HOMEWORK SET 01
Theory of Condensed Matter
UFV/TKL1/99 lecture by Martin Gmitra
Winter Semester 2021, room KNKTFA(Pa9-PKn)

1. *[1 point]* Consider a BCC lattice of touching identical hard spheres and calculate the sphere radius R for a given lattice constant a.

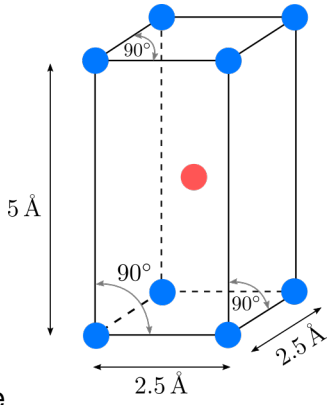
2. *[3 points]* Calculate
   a) volume of the primitive unit cell of BCC lattice
   b) reciprocal volume of the reciprocal lattice to the FCC lattice
   c) volume of the Wigner-Seitz cell in reciprocal space of BCC lattice

3. [*1 point]* Prove that reciprocal lattice of the reciprocal is the direct lattice.

4. *[1 point]* Prove that the reciprocal of a BCC is an FCC lattice and vice versa.

5. *[2 points]* Consider a triangular lattice in 2D with lattice vectors $\mathbf{a}_1 = a\hat{\mathbf{x}}$, $\mathbf{a}_2 = (a/2)\hat{\mathbf{x}} + (a\sqrt{3}/2)\hat{\mathbf{y}}$.
   a) Find the 1st Brillouin zone and write an expression for the equivalent wavevectors within the 1st Brillouin zone.
   b) Draw the 2nd Brillouin zone.

6. *[2 points]* Figure shows the unit cell of a crystal with two different atoms at the relative positions (000) and (½, ½, ½).
   a) What Bravais lattice would you describe to the crystal structure and what is the maximum packing fraction?
   b) Sketch atomic layers along [111], [110] and [210] directions.



7. *[3 extra points]* Lattice planes of a direct lattice can be characterized by the vectors of corresponding reciprocal lattice that are perpendicular to the lattice planes. Notation of the lattice planes follows the notation by the Miller indices (hkl).
   a) Show that the vector of reciprocal lattice $\mathbf{b}_{(hkl)} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to the lattice plane (hkl) of the direct lattice.
   b) Show that the distance d of the (hkl) set of planes in a cubic crystal with lattice parameter a is $d = a/\sqrt{h^2 + k^2 + l^2}$.
   c) Find generalization of the distance formula in b) for orthorhombic crystal.

8. *[2 extra points]* In weakly interacting systems, the interaction between two atoms *i* and *j* is often described by the Lennard-Jones potential, $U(r_{ij}) = 4\varepsilon((\sigma/r_{ij})^{12} - (\sigma/r_{ij})^{6})$, where r_{ij} is the inter atomic distance. Near $T = 0$ K, krypton is an FCC crystal with $\sigma = 0.365$ nm and $\varepsilon = 2.25\ 10^{-21}$ J. Calculate the lattice constant and the binding energy per atom assuming that only interactions between nearest neighbor atoms have to be considered.

HOMEWORK SET 01

Theory of Condensed Matter

UFV/TKL1/99 lecture by Martin Gmitra

Winter Semester 2021, room KNKTFA(Pa9-PKn)