Homework No. 5

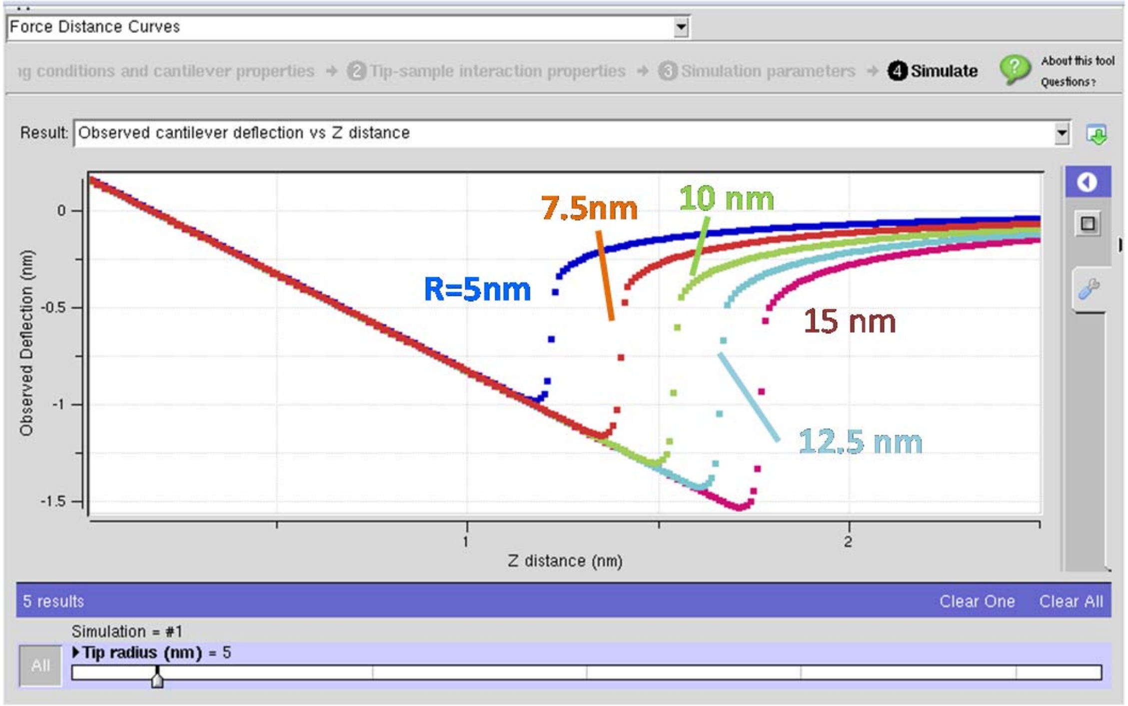
Fundamentals of AFM: Part I

Lectures: P1_Wk5_L1 - P1_Wk5_L6

Problem 1: Does the tip radius change during an AFM experiment?

It is useful to have a simple, *in-situ* test that determines if the tip radius changes during the course of an AFM experiment. One way to monitor the tip radius is to monitor the z location where the jump to contact occurs.

To check this idea further, select the Force Distance Curves application in VEDA. Select the DMT contact model. Use all the default parameters in VEDA **except** for the following. Set the spring constant of the cantilever to 0.1 N/m; choose a hard substrate by making the elastic modulus of the sample equal to 100 GPa. Use the default Hamaker constant of 3.4×10^{-20} J. Perform 4-5 simulations of observed cantilever deflection vs z distance (0<z<3 nm) for different tip radii. Let the tip radius vary between 5 nm and 15 nm.



Force Distance Curves

Result: Observed cantilever deflection vs Z distance

Simulation = #1

Tip radius (nm) = 5

Q1.1. From this simulation, what is the predicted jump to contact distance (z) when the tip radius is 5 nm?

a) about 1.2 nm
b) about 1.4 nm
c) about 1.5 nm
d) about 1.7 nm
e) about 1.8 nm

Q1.2. From this simulation, estimate the accuracy required in a measurement of the z position when jump to contact occurs in order to detect a 1 nm change in tip radius?

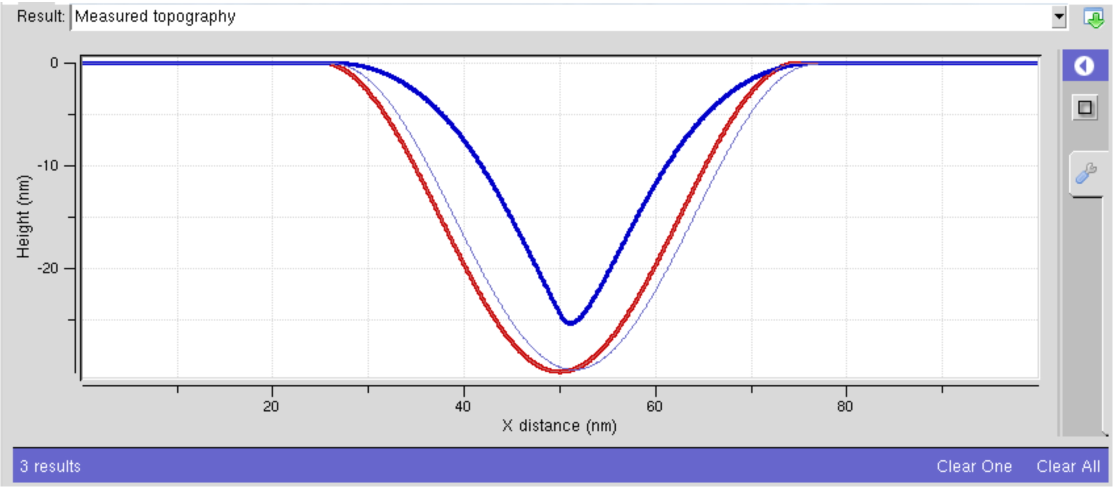
a) a 1 nm change in tip radius corresponds to about a 0.003 nm change in the jump to contact position
b) a 1 nm change in tip radius corresponds to about a 0.05 nm change in the jump to contact position
c) a 1 nm change in tip radius corresponds to about a 0.15 nm change in the jump to contact position
d) a 1 nm change in tip radius corresponds to about a 0.30 nm change in the jump to contact position

Problem 2: Depth of a hole in a flat substrate

Suppose a substrate has a hole that can be modeled as a sinusoid feature. How accurately can a contact mode AFM scan measure the depth of this hole?

To investigate this problem further, select the contact mode scanning application in VEDA. Use the following parameters:

“Operating cond. + Cantilever prop.”			**“Tip-sample interact. prop.: substrate”**	
No. eigenmodes	1		Tip-sample interaction	DMT contact
Cantilever stiffness	0.6 N/m		R_{tip}	10 nm
Q	50		E_{tip}	130 GPa
Set point deflection	2 nm		v_{tip}	0.3
Scan Lines per second	2		a_o	0.2 nm
P	0.0025		H	3.4e-20 J
I	0.0025		E_{sample}	100 GPa
Sampling frequency	1 MHz		v_{sample}	0.3
"Simulation parameters"			**"Tip-sample interact. prop.: Feature"**	
			Geometric feature	Sinusoid
Use default values			Feature height	-30 nm
			Length of feature	50 nm
			Include geometric convolution	Yes
			Specify material properties	no


Result: Measured topography

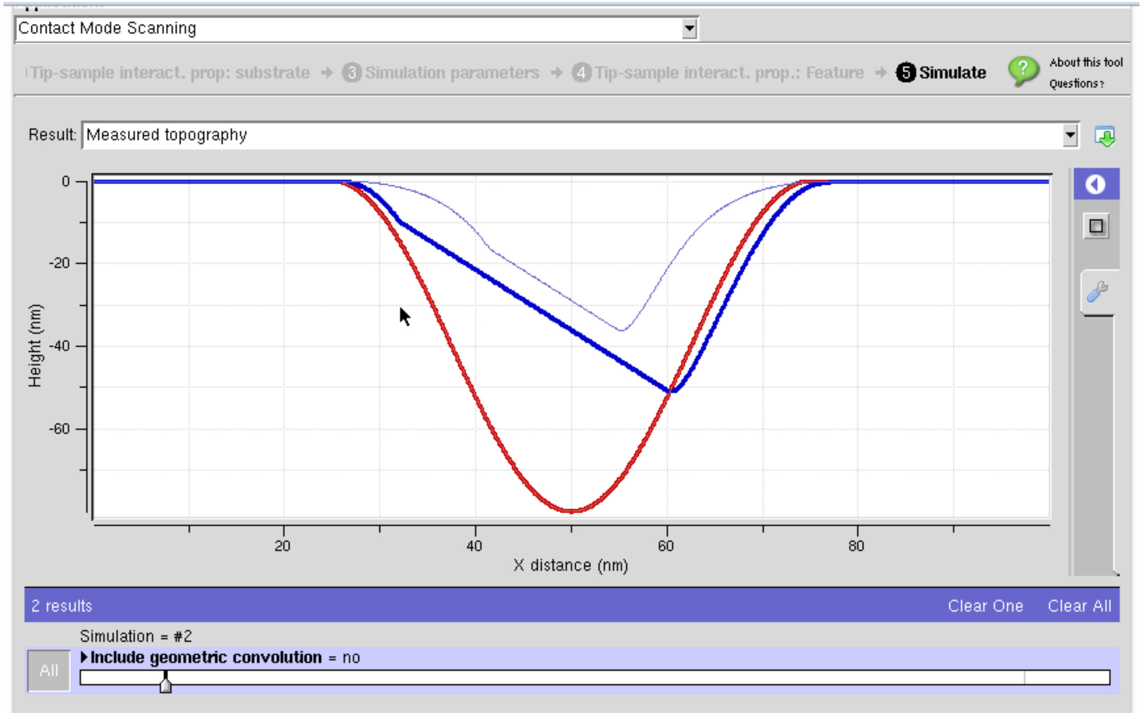
3 results

Q2.1. From this simulation, how deep is the pit as measured from the AFM image?

a) about 5 nm deep
b) about 10 nm deep
c) about 25 nm deep
d) about 30 nm deep

Q2.2. Suppose one pit on the substrate happens to be 80 nm deep instead of 30 nm. Using the same parameters defined above, what would be the apparent depth of the pit as measured from an AFM image?

a) about 15 nm deep
b) about 20 nm deep
c) about 25 nm deep
d) about 35 nm deep


Contact Mode Scanning

Result: Measured topography

2 results

Simulation = #2

Include geometric convolution = no

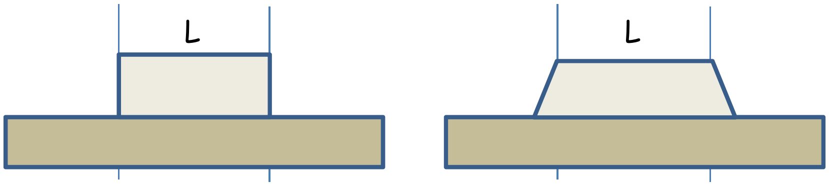
Q2.3. If you performed an experiment and observed the profiles produced by the VEDA simulation generated in Q2.2 above, what course of action might you take next?

a) remove the cantilever and install a different cantilever with a new tip
b) speed up the tip by increasing the number of lines scanned per second
c) readjust the P and I settings to optimize the AFM response
d) readjust the set point conditions so that the set point force increases

Problem 3. Error maps in contact mode AFM

Suppose a substrate has sub-micron features produced by chemical etching. Can a contact mode AFM scan distinguish between rectangular and trapezoidal sidewalls?

Can you distinguish between these
two shapes using contact mode AFM?

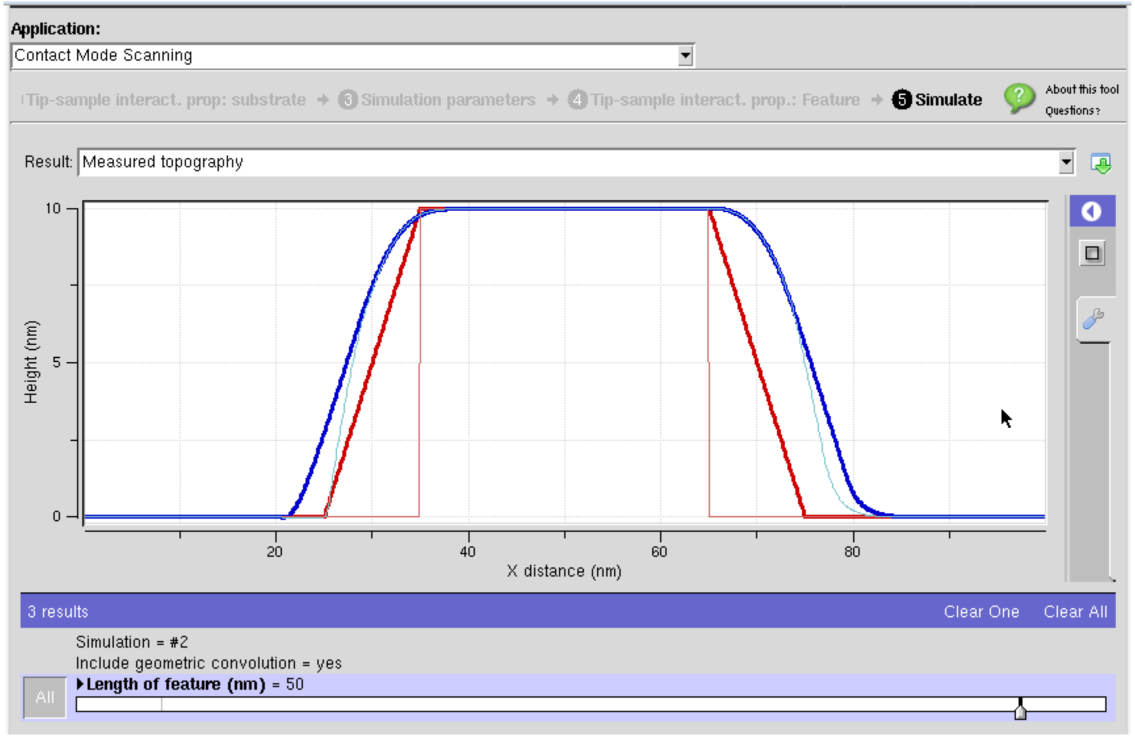


To investigate this problem further, select the contact mode scanning application in VEDA. Use the following parameters:

“Operating cond. + Cantilever prop.”			**“Tip-sample interact. prop.: substrate”**	
No. eigenmodes	1		Tip-sample interaction	DMT contact
Cantilever stiffness	0.6 N/m		R_{tip}	10 nm
Q	50		E_{tip}	130 GPa
Set point deflection	2 nm		ν_{tip}	0.3
Scan Lines per second	2		a_o	0.2 nm
P	0.0025		H	3.4e-20 J
I	0.0025		E_{sample}	100 GPa
Sampling frequency	1 MHz		ν_{sample}	0.3
“Simulation parameters”			**“Tip-sample interact. prop.: Feature”**	
			Geometric feature	Trapezoid
Use default values			Feature height	10 nm
			Length of feature	50 nm
			Length of trapezoid top	30 nm
			Include geometric convolution	Yes
			Specify material properties	no

Initially in the Feature tab, select a trapezoidal geometric feature that is 10 nm high with a 50 nm feature length having a length for the trapezoidal top of 30 nm. Then compare to a trapezoidal geometric feature that is 10 nm high with a 30 nm feature length and a length for a trapezoidal top set to 30 nm (i.e. a rectangular feature).

Make sure you include geometric convolution.



Application: Contact Mode Scanning

Result: Measured topography

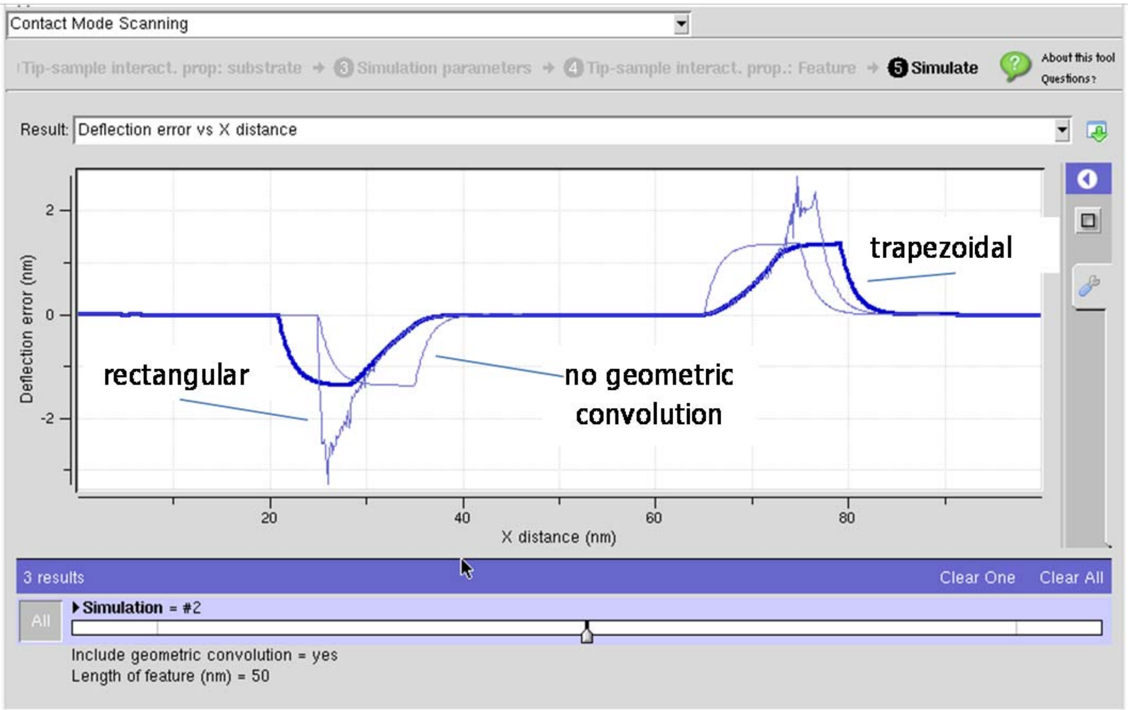
Simulation = #2
Include geometric convolution = yes
Length of feature (nm) = 50

Q3.1. For the scanning parameters selected, is it possible to distinguish between the two geometries from the measured topography?

a) Yes, the differences are quite clear
b) No, there is absolutely no difference in the two contact mode scans
c) The two features look very similar in an AFM scan. Careful measurements would be required to tell them apart.

Q3.2. For the scanning parameters selected, is it possible to distinguish between the two geometries from the deflection error of the cantilever (i.e. an error map)?

a) Yes, the differences in the error map are quite distinct
b) No, there is absolutely no difference in the error map between the two scans
c) The errors look very similar. Careful measurements would be required to tell them apart.



Simulation = #2

Include geometric convolution = yes

Length of feature (nm) = 50

Problem 4. Approach-retract using JKR contact model

After performing an F vs. z experiment, you find a noticeable hysteresis between the approach and retract data even though you believe the sample and tip are clean. Use the JKR contact model to understand the hysteresis.

Open VEDA and under the application window, select “Force Distance Curves”. Set up a simulation using the following parameters. Use the VEDA default parameters for any item not specified below. In the simulations below, you will be adjusting the values in the yellow-shaded boxes.

“Operating cond. + Cantilever prop.”			**“Tip-sample interact. prop.”**	
Operating mode	approach and retract		Tip-sample interaction	JKR contact
No. eigenmodes	1		R_{tip}	10 nm
Cantilever stiffness	2.0 N/m		E_{tip}	130 GPa
Q	50		v_{tip}	0.3
Natural frequency	44 kHz		vdW adhesion force	4 nN
Z approach/retract speed	200 nm/s		E_{sample}	100 GPa
Gamma (z-drag)	3.77e-06		v_{sample}	0.3
Initial separation	3 nm			
Final separation	-1 nm			
“Simulation parameters”				
Num. points plotted	1000			

Q4.1. In the JKR model, there are no long range van der Waal interaction forces between the tip and the sample, but just at contact, an adhesive force develops over an area specified by the JKR contact radius. In VEDA, the magnitude of this adhesive force must be explicitly specified in the “vdW adhesion force” window. The likely origin(s) of this adhesive force might include

i) gravitational attraction
ii) mechanically assisted surface diffusion
iii) chemical forces acting across the tip-sample interface
iv) molecular cross-linking
v) hydrogen bonding
vi) interfacial dipole-dipole interactions at the tip-sample interface

a) all choices except i
b) all choices except i and v
c) all choices are likely origins of the adhesive force
d) all choices except i, ii, iv, and vi

Q4.2. Simulate approach and retract "cantilever deflection vs. z distance" curves for two samples in order to elucidate the role played by the sample's modulus of elasticity. Let one sample have an elastic modulus of 1 GPa, the other a modulus of 100 GPa. From the simulation, what are the pull-off distances for the 1 GPa (and 100 GPa) sample?

a) 0 nm (0 nm)
b) 2.03 nm (2.38 nm)
c) 2.38 nm (2.03 nm)
d) 1.56 nm (1.23 nm)

Application: Force Distance Curves

Result: Observed cantilever deflection vs Z distance

Simulation = #2

Modulus of sample (GPa) = 100

Q4.3. If the adhesive force is the same in both simulations, why is the z pull-off distance different for the two substrates in Q4.2 above?

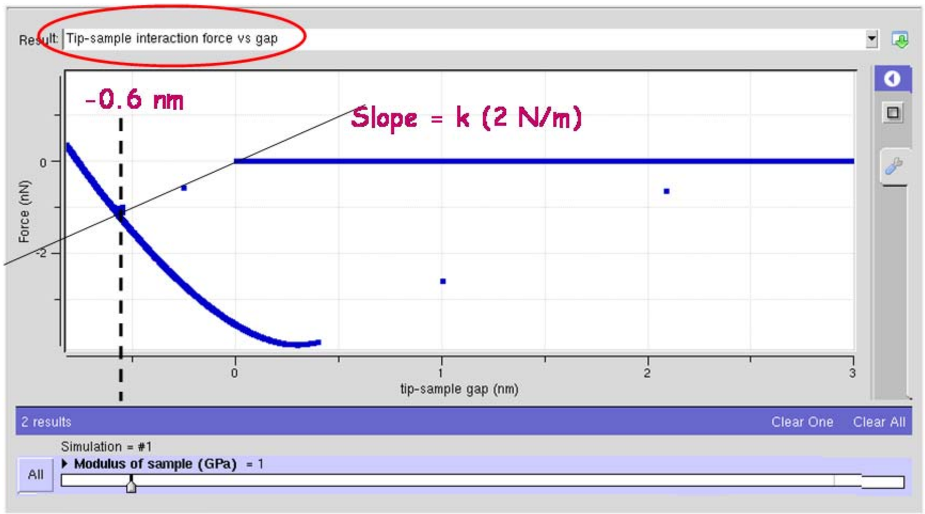
a) the tip breaks when it makes contact with the 100 GPa sample
b) upon tip withdrawal, there is a larger sample deformation for the 1 GPa sample
c) a water meniscus forms
d) non-linearities in the z-piezo motion

Q4.4. Consider the “Force Distance” simulation for the 1 GPa sample. When the tip jumps to contact due to the 4 nN adhesive force, it jumps at z=0. What is the resulting indentation of the 1 GPa sample?

a) D=0.2 nm
b) D=0.4 nm
c) D=0.6 nm
d) D=0.8nm

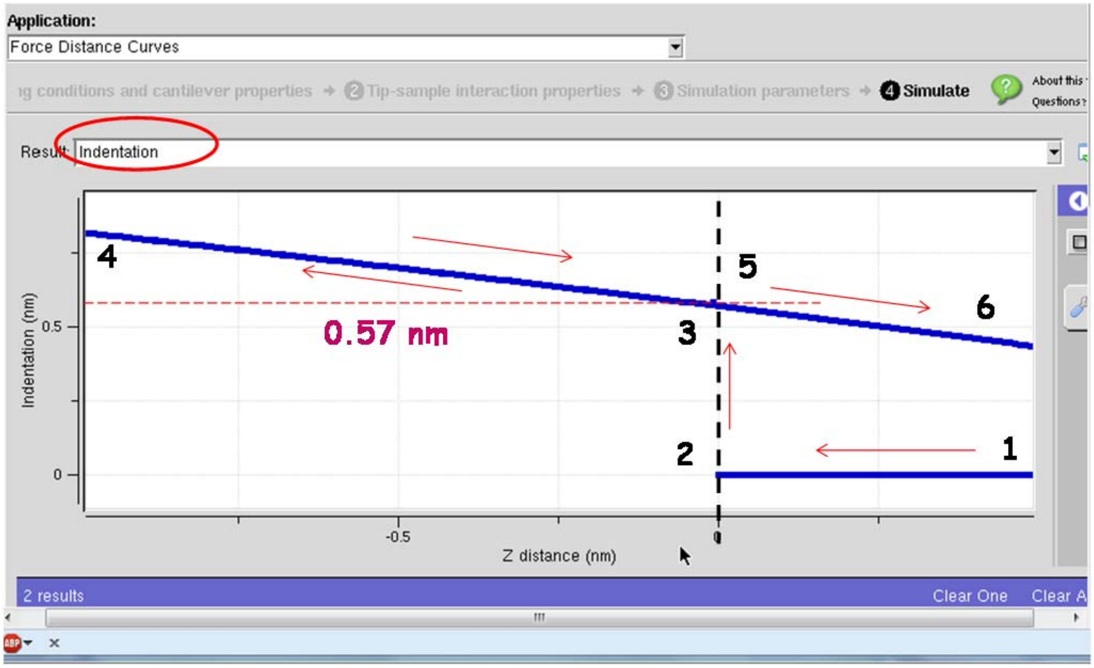
Correct answer is c)

Discussion: Since there are no long-range tip-sample interactions in the JKR model, how does VEDA simulate the jump to contact? The jump to contact occurs at z=0 (which in this case is also the same as d=0 since q=0). The new value of d after the jump is found using the following construction. The value of d is the indentation.


Result: Tip-sample interaction force vs gap

Simulation = #1
Modulus of sample (GPa) = 1

Alternatively, VEDA simulates the indentation directly as shown on the next page.


Application:
Force Distance Curves
ng conditions and cantilever properties
2 Tip-sample interaction properties
3 Simulation parameters
4 Simulate
About this
Questions?
Result: Indentation
Indentation (nm)
0.5
0
-0.5
0
Z distance (nm)
4
5
6
3
2
1
0.57 nm
2 results
Clear One
Clear A

VEDA Worksheet: Force-Distance Curves

Simulation Notes: ______________________________________

Simulation Date:____________

“Operating cond. + Cantilever prop.”		**“Tip-sample interact. prop.”**	
Operating mode		Tip-sample interaction	
No. eigenmodes		R_{tip}	
Cantilever stiffness		E_{tip}	
Q		ν_{tip}	
Natural frequency		vdW adhesion force	
Z approach/retract speed		E_{sample}	
Gamma (z-drag)		ν_{sample}	
Initial separation			
Final separation			
“Simulation parameters”			
Num. points plotted	1000		

VEDA Worksheet: Contact Mode Scans

Simulation Notes: ______________________________________

Simulation Date:____________

"Operating cond. + Cantilever prop."		**"Tip-sample interact. prop.: substrate"**	
No. eigenmodes		Tip-sample interaction	
Cantilever stiffness		R_{tip}	
Q		E_{tip}	
Set point deflection		ν_{tip}	
Scan Lines per second		a_o	
P		H	
I		E_{sample}	
Sampling frequency		ν_{sample}	
"Simulation parameters"		**"Tip-sample interact. prop.: Feature"**	
Num. points plotted	1000	Geometric feature	
		Feature height	
		Length of feature	
		Length of trapezoid top	
		Include geometric convolution	
		Specify material properties	