CHG4359: Assignment 1

Due on October 6, 2010

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Question 1

Problem Statement:

Calculate the increase in surface area for the following conditions:

a. A spherical particle with a radius of 100 μm to be reduced to a group of particles with 10 nm radius
b. A cylindrical wire with a radius of 100 μm and a length of 100 μm to be reduced to a group of wires with 10 nm radius and 100 nm length
c. A cube particle with a length of 100 μm to be reduced to a group of cubes with 10 nm length

Solution:

a.

The surface area of a spherical particle with a radius of 100 μm is calculated as follows:

$$\begin{aligned} SA &= 4\pi R^2 \\ &= 4\pi(100\,\mu m)^2 = 1.257 \times 10^5\ \mu m^2 \end{aligned}$$

The number of particles with a radius of 10 nm in a spherical particle with 100 μm is:

$$\begin{aligned} N &= \frac{V(100\,\mu m)}{V(10nm)} \\ &= \frac{\left(\frac{4\pi(100\mu m\frac{1\times10^{-6}m}{1\mu m})^3}{3}\right)}{\left(\frac{4\pi(10nm\times\frac{1\times10^{-9}m}{1nm})^3}{3}\right)} \\ &= \frac{(1\times10^{-4})^3}{(1\times10^{-8})^3} \\ &= 1\times10^{12} particles \end{aligned}$$

This corresponds to a total surface area of:

$$\begin{aligned} SA &= (1\times10^{12})\times 4\pi\left(10nm\times\frac{1\mu m}{1000nm}\right)^2 \\ &= 1.257\times10^9\ \mu m^2 \end{aligned}$$

The surface area increased by **10000 times**.

b.

The cylindrical wire with a radius of 100 μm and a length of 100 μm has a surface area of:

$$
\begin{aligned}
SA &= 2(\pi r^2) + 2\pi r L \\
&= 2\pi(100)^2 + 2\pi(100 \times 100) \\
&= 1.257 \times 10^5 \mu m^2
\end{aligned}
$$

The number of particles can be calculated as follows:

$$
\begin{aligned}
N &= \frac{V(100\mu m, 100\mu m)}{V(10nm, 100nm)} \\
&= \frac{\pi(100\frac{1\times10^{-6}m}{1\mu m})^2(100\frac{1\times10^{-6}m}{1\mu m})}{\pi(10\frac{1\times10^{-9}m}{1nm})^2(100\frac{1\times10^{-9}m}{1nm})} \\
&= \frac{3.14159265358979323846 \times 10^{-12}}{3.14159265358979323846 \times 10^{-23}} \\
&= 1 \times 10^{11} particles
\end{aligned}
$$

This corresponds to a total surface area of:

$$
\begin{aligned}
SA &= 1 \times 10^{11} \times (2(\pi r^2) + 2\pi r L) \\
&= 1 \times 10^{11} \times \left(2\pi(10nm \times \frac{1\mu m}{1000nm})^2 + 2\pi(10nm \times \frac{1\mu m}{1000nm})(100nm \times \frac{1\mu m}{1000nm})\right) \\
&= 1 \times 10^{11} \times (0.00691150383789754512) \\
&= 6.912 \times 10^8 \mu m^2
\end{aligned}
$$

The surface area increased by approximately **5500 times**.

c.

The cube particle with a length of 100 μm has a surface area of:

$$
\begin{aligned}
SA &= (100 \times 100) + (100 \times 100) + (100 \times 100) + (100 \times 100) + (100 \times 100) + (100 \times 100) \\
&= 60000\, \mu m^2 \\
&= 6 \times 10^{10} nm^2
\end{aligned}
$$

The number of 10nm cubes in the 100 μm cube is calculated as follows:

$$\begin{aligned} N &= \frac{V(100\,\mu m)}{V(10nm)} \\ &= \frac{(100\,\mu m \times \frac{1\times10^{-6}m}{1\mu m})^3}{(10nm \times \frac{1\times10^{-9}m}{1nm})^3} \\ &= \frac{(0.0001)^3}{(1\times10^{-8})^3} = 1\times10^{12} particles \end{aligned}$$

This corresponds to a total surface area of:

$$\begin{aligned} SA &= (1\times10^{12}) \times (10nm)^2 \times (6) \\ &= 6\times10^{14} nm^2 \end{aligned}$$

The surface area increased by **10000 times**.

Question 2

Problem Statement:

Estimate the ratio of surface to bulk atoms in following conditions:

a. Spherical clusters - for cluster of radii 1) 5 μm, 2) 500 nm, 3) 1nm.
b. Cubic clusters - for cluster of length 1) 5 μm, 2) 500 nm, 3) 1nm.

In typical metals the surface atom layer has a thickness of 2 A^o.

Solution:

a.

The fraction of atoms F on the surface of a spherical cluster can be given by Equation 1.

$$F = \frac{4}{N^{1/3}} \tag{1}$$

For **5 μm**:

$$N = \frac{V(5\mu m)}{V(2A^o)}$$
$$= 25000$$

$$F = \frac{4}{N^{1/3}}$$
$$= \frac{4}{(25000)^{1/3}}$$
$$= \mathbf{0.137}$$

For **500 nm**:

$$N = \frac{V(500nm)}{V(2A^o)}$$
$$= 2500$$

$$F = \frac{4}{N^{1/3}}$$
$$= \frac{4}{(2500)^{1/3}}$$
$$= \mathbf{0.295}$$

For **1 nm**:

$$N = \frac{V(1nm)}{V(2A^o)}$$
$$= 5$$

$$F = \frac{4}{N^{1/3}}$$
$$= \frac{4}{(5)^{1/3}}$$
$$= \mathbf{2.34}$$

b.

The fraction of atoms F on the surface of a cubic cluster can be given by Equation 2.

$$F = \frac{6}{N^{1/3}} \tag{2}$$

For **5 μm**:

$$N = \frac{V(5\mu m)}{V(2A^o)} = 1.5625 \times 10^{13}$$

$$F = \frac{6}{N^{1/3}} = \frac{6}{(1.5625 \times 10^{13})^{1/3}} = \mathbf{2.4 \times 10^{-4}}$$

For **500 nm**:

$$N = \frac{V(500nm)}{V(2A^o)} = 1.5625 \times 10^{10}$$

$$F = \frac{6}{N^{1/3}} = \frac{6}{(1.5625 \times 10^{10})^{1/3}} = \mathbf{2.4 \times 10^{-3}}$$

For **1 nm**:

$$N = \frac{V(1nm)}{V(2A^o)} = 1000$$

$$F = \frac{6}{N^{1/3}} = \frac{6}{(1000)^{1/3}} = \mathbf{0.6}$$

Question 3

Problem Statement:

The reaction for the deposition of SiO_2 on the surface is:

$$SiH_{4\,(gas)} + O_{2\,(gas)} \longrightarrow SiO_{2\,(solid)} + 2\,H_{2\,(gas)}$$

Gallium nitride (GaN) is an important wide-band-gap semiconductor. Propose a chemical reaction for the deposition of GaN.

Solution:

The most common method to grow GaN is the chemical vapor deposition (CVD) technique, which involves a chemical reaction of metallic Ga or GaCl and $Ga(CH_3)_3$ as Ga precursors under the presence of ammonia (NH_3) gas as a source of nitrogen. The deposition reaction of the formation of GaN when Ga is directly reacted with NH_3 is represented in Reaction 3 (Chow, 2008):

$$Ga_{(s)} + NH_{3\,(g)} = GaN_{(s)} + \tfrac{3}{2}H_{2\,(g)} \tag{3}$$

Another chemical reaction for the deposition of GaN is highlighted below.

The first step is the reaction between liquid gallium and ammonium chloride (Red'kin et al., 2004):

$$Ga + 3\,NH_4Cl = \underset{\text{trichloroamminegallium}}{GaCl_3NH_3} + 2\,NH_3 + \tfrac{3}{2}\,H_2$$

The main product of this reaction is trichloroamminegallium ($GaCl_3NH_3$).

In the second step, gallium nitride is formed predominantly through pyrolysis of trichloroamminegallium vapor (Red'kin et al., 2004):

$$GaCl_3NH_3 = GaN + 3\,HCl$$

Red'kin et al. (2004) found that the optimal deposition temperature (from the viewpoint of the deposition rate and film quality) was 1000°C.

Question 4

Problem Statement:

How long will it take for the spherical particles in Table 1 to settle, at their terminal velocities under free-settling conditions, through 2m of water at 20°C?

Table 1: Question 4

Substance	Specific Gravity	Diameter (nm)
A	10	100
B	10	10000
C	1	100
D	10	10^7

Solution:

Knowns:

$\rho_{water}\,(at\,20^oC) = 998.2\,kg/m^3$

$\mu_{water}\,(at\,20^oC) = 1.02357 \times 10^{-3}\,kg/m \cdot s$

The specific gravity can be used to calculate the densities of Substances A, B, C, and D using Equation 4:

$$\text{Specific Gravity} = \frac{\text{Density of Substance}}{\text{Density of Water}} = \frac{\rho_{substance}}{\rho_{water}} \tag{4}$$

For Substance A,

$$\begin{aligned}\text{Specific Gravity} = \frac{\rho_{substance}}{\rho_{water}} \implies \rho_{substance} &= (\text{Specific Gravity})(\rho_{water}) \\ &= (10)(998.2) \\ &= 9982\,kg/m^3\end{aligned}$$

Similar calculations were performed for Substances B, C, and D. These values have been summarized in Table 2:

Table 2: Summary of Substance Densities

Substance	Density $[kg/m^3]$	Diameter [m]
A	9982	10^{-7}
B	9982	10^{-5}
C	998.2	10^{-7}
D	9982	0.01

The next step is to determine the regime of settling class for each of the substances. Equation 5 is used to determine *K-Value's*, a dimensionless number that is used to establish the regime. According to (Carpenter, 1983), if the K-value is less than 2.6, then Stokes' law applies. If K is greater than 68.9 but less than 2360, Newton's law applies.

$$K = D_p \left(\frac{g\rho(\rho_p - \rho)}{\mu^2} \right)^{1/3} \tag{5}$$

K-Value calculation for Substance A:

$$\begin{aligned} K &= D_p \left(\frac{g\rho(\rho_p - \rho)}{\mu^2} \right)^{1/3} \\ &= (10^{-7}) \left(\frac{(9.81)(998.2)(9982 - 998.2)}{(1.02357 \times 10^{-3})^2} \right)^{1/3} \\ &= 0.00438 \end{aligned}$$

Similar calculations for B, C, and D were performed. A summary of the K-values is provided in Table 3:

Table 3: K Values and The Regimes

Substance	K Values	Regime
A	4.38×10^{-3}	Stokes Law Applies
B	0.438	Stokes Law Applies
C	0	Stokes Law Applies
D	437.9	Newton's Law Range Applies

Since Substances A, B, and C are all in the Stokes Law Regime, Equation 6 can be used to calculate the terminal velocity.

$$u_t = \frac{gD_p^2(\rho_p - \rho)}{18\mu} \tag{6}$$

Terminal velocity calculation for **Substance A**:

$$
\begin{aligned}
u_t &= \frac{gD_p^2(\rho_p - \rho)}{18\mu} \\
&= \frac{(9.81)(10^{-7})^2(9982 - 998.2)}{18(1.02357 \times 10^{-3})} \\
&= 4.78 \times 10^{-8}\, m/s
\end{aligned}
$$

The terminal velocity of **Substance A** is $\mathbf{4.78 \times 10^{-8}\, m/s}$.

Terminal velocity calculation for **Substance B**:

$$
\begin{aligned}
u_t &= \frac{gD_p^2(\rho_p - \rho)}{18\mu} \\
&= \frac{(9.81)(10^{-5})^2(9982 - 998.2)}{18(1.02357 \times 10^{-3})} \\
&= 4.78 \times 10^{-4}\, m/s
\end{aligned}
$$

The terminal velocity of **Substance B** is $\mathbf{4.78 \times 10^{-4}\, m/s}$.

Terminal velocity calculation for **Substance C**:

$$
\begin{aligned}
u_t &= \frac{gD_p^2(\rho_p - \rho)}{18\mu} \\
&= \frac{(9.81)(10^{-7})^2(998.2 - 998.2)}{18(1.02357 \times 10^{-3})} \\
&= 0\, m/s
\end{aligned}
$$

The terminal velocity of **Substance C** is $\mathbf{0\, m/s}$.

Terminal velocity calculation for **Substance D**:

Since Substance D falls in Newton's regime, we can use Equation 7 to calculate terminal velocity:

$$
u_t = 1.75\sqrt{\frac{gD_p(\rho_p - \rho)}{\rho}} \tag{7}
$$

Plugging known values into Equation 7, we can determine the terminal velocity:

$$
\begin{aligned}
u_t &= 1.75\sqrt{\frac{gD_p(\rho_p - \rho)}{\rho}} \\
&= 1.75\sqrt{\frac{9.81 \times 0.01 \times (9982 - 998.2)}{998.2}} \\
&= 1.644\, \mathrm{m/s}
\end{aligned}
$$

In order to determine the settling time in 2m of water, we simply divide 2m by the terminal velocity. For example, the settling time for Substance A is:

$$\begin{aligned} t &= \frac{2}{u_t} \\ &= \frac{2}{4.78 \times 10^{-8}} \\ &= 4.184 \times 10^{7}\,\mathrm{s} = 11623\,\mathrm{hr} \end{aligned}$$

Similar calculations were performed for Substances B, C and D.

Table 4 presents a summary of terminal velocity and their settling time for each of the substances.

Table 4: Question 4 Summary

Substance	Terminal Velocity [m/s]	Settling Time [hr]
A	4.78×10^{-8}	11623
B	4.78×10^{-4}	1.16
C	0	∞
D	1.64	3.38×10^{-4} (1.215 s)

Question 5

Problem Statement:

Explain the applications of thin films in the fields of energy and environment?

Solution:

It is expected that nanotechnology, especially advances in thin films, may contribute to efficient and low-cost systems for generating, storing, and transporting energy in the near future (Yianoulis and Giannouli, 2008). Thin film nanomaterials provide the opportunity to produce new devices and processes that may enhance efficiencies and reduce costs in many areas. Specific areas include solar photovoltaic systems, hydrogen production, fuel cells, solar thermal systems and energy saving technologies as low e-coatings and electrochromic devices for smart windows.

Examples of how thin films impact the fields of energy and the environment include:

- Solar Thermal Collectors
- Photovoltaics

  Thin films offer significantly cheaper alternative to solar cells made from crystalline silicon. It is cheaper to manufacture and uses one tenth of the silicon as crystalline cells. However, the efficiency of the final product is only 7 to 10 percent. In order to occupy a larger percentage of solar cells, research will be needed to increase this efficiency.

- Electrochromic Smart Windows and Passive Solar and Energy Conscious Design

  Thin films of electrochromic oxides, ion storage layers and transparent conductors are important for smart windows.

- Bendable Batteries

  Engineers from Stanford University have developed bendable batteries by coating a solid support with a thin film of carbon nanotubes and deposited a film of metal-containing lithium compound on top of the nanotubes. These new types of batteries could provide energy sources for many interesting products.

References

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