D43 Training School "Fluids and Solid Interfaces"

Tutroial: Scattering from liquid-Liquid

1. Calculate the scattering length density, ρ for a silicon substrate and hence a value for its critical angle θ_c at a wavelength of 5.0 Å.

[Properties of Si: density = 2.33 g cm^{-3}; atomic weight = 28 g mol^{-1}; neutron scattering amplitude = 0.42×10^{-12} cm].

$$\sum_i b_i = 0.42 \times 10^{-12} \text{ cm} = 0.42 \times 10^{-12} \text{ cm}$$

$$M = 28 \text{ g mol}^{-1}$$

$$\rho = \frac{N_A d \sum_i b_i}{m} = \frac{6.022\times10^{23} mol^{-1} \times 233\ gcm^{-3} \times 0.42\times10^{-12} cm}{28\ gmol^{-1}}$$

$$\rho = 2.1\times10^{-6}\ \text{Å}^{-2}$$

$$\theta_C = \left(\frac{\lambda^2}{\pi}\rho\right)^{1/2} \qquad \theta_C = \left(\frac{5.0^2}{\pi}\times2.1\times10^{-6}\right)^{1/2} = 4.09\times10^{-3}$$

$$\theta_C = 0.23^\circ$$

2. Calculate the difference in the scattering length densities for Iron, for neutron spin aligned parallel and antiparallel to the Fe magnetic moment.

Neutron scattering length, b	9.45 fm
Magnetic moment	2.2 μ_b
Density	7870 kg m^{-3}
Atomic mass	55.845 g mol^{-1}

C = 2.695 fm μ_b^{-1}

$$Number\ density(n) = N_A \times density / AtomicMass = 8.4865 \times 10^{28}\, m^{-3}$$

Scattering length density of Fe for spin up (δ+) and spin down (δ-) neutrons is given by

$$\rho^{\pm} = N \times (b \pm C \cdot \mu_b)$$

$$\rho^{+} = 1.305 \times 10^{-5}\ \text{Å}^{-2}$$

$$\rho^{-} = 4.595 \times 10^{-5}\ \text{Å}^{-2}$$

The difference is 3.290×10^{-5} Å^{-2}

3. Scattering wave vector is defined as;

$$Q = \frac{4\pi \sin\theta}{\lambda}$$

Derive an expression for the resolution $\frac{\Delta Q}{Q}$.

The equation to calculate errors in quadrature is:

$$\sigma_Q^2 = \left(\frac{\delta Q}{\delta \theta}\right)^2 \sigma_\theta^2 + \left(\frac{\delta Q}{\delta \lambda}\right)^2 \sigma_\lambda^2$$

Substituting for Q and partially differentiating with respect to θ and λ;

$$\sigma_Q^2 = \left(\frac{4\pi \cos\theta}{\lambda}\right)^2 \sigma_\theta^2 + \left(\frac{4\pi \sin\theta}{\lambda^2}\right)^2 \sigma_\lambda^2$$

Divide through by Q

$$\frac{\Delta Q}{Q}=\sqrt{\frac{\Delta\lambda^2}{\lambda^2}+\cot^2(\theta)\Delta\theta^2}$$

4. A 20 Å neutron and Airbus A380 leave Sofia airport at the same time bound for Chicago by the same route. Assuming Airbus covers 5600 kilometre in 9 hours, which arrives first at Chicago and by how much. (You may neglect the finite lifetime of neutrons!)

Airbus $Velocity=\frac{dis\tan ce\ travel}{timetaken}=\frac{5600}{9}=622\ Km\ per\ hour=173\ ms^{-1}$

Neutron $Velocity=\frac{h}{m\lambda}=\frac{6.626\times10^{-34}}{\left(1.674\times10^{-27}\times20\times10^{-10}\right)}=198\ JsKg^{-1}m^{-1}$

1 J = 1Nm = 1 kg ms^{-2} m = 1 Kg m^2s^{-2}

Hence Js $Kg^{-1}m^{-1}$ = $Kgm^2s^{-2}Kg^{-1}m^{-1}$ = ms^{-1}

Neutron arrives first by about 68 minutes.

5. What is the energy of 5 Å neutrons in electron-volts, eV?

$$Energy=\frac{m\times v^2}{2}=\frac{m}{2}\left(\frac{h^2}{m^2\times\lambda^2}\right)=\frac{h^2}{2m\times\lambda^2}$$

$$Energy=\frac{(6.626^{-34})}{2\times1.674\times10^{-27}\times(5\times10^{-10})^2}=5.245\times10^{-22}\ J^2s^2Kg^{-1}m^{-2}$$

J^2s^2 $Kg^{-1}m^{-1}$ = $Kg^2m^4s^{-4}s^2Kg^{-1}m^{-2}$ = Kg m^2s^{-2} = J

To convert to eV, divide by the elementary charge:

$$Energy=\frac{5.245\times10^{-22}}{1.602\times10^{-19}}=0.003274\ JC^{-1}(or\ eV)=3.274\ meV$$

6. Calculate the theoretical transmission of 1 mm thick layer of water.

$$T(\lambda) = \exp[-N \times t \times \sigma_{total}(\lambda)]$$

Where t is the path length (0.01 cm) and σ_{total} is total cross-section.

H_2O

M = 18 g mol^{-1}, ρ = 1.00 gcm^{-3} thus N = 3.34 $\times 10^{22}$ cm^{-3}

H:

$\sigma_{coh} = 1.8 \times 10^{-24}$ cm^2, $\sigma_{inc} = 80.3 \times 10^{-24}$ cm^2, $\sigma_{abs} = 0.3 \times 10^{-24}$ cm^2

O:

$\sigma_{coh} = 4.2 \times 10^{-24}$ cm^2, $\sigma_{inc} = 0.0 \times 10^{-24}$ cm^2, $\sigma_{abs} = 0.0 \times 10^{-24}$ cm^2

Hence:

$\sigma_{total} = \sigma_{coh} + \sigma_{inc} + \sigma_{abs} = 2 \times (1.8 + 80.3 + 0.03) \times 10^{-24} + 4.2 \times 10^{-24}$

$\sigma_{total} = 1.69 \times 10^{-22}$ cm^2

T = exp [$-3.34 \times 10^{22} \times 0.1 \times 1.69 \times 10^{-22}$] = 0.57

Absorption cross section is a function of wavelength hence energy. Here the valve is taken for 6 Å neutrons.

7. Small group Exercise:

Computer based analysis of neutron reflectivity data for protein friendly surfaces. This involves analysis of neutron reflectivity data to probe the resistance of a poly (ethylene glycol) (PEG) coated silicon surface to the adsorption of the model protein bovine serum albumin (BSA) from buffered aqueous solution. [**Please see the additional information provided**]