Name: **Quiz-04** **Your ID #:**

ODEs + X-ray diffraction

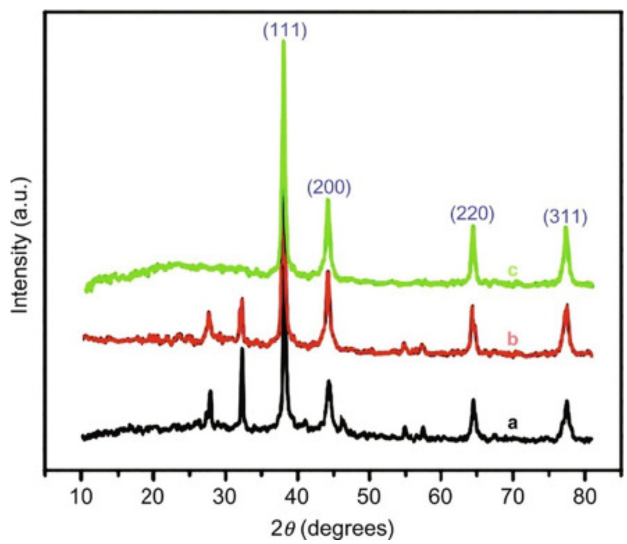
Please answer the below questions:

Instructions:

1. **The Quiz consists of 2 questions (Q1 and Q2) worth a total of 10 points.**
2. **Please submit PDF + code file**
3. **Please submit video (max 2 min) to summarize how did you solve these problems**

Q1 (5pts): Problem 1. (X-ray diffraction)

a) Using Vesta software, generate Sc, Bcc, and Fcc structures of Mg with lattice parameters of a=4.5 Å. Refer to our lecture on Microsoft Teams for more information.
b) Using Vesta, calculate the X-ray diffraction patterns for the Sc, Bcc, and Fcc structures of Mg and export the data in text files.
c) c) Write Python code to calculate the X-ray diffraction pattern for the Bcc structure of Mg.
d) List the first 10 allowed planes [h k l] and the first 5 absent planes in the X-ray diffraction pattern for Bcc structure.
e) Plot all three structures on the same graph (using text files generated in part (b))with result of the Python code from part (c). Your graph should look similar to the below figure.



Q2 (5pts): **Problem 1. (Simple Pendulum)**

The simple pendulum differential equation can be written as

$$\frac{d^2\theta}{dt^2} = -\frac{g}{l}sin\theta$$
$$\frac{d\theta}{dt} = \omega$$

This can be written as a system of first order differential equations as follows:

$$\frac{d\theta}{dt} = \omega$$
$$\frac{d\omega}{dt} = -\frac{g}{l}sin\theta$$

Take $g = 9.8\frac{m}{s2}, l = 1.0$ m, $\alpha = -\left(\frac{g}{l}\right)\sin(\theta)$ and initial positions and velocities $\theta_1 = 0.15\, rad, \omega_1 = 2.0\, rad/s$.

Write a python code to solve the above system of equations and plot

a) $\theta\ vs. t,$
b) $\omega\ vs. t$
c) $\theta\ vs. \omega$
d) Energy J (Joules)

Using the following methods:

a) Euler's method

$$\omega_{n+1} = \omega_n + \alpha_n\, dt$$
$$\theta_{n+1} = \theta_n + \omega_n\, dt$$

b) Euler-Cromer method

$$\omega_{n+1} = \omega_n + \alpha_n\, dt$$
$$\theta_{n+1} = \theta_n + \omega_{n+1}\, dt$$

c) Euler-Verlet method

$$\theta_{n+1} = 2\theta_n - \theta_{n-1} + \alpha_n\,(dt)^2$$
$$\omega_n = \frac{\theta_{n+1}-\theta_{n-1}}{2dt}$$

In the last method, you need to define: $\theta_0 = \theta_1 - \omega_1\, dt + \frac{1}{2}\,\alpha_1\,(dt)^2$

Try values of $dt = 0.5, 0.1,$ and 0.01 and total time = 200.