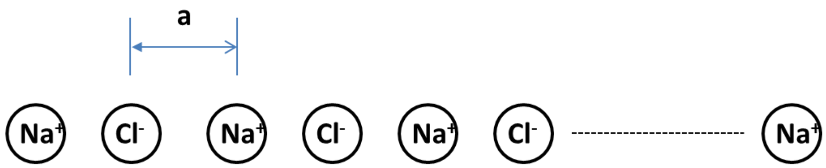
FYS3410 Spring 2016

Module I

Practical assingments:

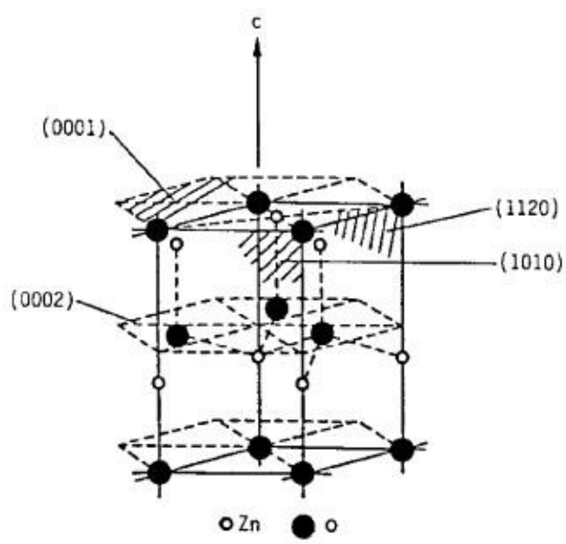
1. Assume infinite one-dimensional (1D) NaCl latice as shown in Fig.1 below.



(a) Choose the basis and the unit cell for this lattice;
(b) Derive an analytical expression for the Madelung constant;
(c) Assume this crystal to be of a finite size varying from 1 to 50 unit cells and plot the evolution of the Madelung constant as a function of the crystal size; analyze the trend for the corresponding cohesive energy evolution;
(d) Is there a condition related to the repulsive/attractive force balance determining potential realization of such crystals? (Comment: no metaphysical or philosophical analysis is required; disregard any consideration of the substrate used; instead, assuming the Pauli repulsion to act similar to that as in 3D NaCl, i.e λ=1keV and ρ=0.32Å, try to calculate and plot/analyze the trend for the equilibrium separation between Na^+ and Cl^- ions as a function of the crystal size)

2. Consider hexagonal close-packed (hcp) crystal (e.g. see Figs 19-21 in Kitells's book).
   (a) Calculate the number of atoms in the unit cell;
   (b) Calculate the characteristic c/a ratio;
   (c) Show that the packing density is 74%;

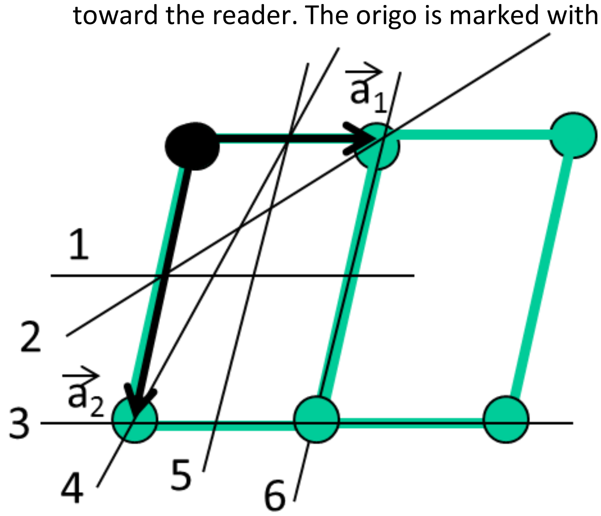
   (d) Deviations from the ideal hcp c/a ratio may be observed in some materials, e.g. in ZnO c/a =1.602. Taking into account alternating "shits" of Zn^+ and O^- ions building this hexagonal structure – conventionally called wurtize, see Fig.2 - try to elaborate what consequences such c/a deviation may result in.



3. Consider a cubic crystal and show that the distance between (hkl)-planes is given by:

$$d_{hkl} = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}}$$

4. Consider specific planes in a triclinic crystal as shown in Fig.3 below. Vector a_3 is directed toward the reader. The origo is marked with a dark spot where a_1 and a_2 are originated.



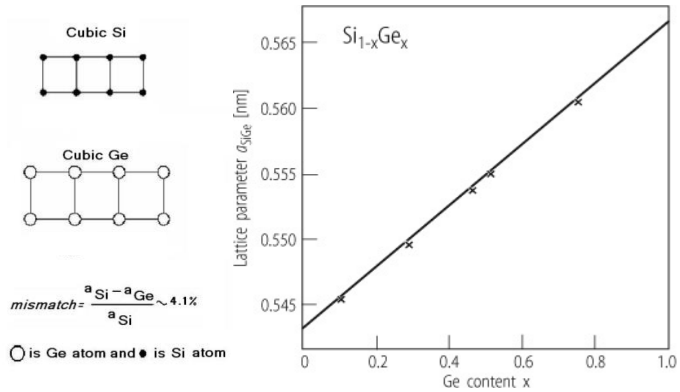
a. What are the Miller indices of the planes 1-6?
b. Make a drawing representing reciprocal lattice points corresponding to the planes in Fig.3;
c. Consider the reciprocal lattice vector *G* corresponding to the (010) planes in the drawing produced when solving problem (b) and an x-ray wave having wavevector *k.* Prove that diffraction is not taking place for any K_G<1/2· |G| where k_G is a projection of *k* vector on *G* direction.
d. Generalize the argument to the rest of the nearest to origo reciprocal points and introduce the Brillouin zone concept on the same graph.

5. Construct 3 first Brillouin zones for a 1D lattice, as well as for 2D and 3D simple cubic lattices.

6. What are limitations to observe crystallographic planes in a real x-ray experiment?

7. Point defects in crystals. Consider, in particular, vacancies.
(a) Show that the minimum free energy in a crystal having N sites is reached only when a certain number of vacancies (n) are available.
(b) Derive an expression for the equilibrium concentration of vacancies (C_V) as a function of temperature (T) and applied stress (σ).
(c) Explain the roles of the activation energy and the activation volume.

8. Consider SiGe alloy. Si and Ge exhibit similar lattice structures, having, however, different lattice parameters, as illustrated in Fig.4 below.



Note, a $Si_{1-x}Ge_x$ film, say $Si_{0.8}Ge_{0.2}$ can be grown on a Si substrate so that the in-plane atomic arrangement in the film is matching that in the substrate, i.e. epitaxy is occurring. The film would then be biaxially compressed as illustrated in Fig.5 below.

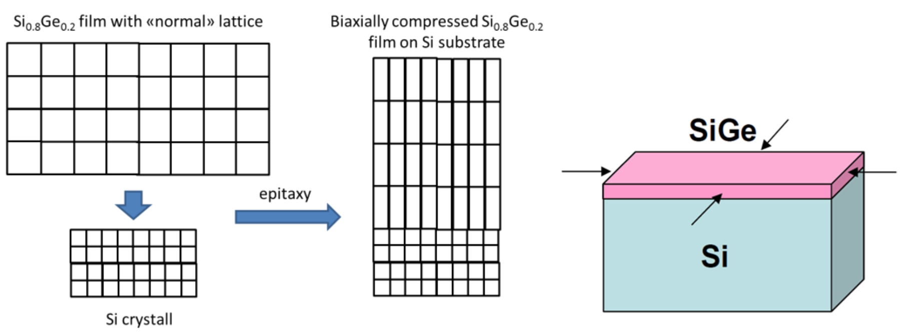
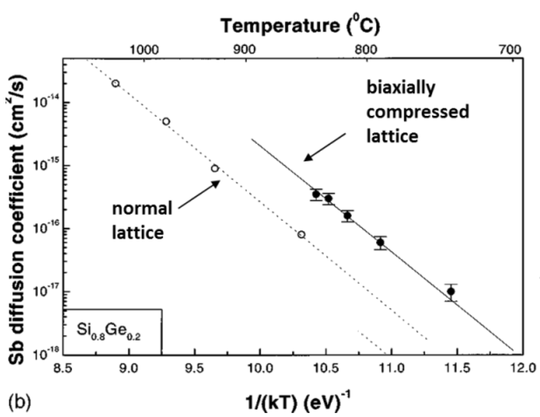


Fig 6 below represents Sb diffusion data in normal and biaxially compressed $Si_{0.8}Ge_{0.2}$.



(a) Estimate the stress occurring effectively in epitaxial $Si_{0.8}Ge_{0.2}$ film manufactured of Si (100) oriented substrate. Use 52GPa for the share modulus of elasticity (μ) and 0.28 for the Poisson ratio (ν).

(a) Assume an x-ray diffraction measurement (λ=1.54Å) of Si and $Si_{0.8}Ge_{0.2}$ crystals as well as $Si_{0.8}Ge_{0.2}$/Si heterostructure. Consider (004) diffraction and make a qualitative drawing showing the diffraction pattern changes in these three samples.

(b) Assuming that Sb diffuses via a vacancy mechanism, estimate the difference in vacancy concentrations in normal and strained $Si_{0.8}Ge_{0.2}$ (use the data in Fig.6).

(c) Estimate the activation volume for Sb diffusion in $Si_{0.8}Ge_{0.2}$.

Note that the stress in a biaxially compressed film may be given as

$$\sigma_0 = -2\mu \frac{\nu+1}{\nu-1} f_m(X), \qquad f_m(X) = 0.0418X,$$

Where $f_m(X)$ is the deformation due to the difference in the lattice parameters and X is the Ge fraction in $Si_{1-X}Ge_X$ alloy [Phys.Rev B 59, 7274(1999)].