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

TMT4320 Nanomaterials, fall 2015

EXERCISE 7

Guidance: Wednesday 14th October, 18:15-20:00, H3
Due date: Friday 16th October, 14:00, boxes outside R7 or on it's learning

PROBLEM 1

a) Carbon nanotubes can be characterized in terms of their structure. What are the three different structures of carbon nanotubes (explain briefly how their structures can be described) and how do their electrical properties differ?

b) How can the different nanotubes be separated from each other and how do you separate carbon nanotubes from other carbon particles? Give examples of two different methods. Do these methods have any negative or positive effect on the carbon nanotube structure?

(These topics have not been covered much in the lectures. Think by yourself, discuss with others, suggest methods, and/or try to find information elsewhere.)

c) An obvious question that has been around since the discovery of carbon nanotubes is how small the smallest SWCNT is. Theoretical calculations predict that the smallest diameter for a stable SWCNT is around 0.4 nm, and there are three possible structures that correspond with this value - chiral vectors (5,0), (3,3) or (4,2). But if we disregard the stability aspect, what are the chiral vectors of the smallest armchair and zigzag nanotubes structurally possible, while still maintaining a 3D structure and without having a hexagon bonding to itself?

d) The C_{60} molecule exhibits some interesting properties.

i. Describe briefly the electronic and chemical properties of the C_{60} molecule.
ii. What happens if C_{60} molecules are close packed with metal atoms occupying the interstitial sites in the structure?
iii. The general formula used to describe the compound in (ii) is A_xC_{60}, where x is an integer from 1 to 6. How do the electronic properties of the compound develop with increasing x? Explain your answer.

The next two problems are not related to the material covered on carbon nanostructures, but is related to previously covered topics. The exercises are good practice for typical final exam questions.

PROBLEM 2

a) Describe two methods to produce Au nanoparticles. What are the benefits and the limitations of the two methods?

b) Describe two methods to produce $BaTiO_3$ nanoparticles. What are the benefits and the limitations of the two methods?

c) Why do we often have to use a different synthesis method to produce $BaTiO_3$ compared to Au?

PROBLEM 3

In liquid-state synthesis of nanoparticles it is often necessary to separate the liquid and the nanoparticles. This can be achieved by sedimentation for a certain period and then decanting the liquid. Sedimentation is the tendency for particles in suspension or molecules in solution to settle out of the fluid in which they are entrained, and come to rest against a wall. This is due to their motion through the fluid in response to the forces acting on them: these forces can be due to gravity, centrifugal acceleration or electromagnetism.

The sedimentation time for a spherical particle with diameter *d* can be calculated according to equation 1 if the thermal forces (diffusion or Brownian motion) are negligible.

$$t = \frac{9h\eta}{2\left(\frac{d}{2}\right)^2\left(\rho_\mathrm{p} - \rho\right)g} \qquad [1]$$

Here *h* is the sedimentation distance, η is the viscosity of the liquid, ρ_p is the density of the particle, ρ is the density of the liquid and *g* is the gravitional constant.

Brownian motion (named after the Scottish botanist Robert Brown) is the seemingly random movement of particles suspended in a fluid (i.e. a liquid or gas). The average Brownian motion length *x* of a particle within the time *t* can be calculated according to equation 2:

$$x = \left(\frac{RTt}{3\pi\eta\frac{d}{2}N_\mathrm{A}}\right)^{1/2} \qquad [2]$$

Here *R* is the gas constant, *T* is the absolute temperature and N_A is Avogadro's constant.

a) Calculate the sedimentation times for three gold nanoparticles with diameters of 1000 nm, 100 nm and 5 nm, respectively, if the nanoparticles are situated at the liquid-atmosphere interface and the nanoparticles are dispersed in hexane with a 10 cm height from the top to the bottom of the liquid.

Viscosity of hexane:	2.923×10^{-4} Ns/m^2	Gravitational const.:	9.807 m/s^2
Density of hexane:	0.6548 g/cm^3	Gas constant:	8.314 J/mol K
Density of gold:	19.3 g/cm^3	Avogadro constant:	6.022×10^{23} mol^{-1}

b) Calculate the average Brownian motion length of the three gold nanoparticles within the sedimentation time at 25 °C.

c) Compare the average Brownian motion length with the sedimentation distance. Can we assume that the thermal forces (Brownian motion) are negligible when we calculate the sedimentation time?

d) How can the sedimentation time of particles be shortened when you are in the laboratory and want to extract the nanoparticles from a dispersion?