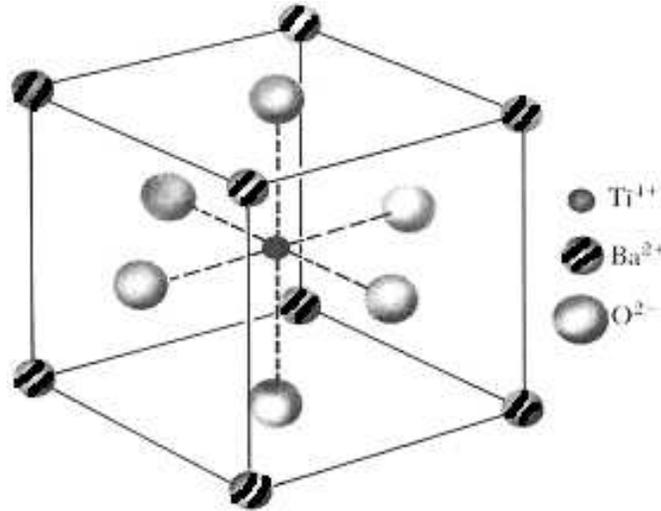


$$\hbar = 1.054 \times 10^{-34} \text{ Js} \quad k_B = 1.38 \times 10^{-23} \text{ J/K} \quad N_{\text{Avogadro}} = 6.022 \times 10^{23} \text{ mol}^{-1}$$

1. (25 points) The crystal structure of barium titanate is shown below with the Ti, O and Ba atoms occupying the body-center, face-center and corner positions of a cubic cell, respectively. This so-called perovskite structure is very important in the field of ferroelectricity. Let us denote the nearest neighbor Ba-Ba distance by d .



- (a) Write down the explicit expressions (in terms of d) for a set of primitive translation vectors \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 and for the corresponding set of primitive reciprocal lattice vectors \mathbf{b}_1 , \mathbf{b}_2 , and \mathbf{b}_3 .
- (b) What is the shape and volume of the first Brillouin zone? If there are 10^{22} BaTiO_3 units in the sample, how many allowed \vec{k} -states are there in the first Brillouin zone and why?
- (c) How many optical phonon branches are there for this material?
- (d) Determine the structure factors for the first two sets of non-zero reciprocal lattice vectors assuming that the atomic form factors are in the ratios 3:2:1 for Ba:Ti:O.
2. (25 points) In this problem no calculations are required. Consider a chain of atoms, all with the same mass, but with two different spring constants (C_1 and C_2) that alternate along the chain. In answering each of the questions below illustrate your answer with a sketch that includes at least four atoms (use X's and O's to represent the two atoms in a unit cell). Sketch, using arrows near each of the four atoms, the normal mode displacements for
- The zone-center acoustic mode;
 - The zone-center optical mode;
 - The zone-boundary acoustic mode;
 - The zone-boundary optical mode.

3. (25 points)

(a) Suppose that an optical phonon branch has, in the vicinity of the zone-center, the form

$$\omega(\mathbf{k}) = \omega_{\max} - \alpha|\mathbf{k}|^2,$$

where $\alpha > 0$. Calculate the density of states (DOS) per unit d -dimensional volume around ω_{\max} for $d = 1, 2, 3$ and sketch of the DOS immediately below and above ω_{\max} .

(b) Consider a dielectric crystal made up of layers of atoms, with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer.

(i) How does the phonon heat capacity scale with temperature in the low-temperature limit? Explain your reasoning.

[NOTE: You can make a semi-quantitative argument which yields the correct scaling but not necessarily the exact numerical prefactors.]

(ii) Suppose instead, as in many layered structures (e.g., graphite) that adjacent layers are very weakly coupled to each other. What form would you expect the phonon heat capacity to approach at extremely low temperatures? Explain your reasoning.

(c) The figure shows the low temperature heat capacity of solid argon. Extract from the figure the Debye temperature T_D .

[NOTE: If you don't remember the needed formula from class and don't have it in your sheet, you should derive it; you will need the integral $\int_0^\infty x^3/(e^x - 1)dx = \pi^4/15$.]

