Lecture: P1_Wk5_L4

Contact Mode Scanning Simulations with VEDA - II

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Contact Mode Scanning in VEDA

Go to the NanoHub at http://nanohub.org/ and login to your account. Locate the VEDA software and launch the tool.

OR access VEDA from the NanoHUB_U course page

Select the "Contact Mode Scanning" application.

For this application, there are five key "tabs" labeled:

❶ **Operating cond. + Cantilever prop.**

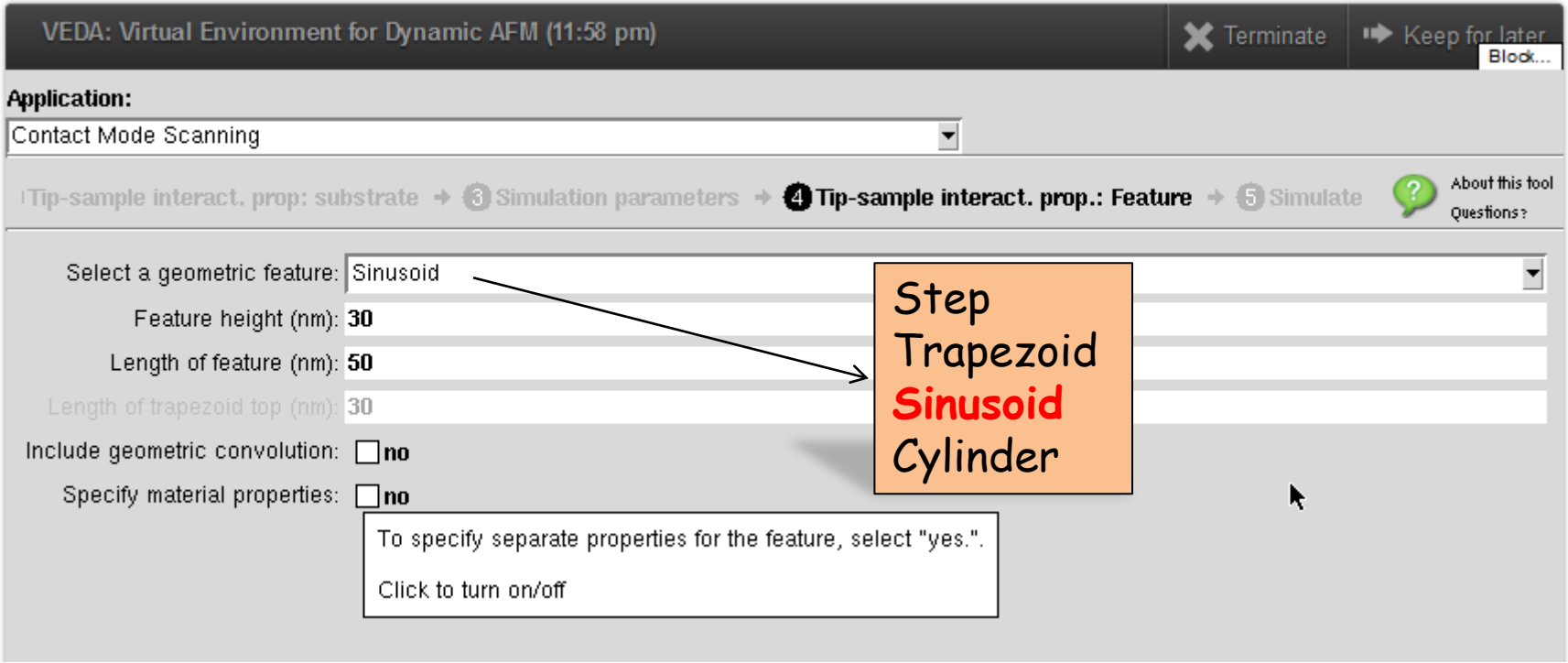
❷ **Tip-sample interact. Prop: substrate**

❸ **Simulation parameters**

❹ **Tip-sample interact. Prop: Feature**

❺ **Simulate**

In this simulation, select "Sinusoid" for the geometric feature



This selection provides a smoothly varying feature to scan in contact mode

Example 1:

Perform a contact mode scanning simulation on a sample that has a **smooth** sinusoidal feature of height 10 nm and a width of 50 nm.

a) Under the **Operating conditions** tab, set the following parameters to specify the cantilever and the controller properties:
   - One eigenmode for the cantilever,
   - Cantilever stiffness of 0.5 N/m,
   - Quality factor of 50,
   - Natural cantilever frequency of 40 kHz,
   - Setpoint deflection of 4 nm,
   - Scan lines/second = 10,
   - Proportional and integral gains of 0.002.

Force Setpoint of 2 nN

b) Under the **Tip-sample interaction properties: substrate** tab, choose the DMT contact to specify the tip-sample interaction. Use the all the specified default values, except change the modulus of the sample to 100 GPa.

c) Under the **Simulation parameters** tab, set the scan size to 100 nm.

Run a simulation and then change the feedback parameters to 0.001.

What do you observe in the measured topography?

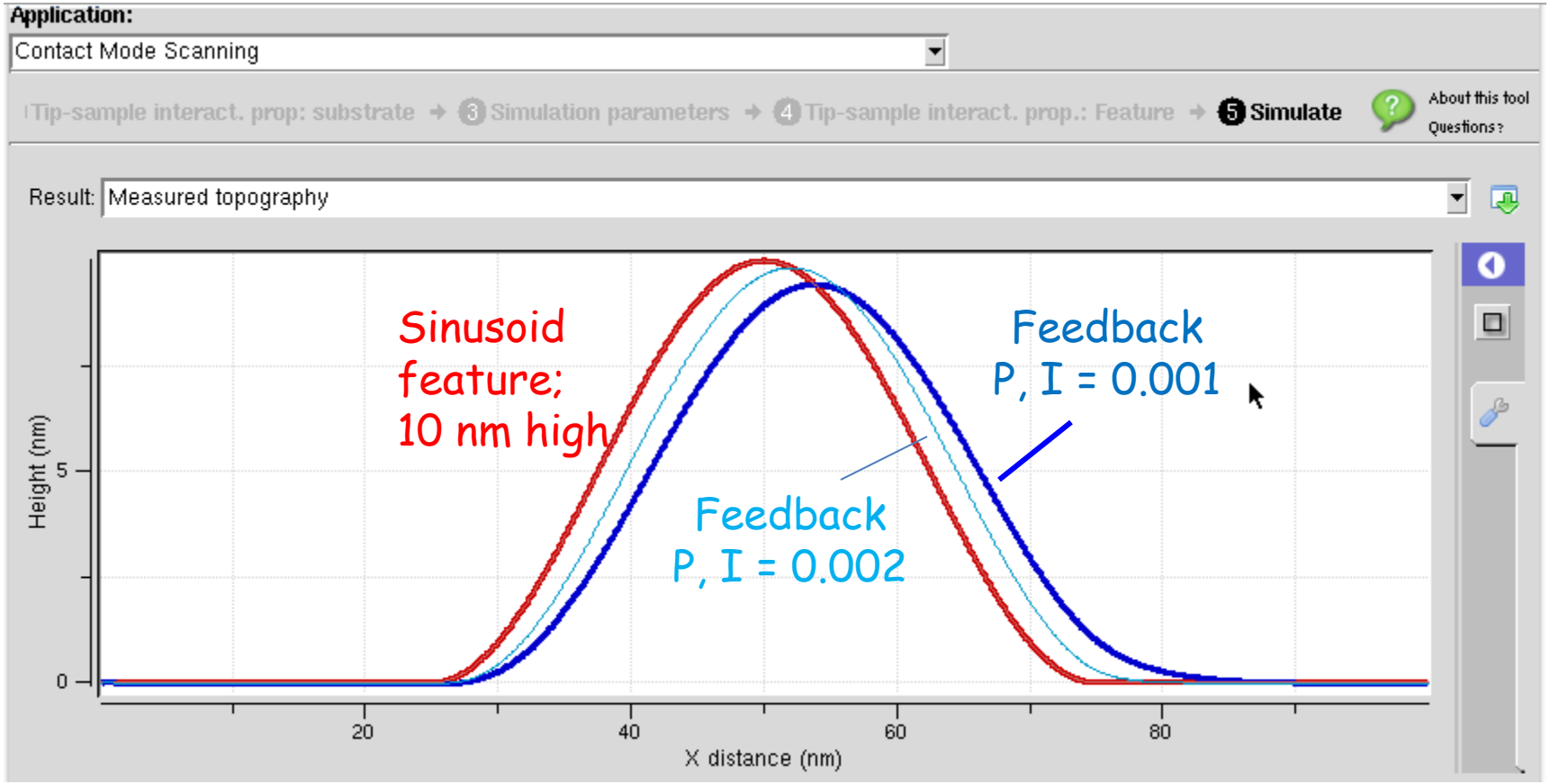
What gain should be selected before running further simulations?

This is a copy of the Echo Input File for the simulation. Many of the parameters are defaults. Many of the listed parameters are not used in this simple example.

exc_choice = 1
operating mode 3 fexcite 3 numModes
1
LockInTC (us) 0.000000000000000E+000
LockInOrder 0
mtip 0
omegad 9.3
Ainitial = 1
omega = 40
Keq = 0.5 k_{cant}=0.5 N/m
Chi = autocalc
Q = 50
sample_freq Mhz 1
sample_freq 1000000.00000000
LineSpeed 10 Scanning speed
SNratio 60
KP 0.002
KI 0.002 P, I feedback gains
Z_feedback_choice 4
HF 10
LF 50 Feature size
LF2 30
LS 100
Feature type 3WantTSCon F
Rtip = 10 R_{tip} = 10 nm
Etip = 130
Poisson_tip = 0.3
mat properties for: input.phase(ts)

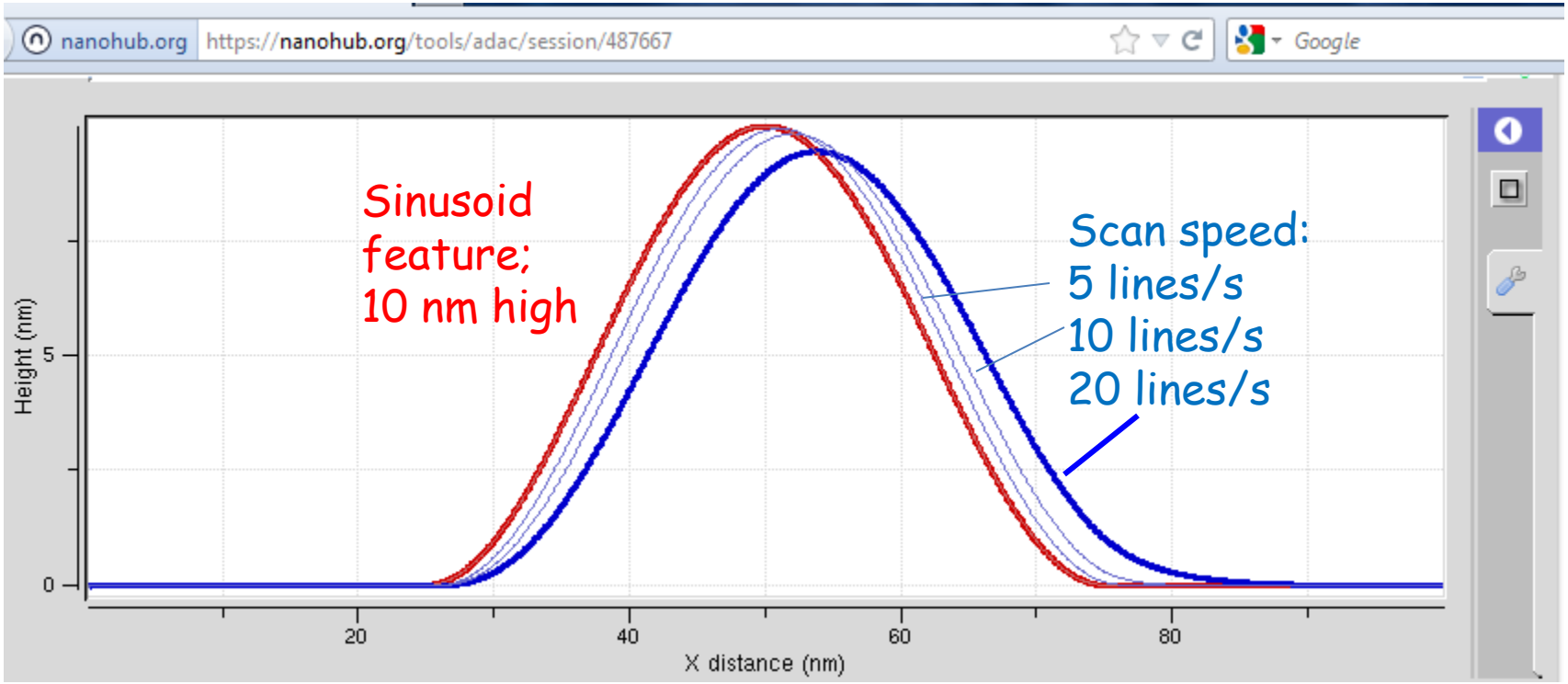
want WLC F
kts_R 10
kts_A 10
Fadhesion 1.4167
A_hamaker 3.4E-20
fts_model 3
want tip squeeze F
want oscillatory F
want hydration F
want v_ie F
electrostatic theta tip 10
electrostatic theta lever 10
electrostatic height 10
electrostatic length 100
electrostatic width 30
VEchoice 1
WantCapAd F
Esample 100 Modulus of sample = 100 GPa
Poisson_sample 0.3
KD 0.001
epsilon 80
sigmat -0.0025
sigmas -0.032
want presiach F
Zrange 0
plotpnts 1000 numincycle 750
Asp 4
transient_allowance

Effect of Feedback Gain



For feedback settings greater than 0.002, the system has a difficult time reaching the set point conditions. Conclude the optimal P,I for this system is 0.002.

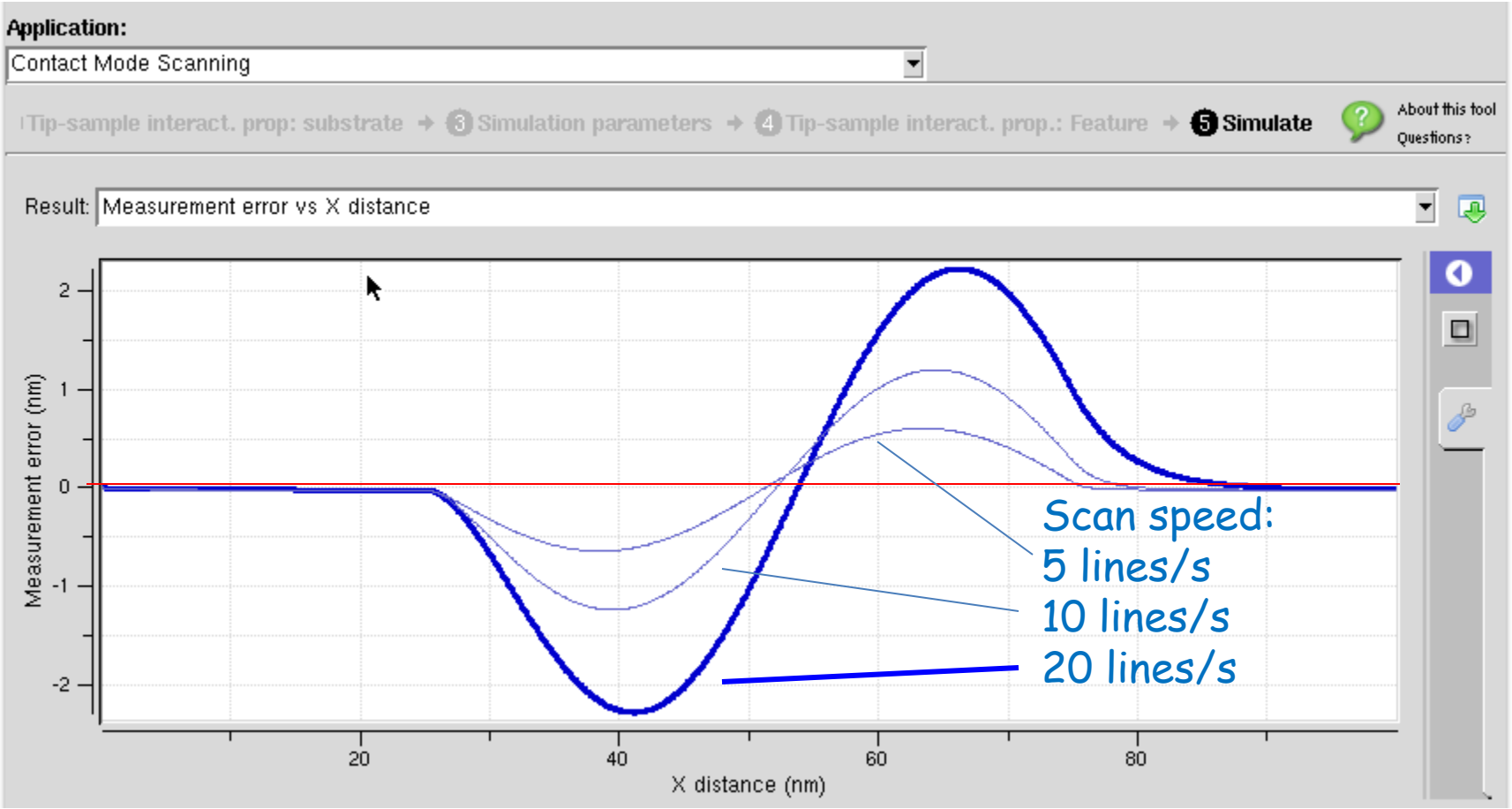
Effect of Scan Speed



The measure topography is shifted "**along the direction of the scan**".

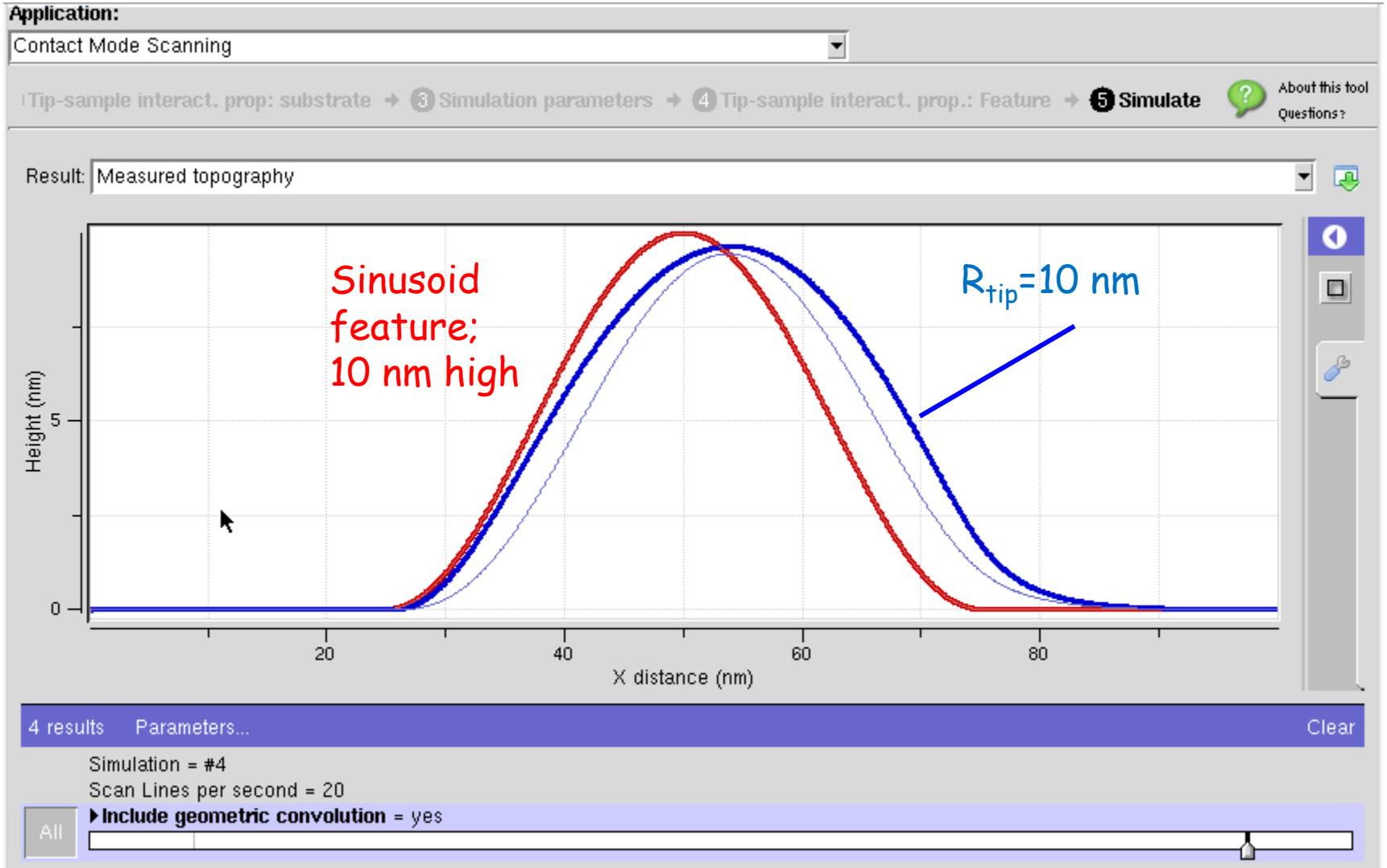
The controller requires a finite time to recognize the change in the topography, which is **always** changing in this example. Meanwhile, the tip position is constantly changing due to the sinusoidal feature.

Error in Topography vs. Scan Speed



In contrast to the square step simulation performed earlier, there is only **one** point on a scan over a smooth feature where the topographical error is zero

Include Tip Dilation
(use 20 lines/s scan rate)



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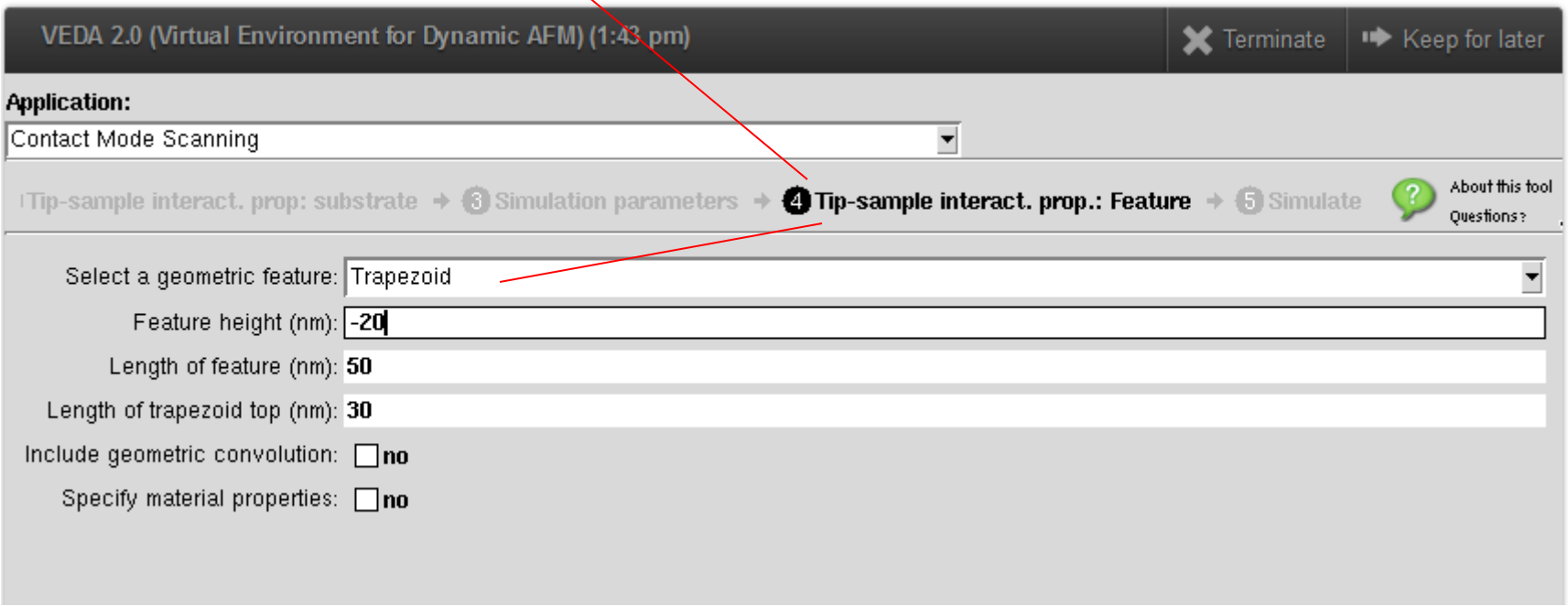
Example 2:

Perform a contact mode scanning simulation over a trapezoidal trench-like feature of depth 20 nm with a width of 50 nm that tapers to a length of 30 nm.

To specify the trapezoidal feature, go to the fourth tab labeled

❹ **Tip-sample interact. Prop: Feature**

and select Trapezoid



a) Under the **Operating conditions** tab, set the following parameters to specify the cantilever and the controller properties:
   - One eigenmode for the cantilever,
   - Cantilever stiffness of 0.5 N/m,
   - Quality factor of 50,
   - Natural cantilever frequency of 40 kHz,
   - R_{tip}=10 nm
   - Setpoint deflection of 4 nm,
   - Scan lines/second = 10,
   - Proportional and integral gains of 0.002.

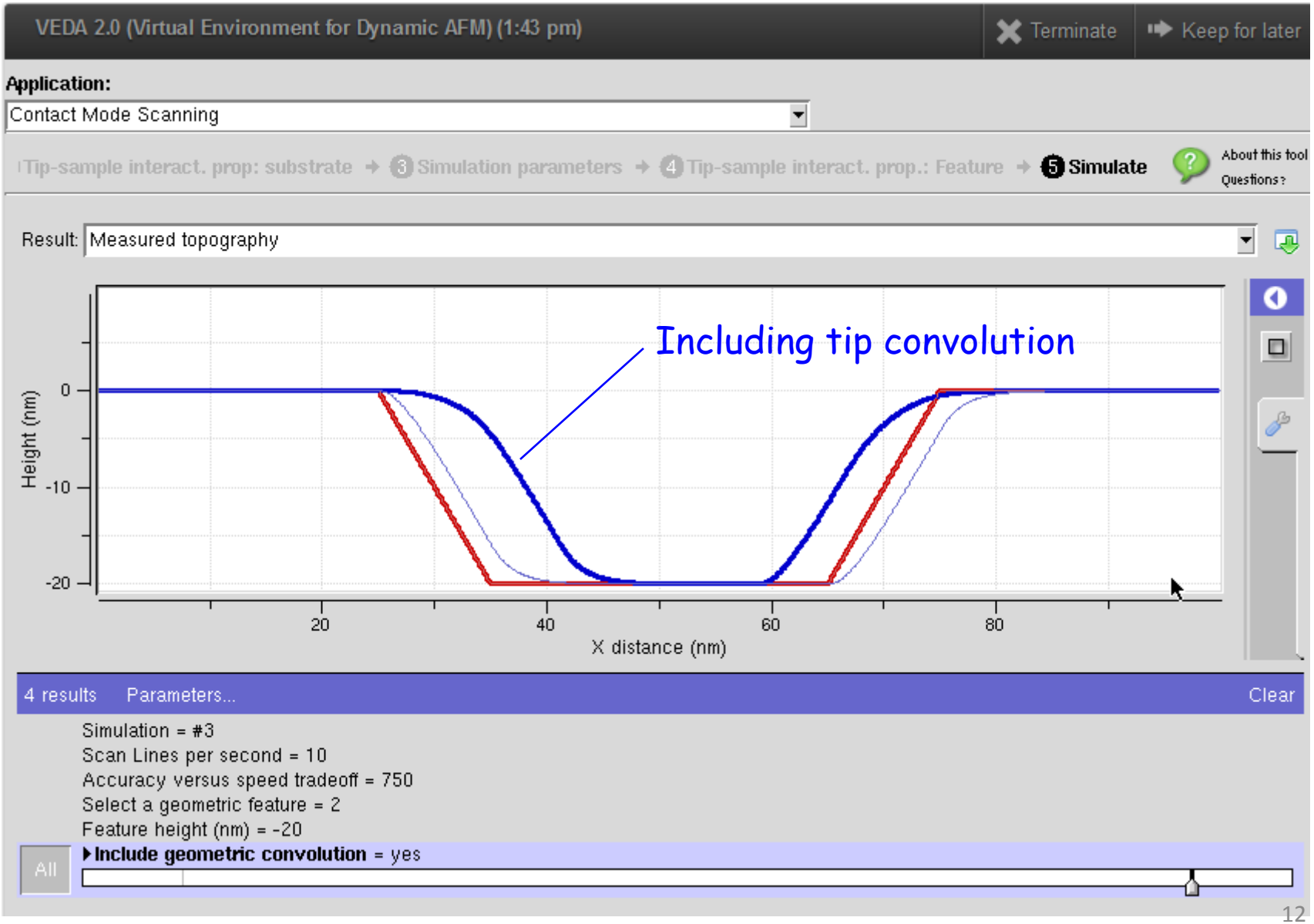
b) Under the **Tip-sample interaction properties:substrate** tab, choose the DMT contact to specify the tip-sample interaction. Use the all the specified default values, except change the modulus of the sample to 100 GPa.

c) Under the **Simulation parameters** tab, set the scan size to 100 nm.

Run a simulation. Run a second simulation including tip convolution effects.

What do you observe in the measured topography?

Include Tip Convolution
(use 10 lines/s scan rate)



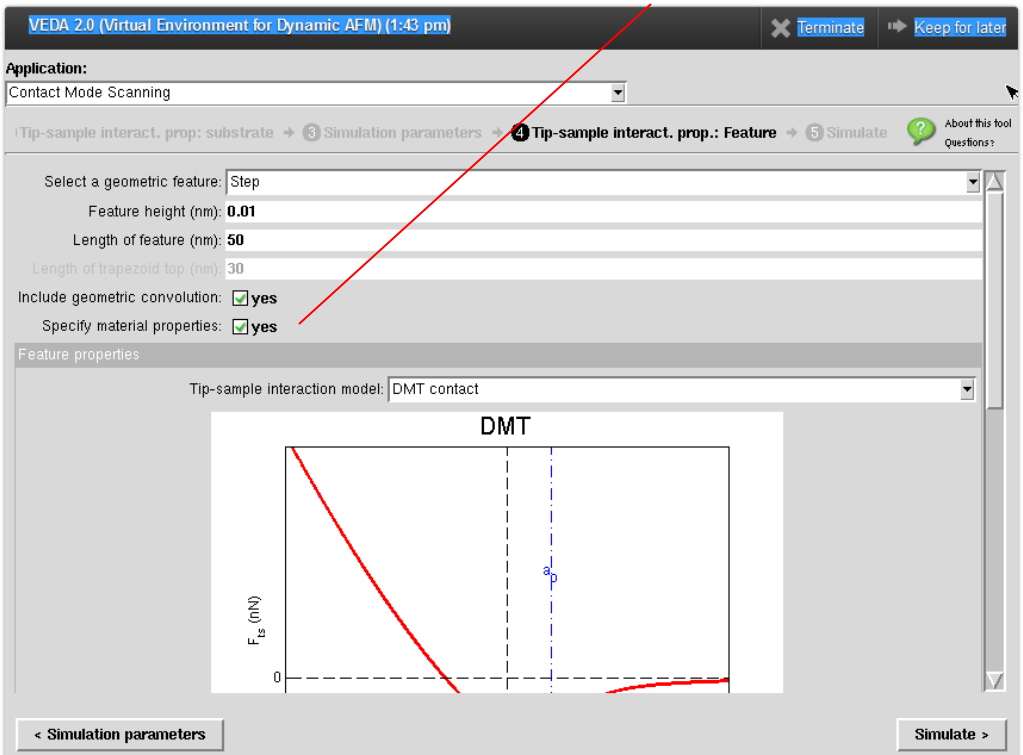
Example 3:

Using the same parameters from the previous simulation, perform a contact mode scanning simulation over a 0.5 nm high feature with a length of 50 nm and having an elastic modulus of 10GPa.

To specify the modulus of the feature, go to the fourth tab labeled

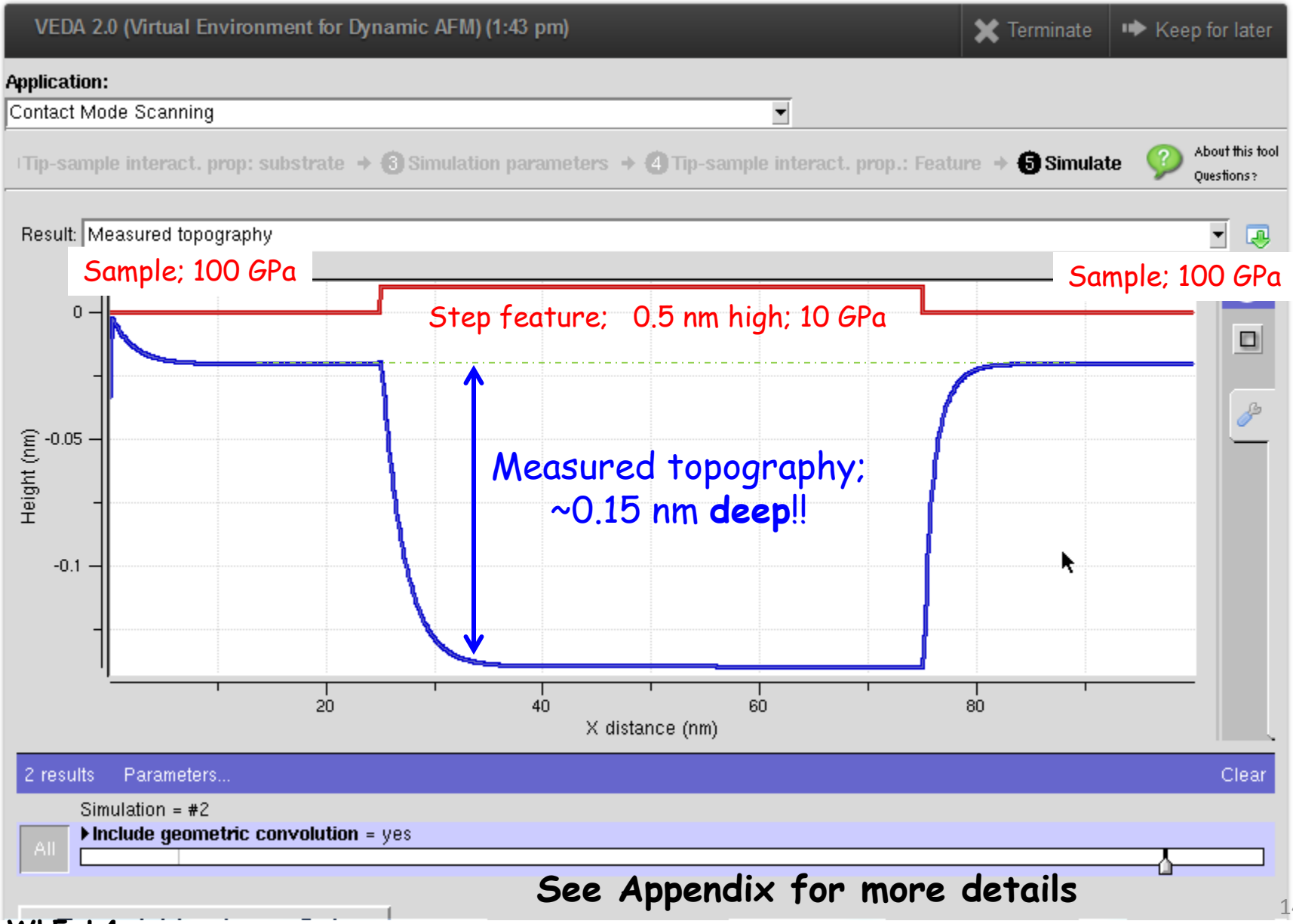
❹ **Tip-sample interact. Prop: Feature**

and click the "Specify material properties" box.



Scroll down and set the elastic modulus of the feature to 10 GPa

Measured Topography



See Appendix for more details

Up Next: Adjusting the feedback gains P and I

Appendix: Example 4

Perform a contact mode scanning simulation over a 1 nm high step with a width of 50 nm. The sample has a modulus of 200 GPa, the step has a modulus of 10 Gpa. What effect does the spring constant of the cantilever have on the measured topography?

a) Under the **Operating conditions** tab, set the following parameters to specify the cantilever and the controller properties:
   - One eigenmode for the cantilever,
   - Cantilever stiffness of 0.1 N/m,
   - Quality factor of 50,
   - Natural cantilever frequency of 40 kHz,
   - R_{tip}=10 nm
   - Setpoint deflection of 2 nm,
   - Scan lines/second = 10,
   - Proportional and integral gains of 0.002.

b) Under the **Tip-sample interaction properties:substrate** tab, choose the DMT contact to specify the tip-sample interaction. Use the all the specified default values, except change the modulus of the sample to 200 GPa.

c) Under the **Simulation parameters** tab, set the scan size to 100 nm.

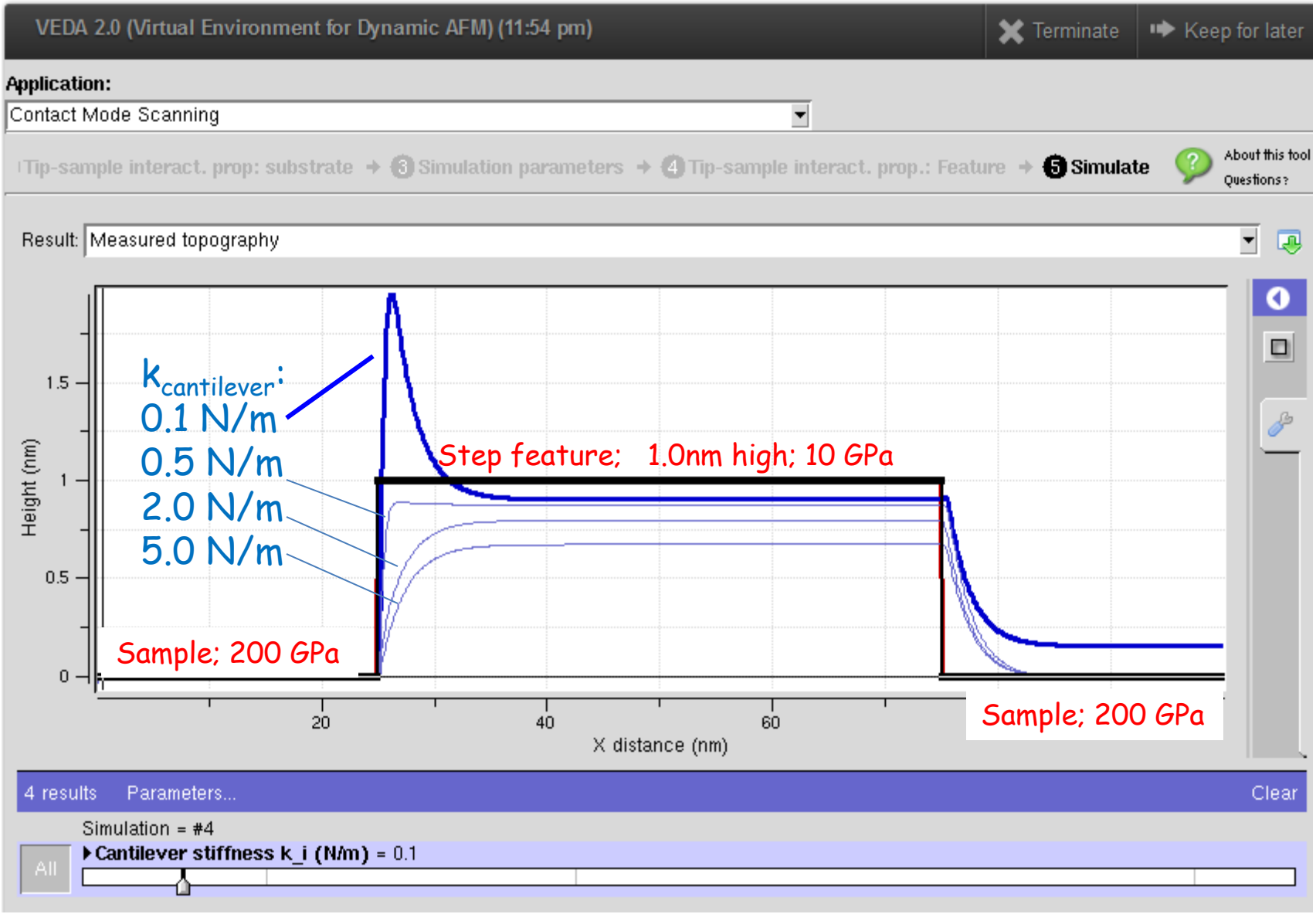
Run a series of simulations for $k_{cantilever}$=0.1, 0.5, 2.0, and 5.0 N/m

What do you observe in the measured topography?

This is a copy of the Echo Input File for the simulation. Many of the parameters are defaults. Many of the listed parameters are not used in this simple example.

exc_choice = 1
operating mode 3 fexcite
3 numModes 1
LockInTC (us)
0.000000000000000E+000
LockInOrder 0
mtip 0
omegad 9.3
Ainitial = 1
omega = 40
Keq = 0.1
Chi = autocalc
Q = 50
sample_freq Mhz 1
sample_freq 1000000.00000000
LineSpeed 10
SNratio 60
KP 0.002
KI 0.002
Z_feedback_choice 4
HF 1
LF 50
LF2 30
LS 100
Feature type 1WantTSCon
T
Rtip = 10
Etip = 130
Poisson_tip = 0.3
mat properties for: input.phase(ts)
want WLC F
kts_R 10
kts_A 10
Fadhesion 1.4167
A_hamaker 3.4E-20
fts_model 3
want tip squeeze F
want oscillatory F
want hydration F
want v_ie F
electrostatic theta tip 10
electrostatic theta lever 10
electrostatic height 10
electrostatic length 100
electrostatic width 30
VEchoice 1
WantCapAd F
Esample 200
Poisson_sample 0.3
KD 0.001
epsilon 80
sigmat -0.0025
sigmas -0.032
want presiach F
mat properties for:
input.phase(feature).group(fp)
want WLC F
kts_R 10
kts_A 10
Fadhesion 1.4167
A_hamaker 3.4E-20
fts_model 3
want tip squeeze F
want oscillatory F
want hydration F
want v_ie F
electrostatic theta tip 10
electrostatic theta lever 10
electrostatic height 10
electrostatic length 100
electrostatic width 30
VEchoice 1
WantCapAd F
Esample 10
Poisson_sample 0.3
KD 0.001
epsilon 80
sigmat -0.0025
sigmas -0.032
want presiach F
Zrange

Topography vs. $k_{cantilever}$



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Include tip convolution effects
R_{tip}=10 nm; topography vs. $k_{cantilever}$