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

TMT4320 Nanomaterials, fall 2015

EXERCISE 1

Guidance: Wednesday 26th August, 18:15-20:00, H3
Due date: Friday 28th August, 14:00, boxes outside R7

PROBLEM 1

a) Find the surface area (m^2/g), length of the edge (m/g), surface energy (J/g) and edge energy (J/g) as a function of particle size for 1 g palladium (Pd) in the form of cubes. If *a* is the length of the sides of the cube, start with a smallest *a* of 2.8×10^{-10} m and calculate for a number of values for *a* up to 0.01 m. Sketch graphically the energy vs particle size curves.

Use the following information in the calculations: Surface energy 2×10^{-5} J/cm^2; edge energy 3×10^{-13} J/cm; density of palladium 12 g/cm^3.

b) Perform the corresponding surface calculations when the particles are spheres instead of cubes.

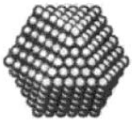
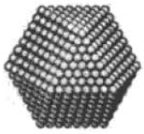
c) Calculate the relative amount of surface atoms as a function of particle size for 1 g palladium in the form of spheres. For small sizes use the information in table 1 below. For larger sizes assume a monolayer of atoms on the surface. Sketch the result graphically.

Use the following information in the calculations: Palladium atomic radius 0.14 nm; Avogadro constant 6.022×10^{23} mol^{-1}; palladium molar mass 106.4 g/mol.

d) Why do small particles tend to be formed as spheres rather than cubes?

e) During a specific growth process of Si nanowires, the nanowires grow as prisms with nearly equal numbers of {211} and {110} faces at the growth temperature of 1000 °C. Estimate the surface energy of the nanowire from the following data: surface energy of the {111} Si = 1.23 Jm^{-2}, ratio of the density of broken bonds on the {211} and {110} faces with respect to the {111} face = 1.41 and 1.22 respectively.

Table 1. The percentage of surface atoms of close-packed full-shell clusters of different sizes.

Full-shell Clusters		Total Number of Atoms	Surface Atoms (%)
1 Shell		13	92
2 Shells		55	76
3 Shells		147	63
4 Shells		309	52
5 Shells		561	45
7 Shells		1415	35