



- (a) Is the honeycomb network a Bravais lattice? If your answer is no, explain how to construct it by beginning with a Bravais lattice.

(b) The perovskite structure (such as $CaTiO_3$ and $BaTiO_3$) is built from three types of atoms. Write and draw primitive and basis vectors that construct this lattice.
- (a) Consider a two-dimensional Bravais lattice that is left invariant after rotation by angle θ around the origin. Suppose the lattice to have points at $(0, 0)$ and $(a, 0)$. By requiring the image of $(a, 0)$ under rotations through $\pm\theta$ to be in the Bravais lattice, find a simple expression that implicitly specifies all possible rotation axes.

(b) Prove that the only allowed axes are twofold, threefold, fourfold, and sixfold. In particular, it is impossible for a Bravais lattice to have a fivefold rotation axis.
- The following table shows the number of the first, second, third, and fourth neighbors and their distances for each atom in the simple cubic lattice. Construct the same table for the FCC and BCC lattices, up to the fourth neighbors. The parameter (a) is always the cube edge.

Table 1: Neighbors of the sc lattice

Neighbor	#	$ \frac{\mathbf{a}}{a} $
1	6	1
2	12	$\sqrt{2}$
3	8	$\sqrt{3}$
4	6	2

- (a) Compare the area packing fraction for triangular and square Bravais lattices.

(b) It is difficult to avoid asking why elements choose the crystal structure they do. Without a quantitative theory of cohesion, this question cannot be answered in detail. However, simple arguments can explain a great deal. Many atoms are held together by isotropic attraction that favors packing them as closely as possible. The concept of packing can be addressed by setting the distance between the nearest neighbors in a given lattice to 2, putting unit spheres on each lattice site, and asking what portion of space is occupied by the spheres. This number is the packing fraction and is displayed in [Table 2](#).

Verify the packing fractions listed in [Table 2](#). The packing argument explains the great frequency of the hcp and fcc structures, although it cannot explain how crystals would choose between them.



Table 2: Packing fractions for various crystal structures

Structure	Packing Fraction
hcp	0.74
fcc	0.74
bcc	0.68
sc	0.52
diamond	0.34

5. Consider a collection of particles in three dimensions whose energy is

$$\mathcal{E} = \frac{1}{2} \sum_{i \neq j} \phi(r_{ij}) \quad (1)$$

with

$$\phi(r) = \begin{cases} \phi_0 \exp(-r) \left(\frac{1}{r^3} - 1 \right) & \text{if } r < 1.5 \\ 0 & \text{else,} \end{cases} \quad (2)$$

where r_{ij} is the distance (measured, say, in Å) between particles i and j . Compare the energies of the bcc, fcc, and hcp lattices. Find the lattice spacing leading to the minimum energy for each of these three lattices, and find the state of lowest overall energy.