

# Lecture: P1\_Wk5\_L4

Contact Mode Scanning Simulations with VEDA - II

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for VEDA overview: Rev. Sci. Instrum. 83, 013702 (2012).

# 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:

- ① Operating cond. + Cantilever prop.
- ② Tip-sample interact. Prop: substrate
- ③ Simulation parameters
- ④ Tip-sample interact. Prop: Feature
- ⑤ Simulate

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

VEDA: Virtual Environment for Dynamic AFM (11:58 pm) [X] Terminate [▶] Keep for later [Block...]

Application:  
Contact Mode Scanning

Tip-sample interact. prop: substrate → 3 Simulation parameters → 4 Tip-sample interact. prop.: Feature → 5 Simulate [?] About this tool Questions?

Select a geometric feature: Sinusoid

Feature height (nm): 30

Length of feature (nm): 50

Length of trapezoid top (nm): 30

Include geometric convolution:  no

Specify material properties:  no

To specify separate properties for the feature, select "yes".  
Click to turn on/off

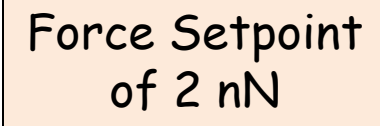
Step  
Trapezoid  
**Sinusoid**  
Cylinder

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.
- 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.



Force Setpoint  
of 2 nN

**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) 0.0000000000000000E+000
LockInOrder 0
mtip 0
omegad 9.3
Ainitial = 1
omega = 40
Keq = 0.5
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 10
LF 50
LF2 30
LS 100
Feature type 3WantTSCon F
Rtip = 10
Etip = 130
Poisson_tip = 0.3
mat properties for: input.phase(ts)
```

$k_{cant} = 0.5 \text{ N/m}$

Scanning speed

P, I feedback gains

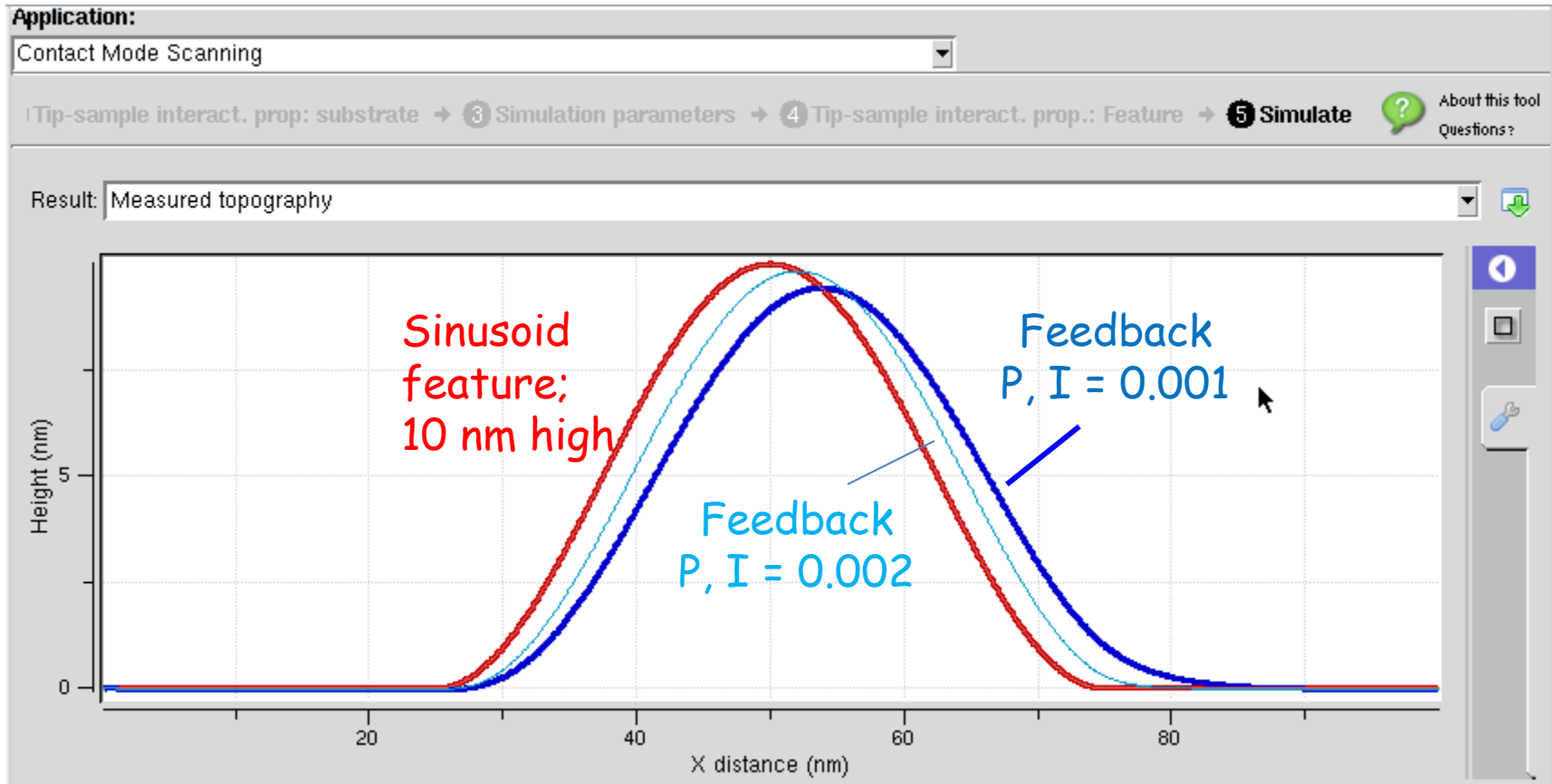
Feature size

$R_{tip} = 10 \text{ nm}$

```
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
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
```

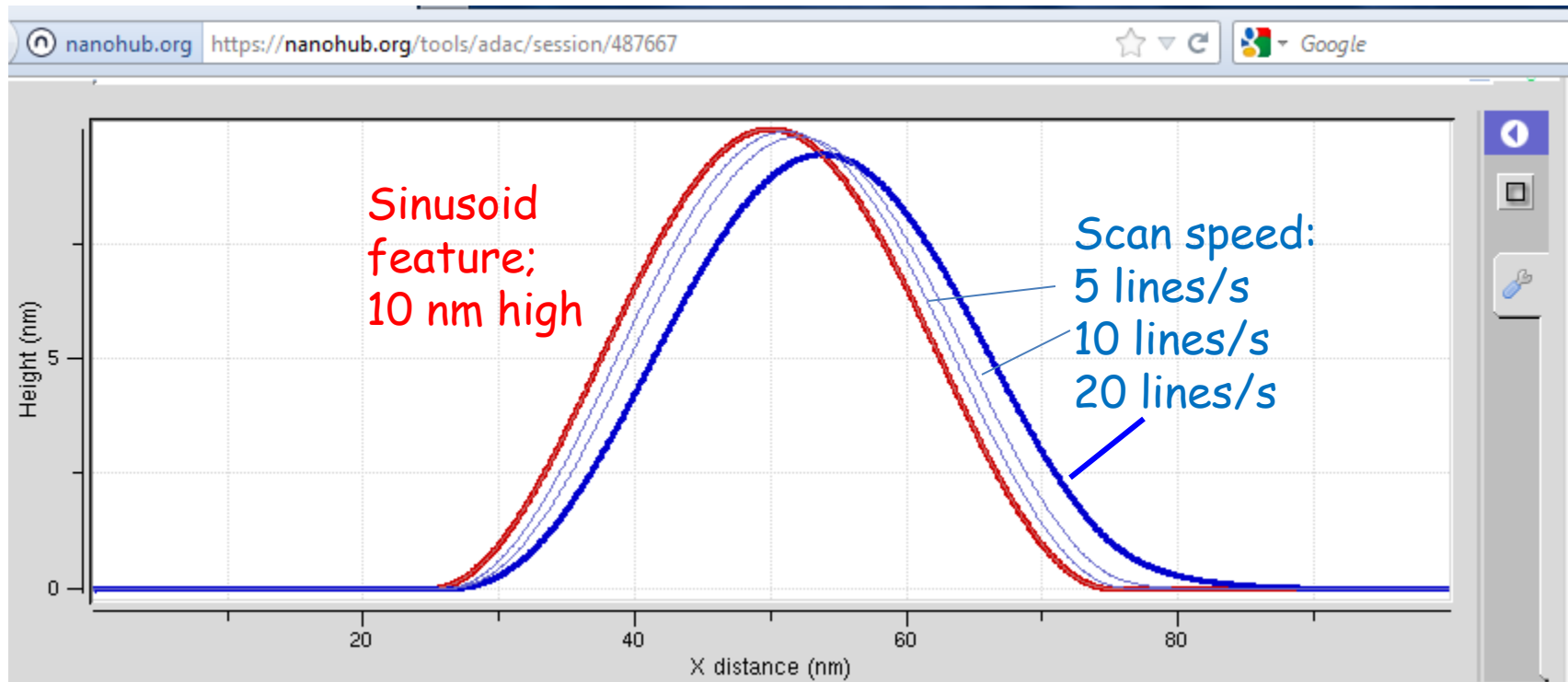
Modulus of sample = 100 GPa

# 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.

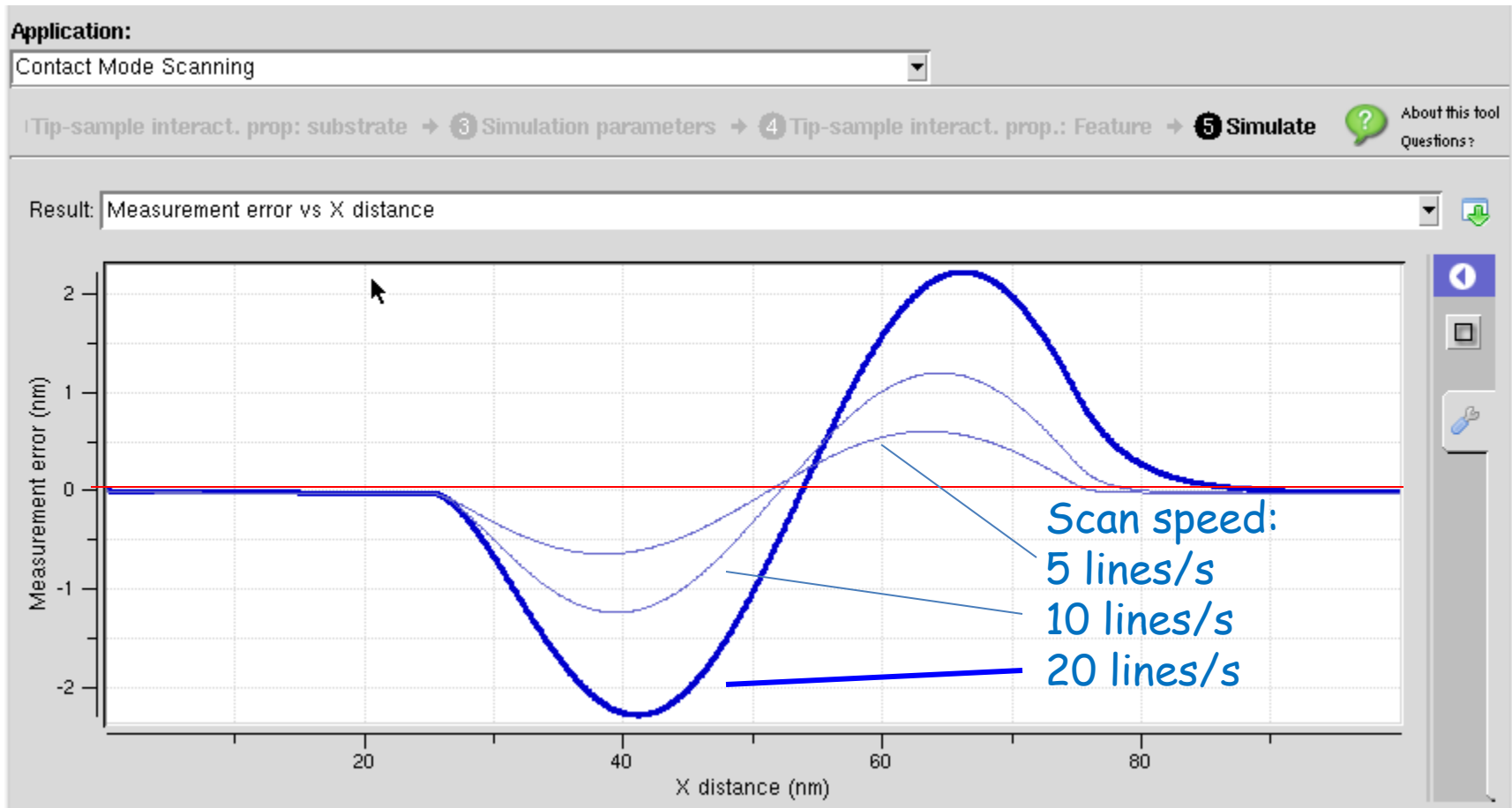
# Effect of Scan Speed



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.

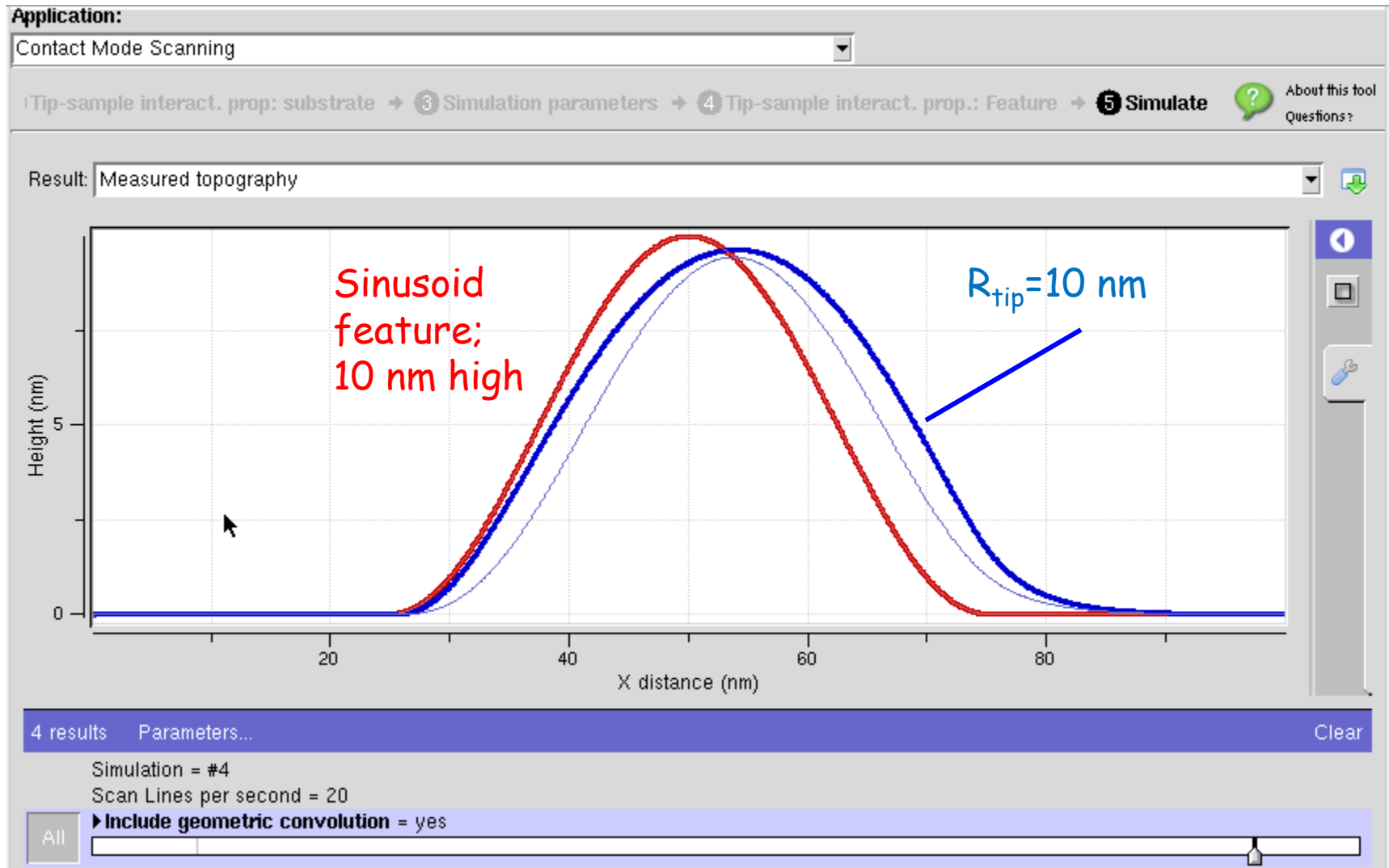
# Error in Topography vs. Scan Speed



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)



## 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 **④ Tip-sample interact. Prop: Feature** and select Trapezoid

VEDA 2.0 (Virtual Environment for Dynamic AFM) (1:43 pm) ✕ Terminate ▶▶ Keep for later

**Application:**  
Contact Mode Scanning

① Tip-sample interact. prop: substrate → ③ Simulation parameters → **④ Tip-sample interact. prop.: Feature** → ⑤ Simulate ? About this tool Questions?

Select a geometric feature: Trapezoid

Feature height (nm): -20

Length of feature (nm): 50

Length of trapezoid top (nm): 30

Include geometric convolution:  no

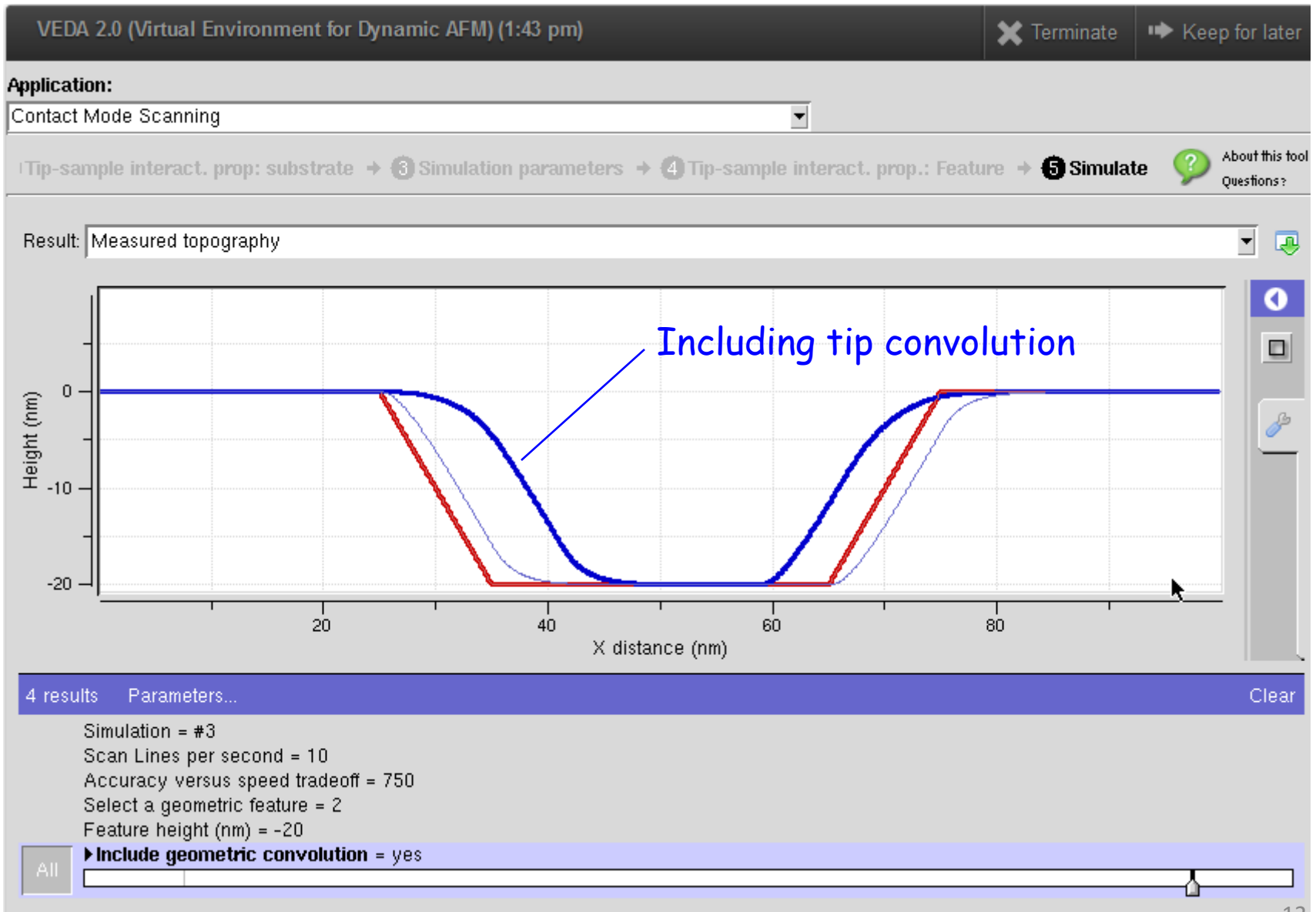
Specify material properties:  no

- 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,
  - $R_{\text{tip}}=10$  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 10 GPa.

To specify the modulus of the feature, go to the fourth tab labeled **④ Tip-sample interact. Prop: Feature** and click the "Specify material properties" box.

VEDA 2.0 (Virtual Environment for Dynamic AFM) (1:43 pm) [Terminate] [Keep for later]

Application: Contact Mode Scanning

① Tip-sample interact. prop.: substrate → ② Simulation parameters → ④ Tip-sample interact. prop.: Feature → ⑤ Simulate [About this tool Questions?]

Select a geometric feature: Step

Feature height (nm): 0.01

Length of feature (nm): 50

Length of trapezoid top (nm): 30

Include geometric convolution:  yes

Specify material properties:  yes

Feature properties

Tip-sample interaction model: DMT contact

DMT

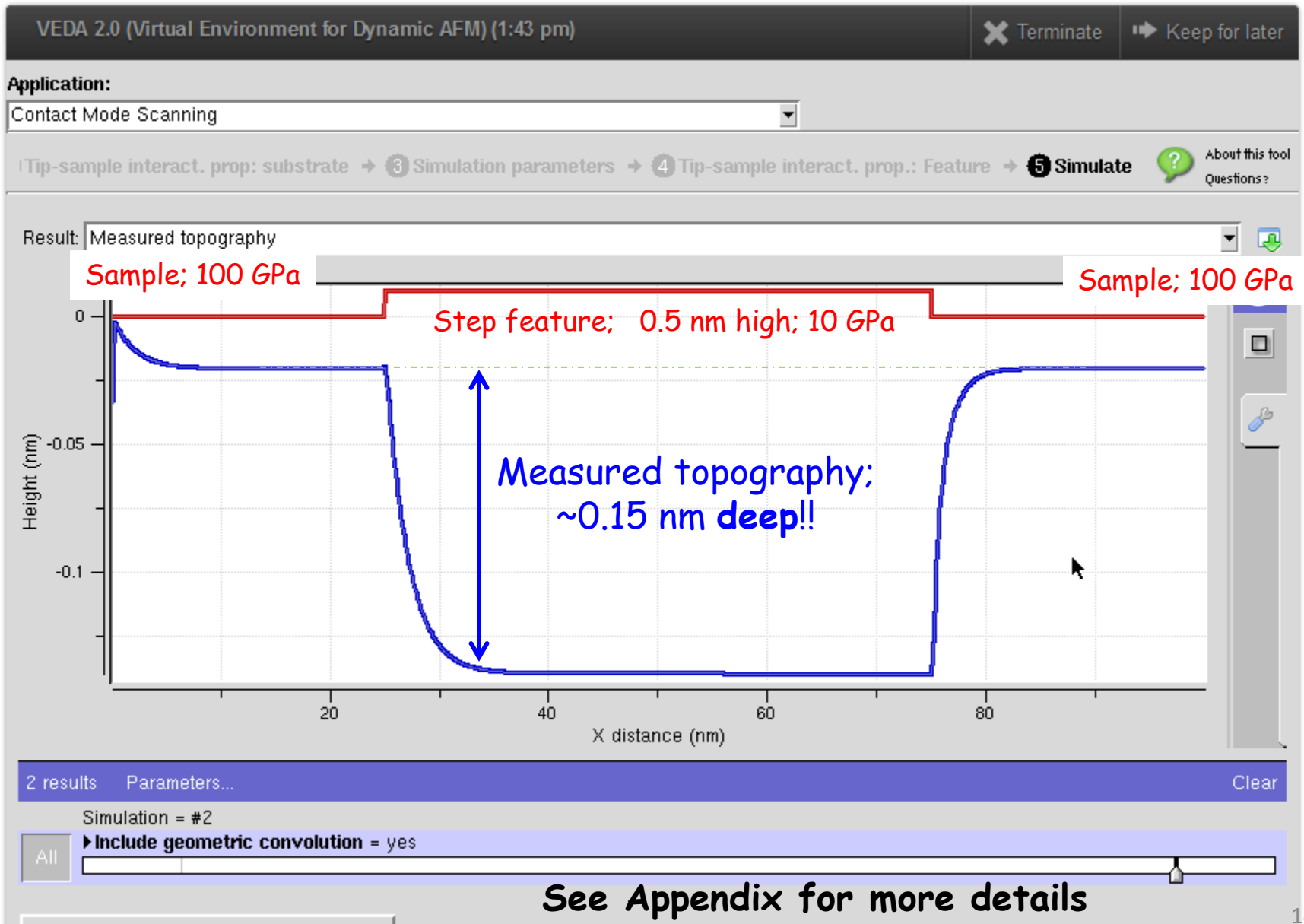
$F_{ts}$  (nN)

0

< Simulation parameters [Simulate >

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

# Measured Topography



**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,
  - $R_{\text{tip}}=10$  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  $k_{\text{cantilever}}=0.1, 0.5, 2.0, \text{ and } 5.0$  N/m

What do you observe in the measured topography?

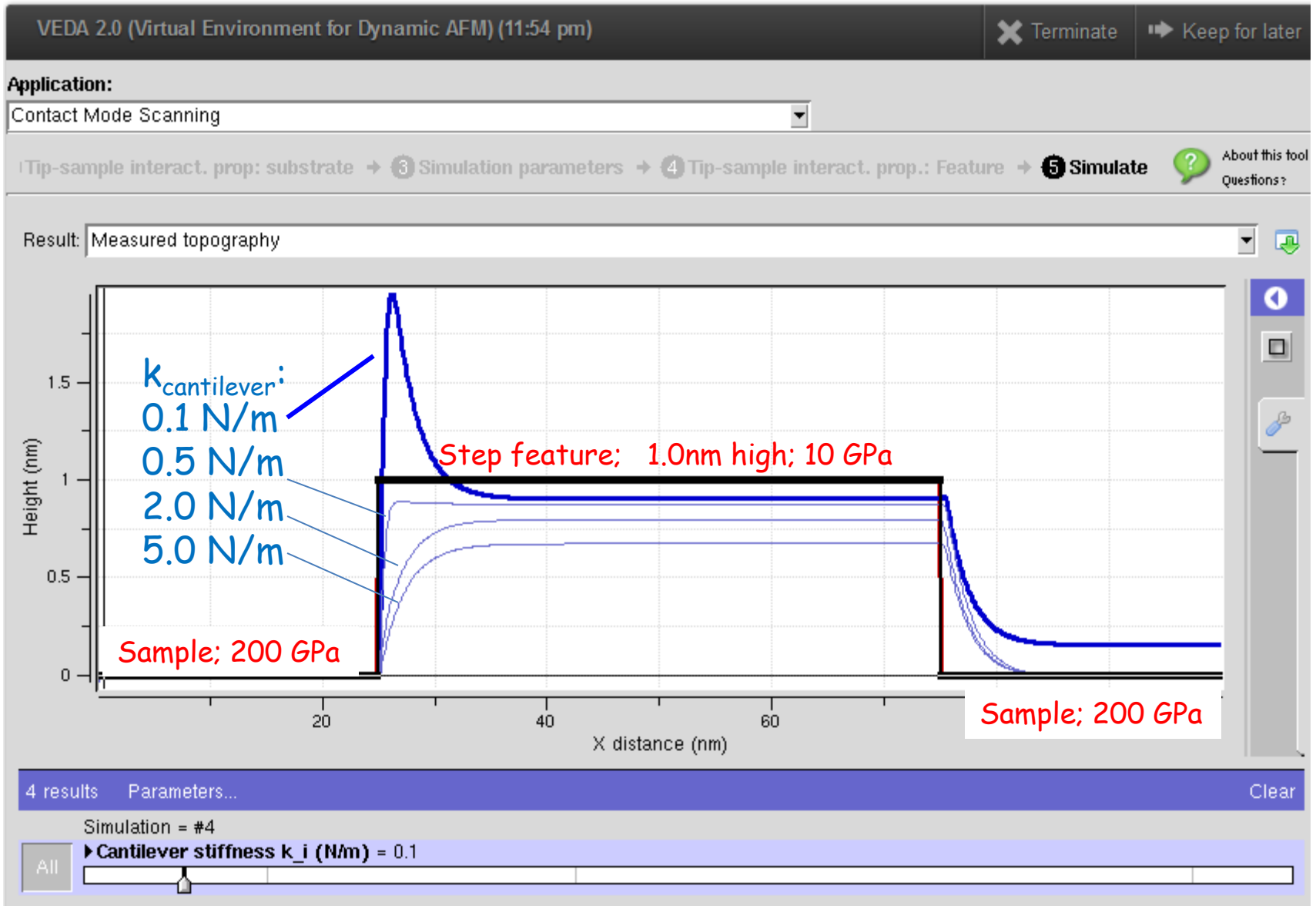
This is a copy of the Echo Input File for the simulation. Many of the parameters are defaults. Many of the listed parameters are not used in this simple example.

```

exc_choice =          1                Poisson_tip = 0.3                want WLC F
operating mode      3 fexcite          mat properties for: input.phase(ts)  kts_R 10
3 numModes         1                want WLC F                kts_A 10
LockInTC (us)      0.0000000000000000E+000  kts_R 10                Fadhesion 1.4167
LockInOrder        0                kts_A 10                A_hamaker 3.4E-20
mtip 0             Fadhesion 1.4167          fts_model          3
omegad 9.3         A_hamaker 3.4E-20        want tip squeeze F
Ainitial = 1       fts_model          3                want oscillatory F
omega = 40         want tip squeeze F        want hydration F
Keq = 0.1          want oscillatory F        want v_ie F
Chi = autocalc    want hydration F          electrostatic theta tip 10
Q = 50             want v_ie F              electrostatic theta lever 10
sample_freq Mhz 1  electrostatic theta tip 10  electrostatic height 10
sample_freq 1000000.000000000        electrostatic theta lever 10  electrostatic length 100
LineSpeed 10       electrostatic height 10   electrostatic width 30
SNratio 60         electrostatic length 100  VEchoice          1
KP 0.002           electrostatic width 30    WantCapAd F
KI 0.002           VEchoice          1                Esample 10
Z_feedback_choice  4                WantCapAd F        Poisson_sample 0.3
HF 1               Esample 200            KD 0.001
LF 50              Poisson_sample 0.3     epsilon 80
LF2 30             KD 0.001               sigmat -0.0025
LS 100             epsilon 80              sigmas -0.032
Feature type      1WantTSCon        sigmat -0.0025      want presiach F
T                 sigmas -0.032          Zrange
Rtip = 10         want presiach F
Etip = 130        mat properties for:
                  input.phase(feature).group(fp)

```

# Topography vs. $k_{\text{cantilever}}$



# Include tip convolution effects

## $R_{\text{tip}} = 10 \text{ nm}$ ; topography vs. $k_{\text{cantilever}}$

