Homework No. 5 (Based on week 5 lectures)

1. In order to understand some aspects of Kelvin Probe Force Microscopy let us consider a few key equations for the electrostatic force between the tip and the sample. The following relation was shown in the class notes:

   $$F_{electrostatic} = -\frac{1}{2}\frac{dC}{dz}\left[V_s(x,y) - \left(V_{DC} + V_{AC}\sin\left(\omega_{elec}t\right)\right)\right]^2$$

   To this let us add an analytical expression for the Capacitance from (L. Fumagalli et al, Nanotechnology, 20(39), 2009)

   $$C = 2\pi\varepsilon_0 R \ln\left[1 + \frac{R\sin(\theta)}{z + h/\varepsilon_r}\right] + K(R,\theta)$$

   which represents an expression for the capacitance formed between the apex of an AFM conducting tip of radius $R = 10nm$ and semi-cone angle $\theta = 30\,\text{degrees}$ and a sample consisting of a thin dielectric layer of height $h = 10nm$ and relative dielectric constant $\varepsilon_r = 20$ deposited on a conducting substrate. $\varepsilon_0 = 8.8542 \times 10^{-12}$ farads per meter ($\text{F}\cdot\text{m}^{-1}$) is the vacuum permittivity and z is the gap between the tip and the surface of the dielectric layer. $K(R,\theta)$ is a geometric term which is independent of tip sample gap z and thus does not contribute to the force gradient. As discussed in class there is also a stray capacitance that should be included to this apex capacitance but for the sake of simplicity let us assume here that only the apex capacitance is significant.

What is the magnitude of dC/dz when $z = 10nm$?

(a) 722 nanoFarad/meter
(b) 366 picoFarad/meter
(c) 722 microFarad/meter
(d) 366 miliFarad/meter

2. From the expressions of electrostatic force and apex capacitance provided in the previous page, which of the following statements about KPFM data on this sample are correct?
   a. The contact potential image would contain information related to the viscosity of the sample.
   b. The contact potential image would contain information related to contact potential difference and/or trapped surface charges on the dielectric.
   c. The $2\omega_{elec}$ amplitude maps variations contact potential difference and/or trapped surface charges on the dielectric
   d. The $2\omega_{elec}$ amplitude maps variations in local height of the dielectric film, its relative dielectric constant.
   e. (a) and (c)
   f. (a) and (d)
   g. (b) and (c)
   h. (b) and (d)

3. We would like to simulate F-Z curves between a Si tip and a mica surface in saline solution in this problem. For this log on to VEDA, and load the "Force-Distance Curves" tool. Load the "Example 1:Approaching and retracting from a sample modeled using DMT contact". Make the following changes to the parameter values that automatically load with this example:

- Under *operating conditions and cantilever properties* tab, change the Q factor to 2 (which is more relevant for water), and reduce the resonance frequency to 10kHz. Furthermore, please make the starting Z distance=20nm and final Z distance =-20nm. Also make the cantilever stiffness= 10 N/m
- Under the *Tip-sample interaction properties* tab, change the tip-sample interaction model from DMT to DMT+DLVO(liquids). The charge density numbers that auto-populate are typical for those for Si and mica in saline solutions. Also change the Young's modulus of the sample to 170GPa to mimic micas elasticity and the van der Waals adhesion force = 0.25 nN. Finally change the Debye length to 0.01 micrometers (10 nm for a moderate concentration buffer)
- Now hit the *simulate* button, and in the results, choose to graph "Observed cantilever deflection vs Z" . Repeat for retraction, making the starting Z distance=-20nm and final Z distance =+20nm
- By comparing approach and retraction curves (cantilever deflection vs. Z) and noticing there is almost no hysteresis there is no visible snap-in or pull-off instability observed in this graph.
- Repeat these approach/retract simulations for a few evenly spaced decreasing values of cantilever stiffness (down to 0.01 N/m) leaving everything else unchanged

Below what cantilever stiffness do you observe a clear hysteresis between approach and retraction curves (i.e snap-in/pull-off)?

a. For any cantilever stiffness there is a snap-in phenomenon
b. For any k<5 N/m a clear snap-in can be seen
c. For k<0.1 N/m there is a clear snap in
d. Only when k<0.01 N/m does one see a snap-in