Department of Materials Science and Engineering
Norwegian University of Science and Technology

TMT4320 Nanomaterials, fall 2015

EXERCISE 2

Guidance: Wednesday September 2nd, 18:15-20:00, H3
Deadline for handing in: Friday September 4th, 14:00, boxes outside R7

PROBLEM 1

The face-centered cubic unit cell is shown in figure 1 below (the black spheres in the box defines the face-centered cubic lattice). The crystal surface with Miller index (111) is also illustrated in the figure and is normal to the vector [111]. The crystal surfaces (110) and (100) are similarly defined as the planes normal to the vectors [110] and [100].

Several metals have a close-packed structure with the fcc symmetry. The atomic arrangement of a crystal with the fcc lattice is illustrated in figure 1 to the right. The crystal surfaces (111), (110) and (100) are illustrated in the figure.

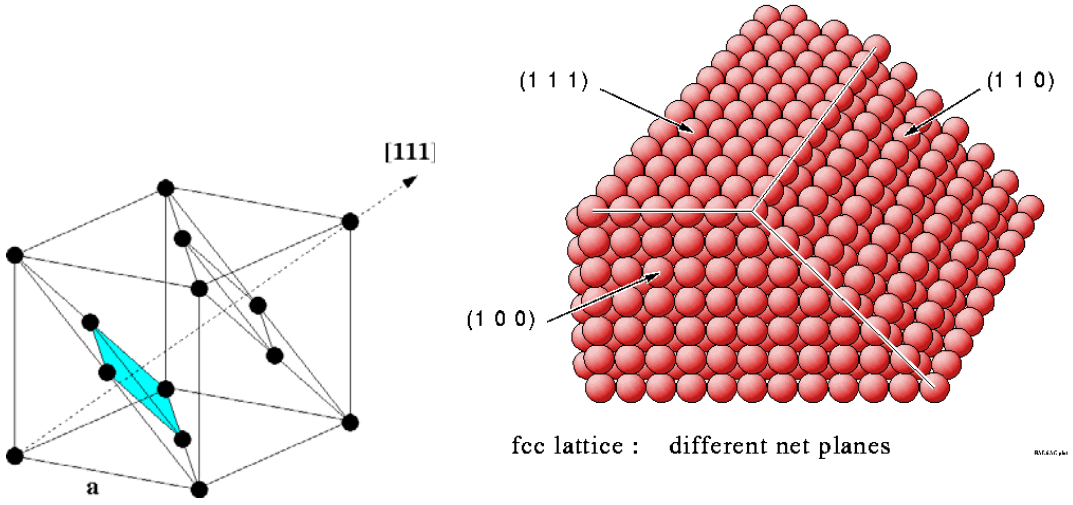

Figure 1. (left) The fcc unit cell. (right) The atomic arrangement of a crystal with the fcc lattice.

a) Rank the three crystal surfaces (111), (110) and (100) according to their surface atomic density (the number of surface atoms per unit area).

b) Each atom in a closed-packed structure is bonded to 12 other atoms (the coordination number is 12). How many bonds per atom are broken for the atoms at the (111), (110) and (100) crystal surfaces?

c) The surface energy γ of a crystal surface can be estimated by:

$$\gamma = \frac{1}{2} N_b \rho_a \varepsilon$$

where N_b is number of broken bonds, ρ_a is the surface atomic density (the number of surface atoms per unit area) and ε is the average bond energy, which can be assumed to be unchanged if the atom is located at the surface.

Rank the three crystal surfaces (111), (110) and (100) according to their surface energy by using this simple model.

PROBLEM 2

a) How is the lattice parameter of a single fcc metal nanoparticle (for instance copper, Cu) with a clean surface affected by the nanoparticle size (qualitatively)?

b) How is the lattice parameter of a single $BaTiO_3$ nanoparticle with cubic crystal structure and a clean surface affected by the nanoparticle size (qualitatively)?

c) Explain the difference in the behavior of the lattice parameter as a function of the size for these two types of nanoparticles.

PROBLEM 3

Why are species (molecules, atoms, ions) adsorbed on edges and/or corners more stable and desorb at higher temperatures than species adsorbed on flat surfaces? Explain.