

**Problem set #1**

1. A Copper Oxide Layer

The common building blocks for most high temperature (high  $T_c$ ) superconductors are copper oxide layers, as depicted in Fig. 1. Assume the distance between copper atoms (filled circles) is  $a$ .

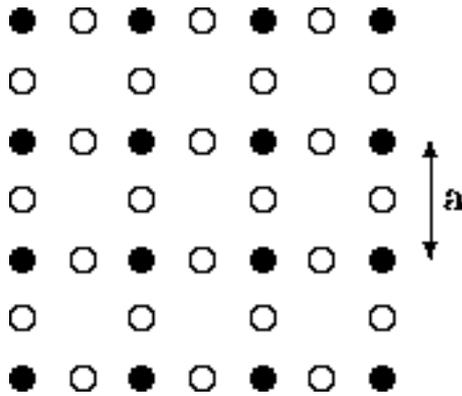


Fig. 1

(a) Sketch the 2D Bravais lattice of a single copper oxide layer and indicate the fundamental translation vectors  $(\vec{a}, \vec{b})$  which can be used to define the 2D primitive unit cell. What is the primitive unit cell, and what is the basis?

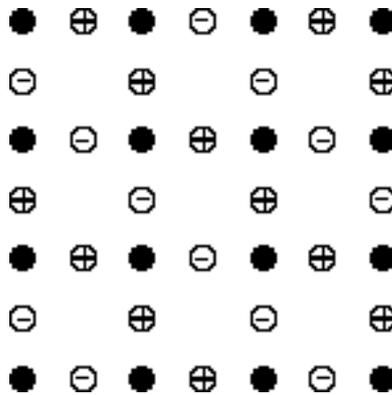
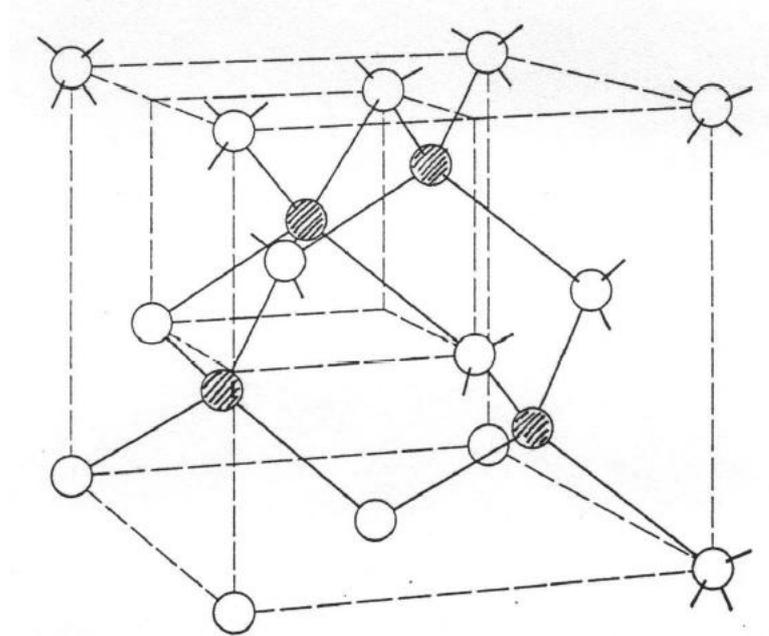


Fig. 2

(b) In  $LaCuO$  one discovers, at closer inspection, that the copper oxide lattice is actually not flat, but that the oxygen atoms are moved a small amount out of the plane (“up” or “down”) in an alternating fashion (see Fig. 2. a + means up and a - means down) What is the primitive cell and lattice spacing for this crystal? What is the basis?

2. Gallium Arsenide

A conventional (cubic) unit cell of gallium arsenide, GaAs, is shown below. Note the similarity to the diamond structure. The gallium atoms are indicated by shaded circles and the arsenic atoms by open circles.



- How many atoms of each type are contained in the conventional cell?
- To which space lattice type does this crystal belong?
- Give a set of fundamental translation vectors  $(\vec{a}, \vec{b}, \vec{c})$  which can be used to define the primitive unit cell. Express your answer in cartesian coordinates  $(\hat{x}, \hat{y}, \hat{z})$ . How many atoms are there in the primitive cell?

3. Calcium Fluoride

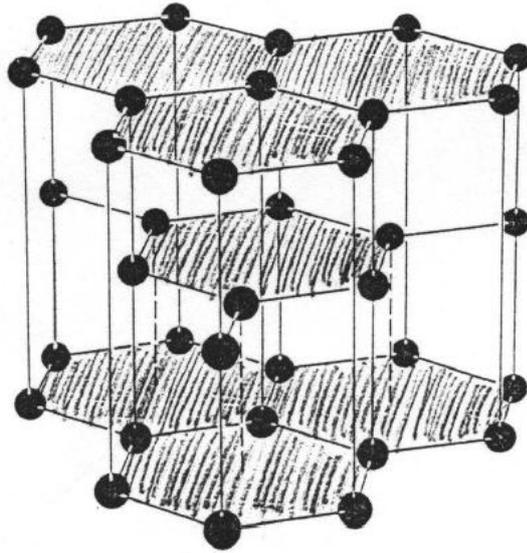
Calcium fluoride,  $\text{CaF}_2$ , has a structure based on the fcc lattice and a basis with Ca at  $(000)$  and F's at  $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$  and  $(\frac{3}{4}\frac{3}{4}\frac{3}{4})$ . Draw a projection diagram and sketch one conventional (cubic) unit cell of the structure.

4. Packing Fraction

Show that the maximum proportion of the available volume which may be filled by hard spheres arranged on various lattices is: simple cubic, 0.50; body-centered cubic, 0.68, face-centered cubic, 0.74; diamond, 0.34.

5. Graphite

Graphite, a form of elemental carbon, is made up of planes of atoms as shown below.



In each plane the atoms are at the corners of open hexagons. The odd-numbered layers are all identical when viewed from above. All even-numbered layers are also identical, but they are shifted with respect to the odd layers. Describe this structure by giving the lattice type, the primitive unit cell, and the basis.