P9826b Winter 2013

## March 13, 2013

## Homework Assignment #1 (due on March 25, 2013)

## **Problems:**

1. (3 points) XPS spectrum for unknown sample is presented below with exact binding energies list. Identify the peaks (element and transition) at the listed binding energy positions.



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	1	2	3	4	5	Total
mark						
out of	3	4	3	2	3	15

2. (4 points) In Rutherford backscattering spectrometry, the kinematics of the collisions and the scattering cross section are independent of the chemical bonding, but only dependent on the masses of the target atoms. The diagram of the collision events is shown below:



In the collision, energy is transferred from the moving particle to the stationary target atom; the reduction in energy of the scattered particle depends on the masses of incident and target atoms and provides the signatures of the target atoms.

Assuming that an incident energetic particle of mass  $M_1$  has velocity  $v_0$  and energy  $E_0$ , and target atom of mass  $M_2$  is at rest. After the collision, the values of the velocities  $v_1$  and  $v_2$ , the projectile and target atoms are determined by the scattering angle  $\theta$  and recoil angle  $\phi$ .

One can write equations for conservation of energy, and conservation of momentum parallel and perpendicular to the direction of incidence (3 equations total, see lecture notes). One can go through a page of algebra to get the following expression for the energy of projectile  $(M_1)$  after collision:

$$E_{1} = E_{0} \left[ \frac{\left(M_{2}^{2} - M_{1}^{2} \sin^{2} \theta\right)^{1/2} + M_{1} \cos \theta}{M_{2} + M_{1}} \right]^{2}$$

(a) Assuming that M<sub>1</sub><M<sub>2</sub>, find the ration of  $\frac{E_1}{E_0}$  at direct backscattering condition ( $\theta$ =180<sup>0</sup>).

Show the details of your calculations.

$$E_{1} = E_{0} \left[ \frac{\left( M_{2}^{2} - M_{1}^{2} \times 0 \right)^{1/2} + M_{1} (-1_{-}}{M_{2} + M_{1}} \right]^{2} = \left( \frac{M2 - M1}{M2 + M1} \right)^{2}$$
  
$$\frac{E1}{E0} = \left( \frac{M2 - M1}{M2 + M1} \right)^{2}; \text{ when } M1 << M2 \Longrightarrow \frac{E1}{E0} = 1$$

(b) Assuming collision where  $M_1=M_2$ , and the incident particle is at rest after the collision, with all the energy transferred to the target atom, a feature well known in billiards. Find the ration of  $\frac{E_2}{E_0}$  as a function of  $M_1$ ,  $M_2$  and angle  $\phi$ .

$$\frac{E2}{E0} = \frac{4M_1M_2}{(M_1 + M_2)^2} \cos^2 \phi$$

(c) Under which conditions the maximum value of  $\frac{E_2}{E_0}$  (or the maximum energy transfer)?  $\frac{E2}{E0} = \frac{4M_1M_2}{(M_1 + M_2)^2} \cos^2 \phi;$   $\frac{E2}{E0}$  has maximum value = 1, when  $\phi = 0$ ,  $M_1 = M_2$ 

(d) If you use alpha particles ( $M_1$ =4a.m.u.) with incident energy  $E_0$ =2MeV, detector is at  $\theta$ =180<sup>0</sup>; and your target is ~100 Å thick gold film on top of silicon substrate<sub>)</sub>, find your energy positions of Si and Au elements in Rutherford Backscattering spectrum. Draw RBS spectrum schematically but mark energy positions for all observed features.



3. (3 points) Silicon nanocrystals (Si-ncs) embedded in SiO<sub>2</sub> exhibit strong luminescence at room temperature and are of interest in the drive to produce silicon photonic devices that are compatible with silicon processing techniques. Formation of Si-ncs can be done using ion implantation of excess silicon into an SiO<sub>2</sub> film, followed by high temperature annealing (nucleation and growth via Ostwald ripening).

(a) Your sample is composed of 100nm  $SiO_2$  film on top of Si(001) substrate. Use SRIM to find the incident energy of Si ions to place excess Si atoms in the middle of  $SiO_2$  layer (assume that implantation angle is 10 degrees).

If you used SiO<sub>2</sub> density of 2.2 g/cm<sup>2</sup>, the incident ions energy is ~33keV

(b) To achieve excess silicon in SiO<sub>2</sub> layer, one has to use implantation dose as high as  $1 \times 10^{17}$  Si atoms/cm<sup>2</sup>. As a result of Si-ncs formation SiO<sub>2</sub> layer expands or "swell" to some degree, and thickness of SiO<sub>2</sub> layer becomes larger. Calculate this increase in SiO<sub>2</sub> layer thickness, assuming simplified model when 100% of implanted Si form Si-ncs that are cubic in shape with the dimensions  $d=3 \times 1$  attice constant of Si ( $a_{Si}$ ). (As a reminder, Si has a diamond lattice structure with the lattice constant a=5.43Å). Hint: you may choose to calculate (*i*) number of Si atoms in unit cell; (*ii*) how many Si atoms per cm<sup>-3</sup>.)

Si has a diamond lattice structure: 8 atoms/unit cell

 $\Rightarrow$  4.99×10<sup>22</sup> atoms/cm<sup>3</sup>

You expect change in thickness by  $1 \times 10^{17}/4.99 \times 10^{22} = 2 \times 10^{-6}$  cm = 20nm

(c) During implantation process, some fraction of Si and O atoms will be sputtered. Use SRIM to estimate the total sputtering effect with running simulation with 1000 incident ions, extracting sputtering yield of Si and O, and extrapolating to the dose of  $1 \times 10^{17}$  Si atoms.

Sputtering yield of Si: 0.55 atoms/ion  $\Rightarrow$  total sputtering yield 0.55×10<sup>17</sup> atoms

*O*: 1.80 atoms/ion  $\Rightarrow$  total sputtering yield 1.8×10<sup>17</sup> atoms

(d) Compare your sputtering results in (c) with "swelling" results in (b), and comment on whether you should use your ion energy for the Si-ncs formation.

*Mass of sputtered Si atoms*= $0.55 \times 10^{17}$  *atoms*× 28.08 g/mol / 6.022 × $10^{23}$ = $2.56 \times 10^{-6}$ g *Mass of sputtered O atoms*= $1.8 \times 10^{17}$  *atoms*× 16 g/mol / 6.022 × $10^{23}$ = $4.78 \times 10^{-6}$ g

Assuming that  $SiO_2$  layer was sputtered (density of 2.2 g/cm<sup>2</sup>),  $SiO_2$  layer was reduced by"

 $(2.56 \times 10^{-6} + 4.78 \times 10^{-6})g/(2.27 g/cm^3 \times 1 cm^2) = 32.3 nm$ 

Incident energy of 33keV can be used for Si-ncs formation. Implanted Si atoms are at a depth of 50 nm, at the same time top 32.3 nm of SiO<sub>2</sub> is sputtered of, as a result the layer containing Si nanoparticles is closer to the top surface, and total thickness of Si NP in SiO<sub>2</sub> layer is < 100nm.

4. (2 points) In your own words explain the meanings of matrix effects in SIMS.

Secondary ion yields depend the energy of the incident ions, mass of the incident particles, material properties (ionization potential and electron affinity), and strongly dependent on the chemical environment.

5. (*3 points*) (a) When measuring spherical particles of less than 10 nm on a substrate with an atomic force microscope, an experienced operator uses the height of the sphere to estimate the size of the object. Explain why, instead of using the measured lateral dimension (size) of the sphere, he/she selects to do so.

Using a simple geometrical argument we see that when the size of a particle is smaller than the size of the tip, the shape of the object cannot be resolved, as depicted by the curve in the diagram below. However the vertical displacement at the highest point can be deduced from the cross-section curve of the image at the location of the particle and the size can be calculated by using this value as the diameter of the sphere.

(b) Explain why phase shift imaging in AFM may be useful in differentiating composite materials. Hint: Think about AFM tip as of a forced oscillator.

If we consider the AFM tip as a forced oscillator, the corresponding differential equation would

be  $m\frac{d^2z}{dt^2} + c\frac{dz}{dt} + kz = F_0 \cos \omega t$ , where c is the damping coefficient, m is the mass of the

cantilever,  $F_o$  and  $\omega$  are the force and amplitude applied to the piezoelectric, respectively. The equation above can be solved as the differential equation. Solution is  $z = A(\cos(\omega t + \phi), where \tan(\phi) \propto \omega/(\omega_0^2 - \omega^2)$ .

By varying the damping coefficient  $\omega$  the phase shift also changes, and since variation in composition of the sample corresponds to variation in the damping coefficient, this can tell us about composition of the sample.