

Problem session 1

A. Problem 1

Consider first a simple cubic (sc) lattice (see, for example, Fig.8 in p.9 of Kittel). Write down the primitive vectors of this lattice. Further, please write down basis vectors in a conventional unit cell of the face centered cubic (fcc) lattice. Choose a primitive cell for the fcc lattice and write down its unit vectors. Remember, the primitive cell contains only one atom and fills all space when translating.

B. Problem 2

Consider two binary oxides – ZnO and CdO – that, at equilibrium conditions, crystallize into so called wurtzite and rock salt structures, respectively. Note, “rock salt” means nothing else than a well known sodium chloride or a modification of the fcc lattice - see, for example, Figs.15 and 16 in p.13 of Kittel, while “wurtzite” is a modification of the hexagonal close-packed (hcp) structure as, for example, shown in Fig.21 in p.16 of Kittel. Firstly, sketch the corresponding lattice structures. Further, please determine primitive and basis vectors describing both ZnO and CdO.

C. Problem 3

Derive that for an ideal hcp structure the c/a ratio is equal to 1.633 (angular parameter for hcp lattice may be taken from Table I in p.9 of Kittel). What is the c/a value in a real ZnO crystal (please search for c and a values in literature)? Please consider a question – qualitatively – why these two relatively similar II-VI compounds – ZnO and CdO – crystallizes into different structures?

D. Problem 4

The coverage of a lattice structure is the maximum fraction of space filled by non-overlapping spheres centered on the sites of the lattice. Show that the coverage of sc, fcc, and hcp lattices are 52, 74, and 74 %, respectively.

C. Problem 5

Consider the Miller system of indices of planes as illustrated in Fig.13 in p.12 of Kittel. Please, make a sketch the (010) , $(20\bar{1})$ and $(1\bar{2}1)$ planes in a sc lattice. Consider next the planes with indices (100) and (001) of the fcc lattice, where the indices refer to the conventional cubic unit cell. What are the indices of these planes when referred to the axis of the fcc primitive cell? Interpretations in Fig.11 in p.11 of Kittel may be readily considered.