Name: _____

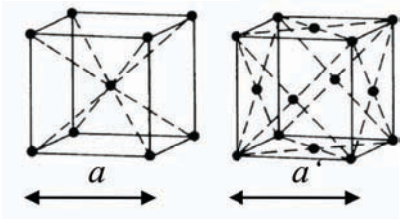
Advanced Solid State Physics — Prof. Dr. W. Kuch
Winter semester 2014/2015
1st exercise sheet

Submission: Tuesday, 21. October 2014 before the lecture
(or drop until 10 o'clock on the same day in mailbox between rooms 1.2.38 and 1.2.40)

1. Influence of surface properties (*) (4 points)

Determine the relative amount of low-coordinated atoms (atoms at surfaces, edges, corners) in a cuboid of n atoms edge length. Assume a simple cubic crystal structure.

2. Structural bcc-to-fcc transition („Bain Path“) (**) (4 points)

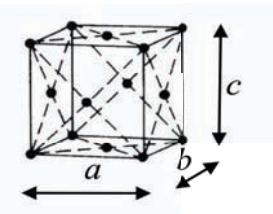


Iron has a *bcc* crystal structure at room temperature with a lattice constant a = 2.87 Å.

a) Calculate the lattice constant a' of an *fcc* structure that has the same atomic density.

b) Calculate the distance between lattice planes defined by Miller indices (100) as well as the nearest neighbor distance of atoms within these lattice planes for *bcc* Fe and for the *fcc* crystal from a).

3. Lattice distortion (**) (4 points)



Nickel has an *fcc* crystal structure at room temperature with a lattice constant a = 3.52 Å. Ultra-thin nickel films on a copper single crystal adopt a tetragonally distorted structure (*fct*, face-centered tetragonal), in which Ni has within lattice planes with Miller indices (001) the lattice constant of Cu ($a = b$ = 3.61 Å), while the distance between these lattice planes is reduced to c = 3.40 Å. The elastic energy needed for this distortion is 17 meV/atom. Estimate from that energy the pressure that would be necessary to yield the same tetragonal distortion in a Ni single crystal.
(Assumptions: Constant Young's modulus, force from pressure = stress is applied perpendicular to (001) lattice planes.)