STATE UNIVERSITY OF NEW YORK AT BUFFALO
Department of Mechanical and Aerospace Engineering

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HOMEWORK NO. 1

Problem 1

Sodium oxide (Na_2O) is an ionic solid that exhibits the crystal structure shown in Fig. 1. The O^{2-} ions occupy the atom sites of an FCC structure while the Na^+ ions occupy all of the tetrahedral interstitial sites of the anion FCC structure.

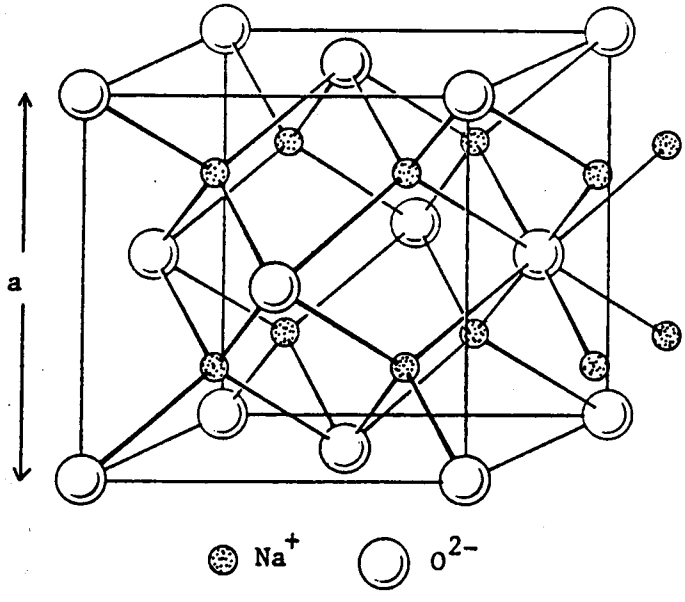

Fig. 1 The unit cell of Na_2O.

(3%) (a) Give the number of Na^+ ions per unit cell.

(3%) (b) Give the number of O^{2-} ions per unit cell.

(3%) (c) How many O^{2-} ions surround a Na^+ ion?

(3%) (d) How many Na^+ ions surround an O^{2-} ion?

(3%) (e) On which Bravais lattice is the crystal structure of Na_2O based?

(3%) (f) Give the number of Na^+ ions and the number of O^{2-} ions in the basis.

(6%) (g) The lattice constant is a, as indicate in Fig. 1. Give the relationship between a and the cation radius r and the anion radius R.

(10%) (h) Calculate the density of Na_2O.

Problem 2

Consider the two-dimensional space lattice shown in Fig. 2, where the parallelogram shown by solid lines is a unit cell. All four edges of the parallelogram are equal in length. The hexagon shown by dashed lines is another unit cell.

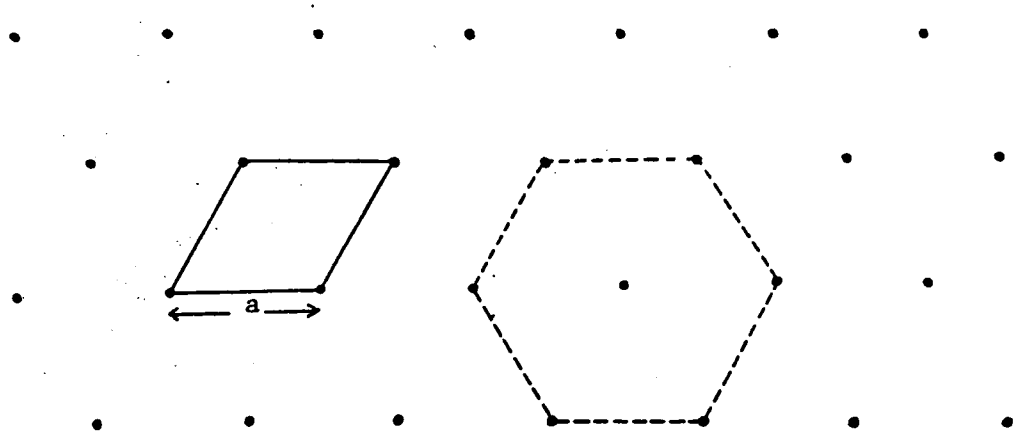

Fig. 2 A two-dimensional space lattice.

(3%) (a) Give the number of lattice points per unit cell for the parallelogram unit cell.

(3%) (b) Give the number of lattice points per unit cell for the hexagonal unit cell.

(3%) (c) Which unit cell is the primitive unit cell?

(13%) (d) A hypothetical two-dimensional crystal structure is based on the lattice shown in Fig. 2, and has two atoms in the basis. The positions of the two atoms associated with the lattice point A are indicated by X in Fig. 3. One atom in the basis is at the lattice point A; the other atom in the basis is at point B, which is such that the distance AB is 1/3 of the distance AC. By repeating the basis at every lattice point, sketch the crystal structure.

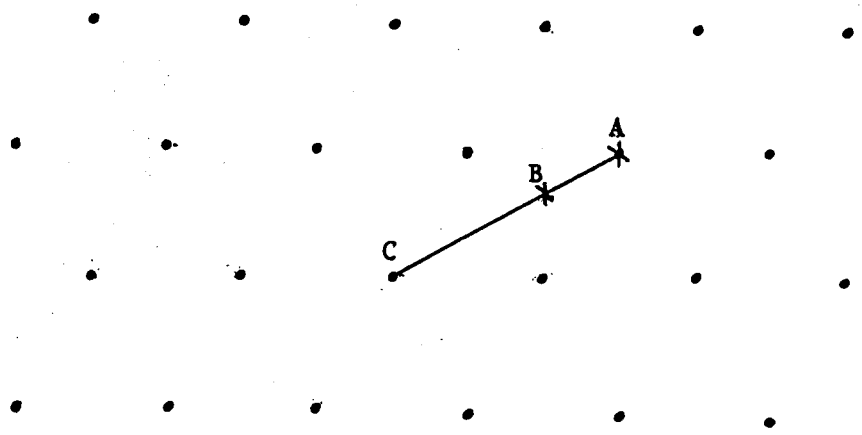

Fig. 3 A basis for the lattice of Fig. 2.

(6%) (e) What is the coordination number of the two-dimensional crystal structure obtained in (d)?

(6%) (f) The lattice constant is a, as indicated in Fig. 2. Assume that nearest neighbor atoms touch each other in this crystal structure, give the relationship between a and the atomic radius r.

Problem 3

Lead is FCC with atomic radius 1.750 Å. What is the volume of its unit cell?

Problem 4

Magnesium is HCP and has nearly spherical atoms with a radius of ~1.61 Å. What is its density? For Mg, $\frac{c}{a} = 1.62$. Hint: $a = 2r$ for HCP.

Problem 5

The electron energy levels for a copper atom are $E_K = -8982$ eV, $E_L = -933$ eV, and $E_M = -75$ eV. Calculate (a) the K_α photon energy, (b) the K_β photon energy, (c) the L_α photon energy, (d) the KLL Auger electron energy, and (e) the LMM Auger electron energy.

Problem 6

The K shell electron energy for nickel is $E_K = -8333$ eV and the wavelengths of the NiK_α and NiK_β photons are 0.1660 nm and 0.1500 nm, respectively. (a) Draw an energy-level diagram for a nickel atom. Calculate (b) the KLL and (c) the LMM Auger electron energies for nickel.