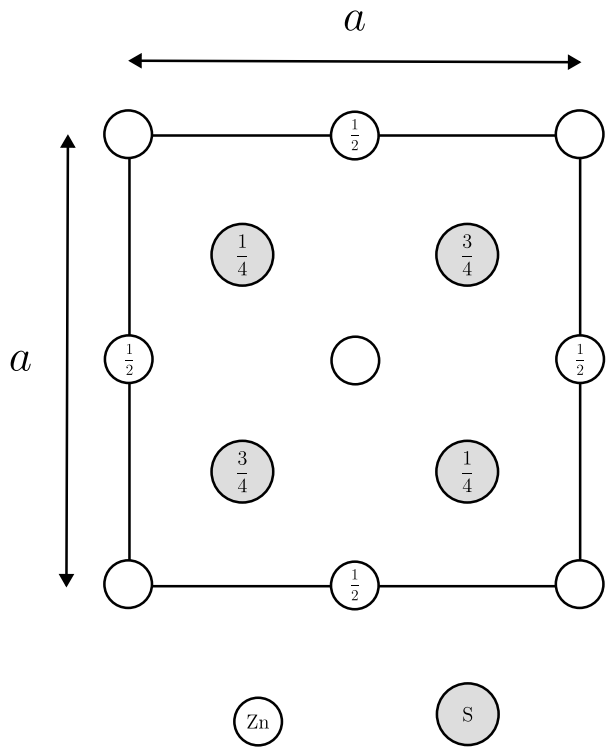
Please complete the following questions. You are allowed to work in groups but remember to show your own work.

Problem 1. (Zincblende Structure)

The diagram below shows a representation of the unit lattice structure of a common zinc ore, zincblende (ZnS), in the xy-plane (z axis is out of the page). The numbers shown next to each atom represents their height as a fraction of a within the unit cell (bottom layer is $z = 0$ and top layer is $z = a$). Atoms without numbers are either on the top layer or the bottom layer.



(a) Make a sketch of the lattice in the xz-plane.

(b) Give a lattice basis for this structure.

(c) The accepted value of ZnS lattice constant is $a = 5.41$ Å. Find the nearest neighbor distances of Zn-Zn, Zn-S, and S-S.

(d) How many Zn atoms per unit cell are there? What about S atoms?

(e) Describe what you notice about the type of Bravais lattice formed by each "sublattice" of each atom type.

Problem 2. (Atomic Packing Fractions)
In class, we calculated the atomic packing fraction of a body-centered cubit (BCC) lattice to be 68%.

(a) Show that the APF of a simple cubic lattice is 52%.

(b) Show that the APF of a Face-centered cubic (FCC) is 74%.

Problem 3. (Reciprocal Lattice Vectors)
We claimed in class that we can use the primitive lattice vectors $(\vec{a}_1, \vec{a}_2, \vec{a}_3)$ to construct reciprocal lattice primitive vectors

$$\vec{b}_1 = \frac{2\pi \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$
$$\vec{b}_2 = \frac{2\pi \vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$
$$\vec{b}_3 = \frac{2\pi \vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

(a) Write down both the mathematical definition of the reciprocal lattice and then try to explain what a reciprocal lattice is in your own words.

(b) Confirm that these vectors obey the identity

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$$

(c) Show that the identity above ensures that $\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$ is a reciprocal lattice vector.

Problem 4. (FCC Reciprocal Lattice)
Show that the reciprocal lattice of a FCC lattice with lattice constant a is a BCC lattice with lattice constant $\frac{4\pi}{a}$.

Problem 5. In lecture, we claimed that the Laue condition is equivalent to the Bragg condition. Let's show that that is the case.

Consider a wave with momentum $\vec{k}$ incident at an angle θ from a family of planes with spacing d. The scattered wave has momentum $\vec{k}'$.

(a) State the Laue condition and explain what it physically represents.

(b) Let $\vec{G}$ be a reciprocal lattice vector perpendicular to the incident lattice plane. Show that

$$-\hat{k} \cdot \hat{G} = \sin\theta = \hat{k}' \cdot \hat{G}$$

(c) Show that the Laue condition can be rewritten as

$$\frac{2\pi}{\lambda}(\hat{k}' - \hat{k}) = \vec{G}$$

(d) Dot both sides of the previous equation with $\hat{G}$ and show that

$$2d \sin\theta = \lambda$$

Problem 6. (X-ray Scattering)

You shoot a powdered sample of Pd metal with a beam of monochromatic X-rays of wavelength 0.162 nm. The resulting intensity spectrum has peaks at angles 42.3°, 49.2°, 72.2°, 87.4°, and 92.3° from the incident beam.

(a) Determine the cubic lattice type of this metal.

(b) Estimate the lattice constant of Pd metal.

(c) Estimate the dimensions of a 0.5 mol palladium crystal sample.

Problem 7. (Lennard-Jones Potential)

In computational physics, molecular structures are very commonly simulated to have an interatomic potential of the following form

$$\phi(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right].$$

where ϵ and σ are constants. This is called the Lennard-Jones potential. This is actually a terrible potential for modeling solids but it's still a good potential to know since it's the "default" potential for most simulation packages.

(a) Find the interatomic distance, a, of two atoms bound by this potential.

(b) What is the energy of two atoms bounds by a Lennard-Jones potential at equilibrium?

(c) Based on your answer above, what does the constant ϵ represent?

(d) Expand the potential around the equilibrium length a up to third order in r. Find estimates for the Young's modulus, Y, and the coefficient of thermal expansion, α in terms of the L-J coefficients, σ and ϵ.

(e) Solid Argon can be simulated using the Lennard-Jones potential with coefficients $\epsilon = 10$ meV and $\sigma = 0.34$ nm. Use these values to estimate the Y and α of solid Argon.

Problem 8. (**Extra Credit:** Classical Thermal Expansion)

You are not required to do this problem but in case you were wondering why the coeffient of thermal expansion is

$$\alpha \approx \frac{k_B \phi'''(a)}{2a(\phi''(a))^2}$$

this problem shows you how to get it.

Let's start with the usual taylor expansion of the interatomic potential. Like we discussed in lecture, at a non-zero temperature the actual "bond length" is the average distance you get when you oscillate about the two turning points set by the total available thermal energy, $k_B T$. That is, $a \approx \langle r \rangle$, where $\langle \cdot \rangle$ denotes the average.

In statistical mechanics, we compute these averages using the Boltzmann weight for a given state:

$$\langle r(T) \rangle = \frac{\int_{-\infty}^{\infty} r e^{-\phi(r)/k_B T} dr}{\int_{-\infty}^{\infty} e^{-\phi(r)/k_B T} dr}$$

These integrals are generally very hard/impossible to compute analytically, so we need to rely on expanding the exponentials.

You will need the following expansion:

$$e^{-\phi(r)/k_B T} \approx e^{-\frac{\phi''(a)}{2k_B T}(r-a)^2} \left[1 + \frac{\phi'''(a)}{6k_B T}(r-a)^3\right] \tag{1}$$

(a) Note that we have two expansions, the original Taylor expansion of the potential, ϕ, and the expansion (1) above of the exponential. Using your own words, explain what in the original Taylor expansion, allows us to expand the exponential.

(b) Use the expansion to find an expression for $\langle r(T) \rangle$.

(c) Use your result from part (b) along with the definition of the coefficient of thermal expansion to show

$$\alpha = \frac{1}{L}\frac{\Delta L}{\Delta T} \approx \frac{k_B \phi'''(a)}{2a(\phi''(a))^2}$$

(d) Now, let's think about where this approximation is valid. Based on the two expansions we used, give a reasonable bound for the temperatures at which this is a valid estimate for α. Note that you don't have any numbers so I'm not asking for a numerical bound.

Hint: In expansion (1), what term needs to dominate for it to be a valid expansion and what does that say about $|r - a|$? Now use that to justify the original Taylor expansion.