Deconvolution of Atomic Force Microscopy Data From the Effects of Destructive Indentation and Rigid Body Motion of Embedded Particles In Heterogeneous Systems

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Research Question/Motivation

- Atomic Force Microscopy (AFM) used by researchers to characterize soft materials at micron and submicron length scales
- Experimental AFM data is easily convoluted by many structural effects
- Investigate/study the effects of destructive indentation and rigid body motion of embedded particles on AFM data

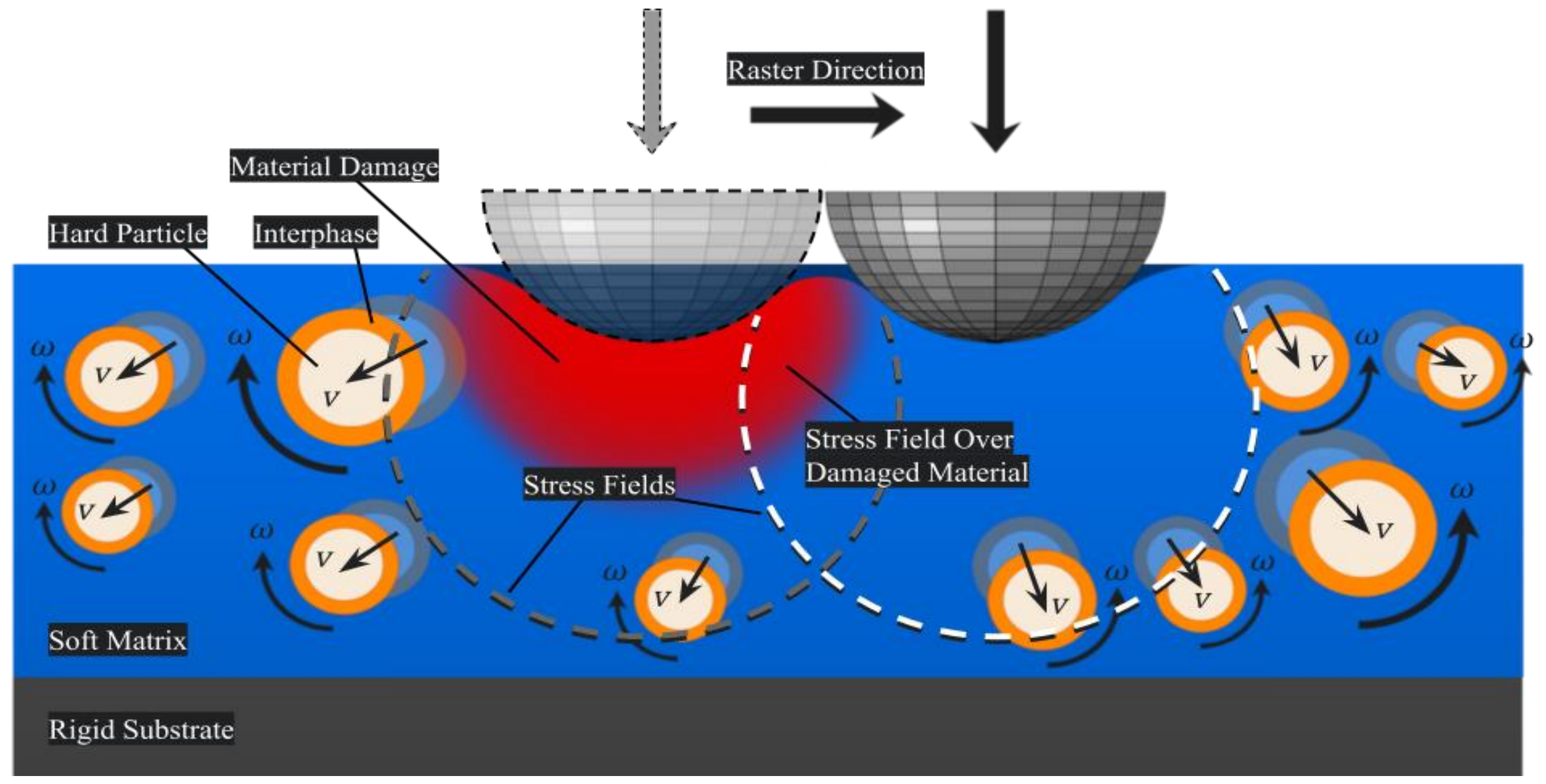


Figure 1 Destructive AFM indentation causing material damage (plasticity) to a soft polymer matrix and rigid body motion undergone by embedded hard particles under indentation load

Methods

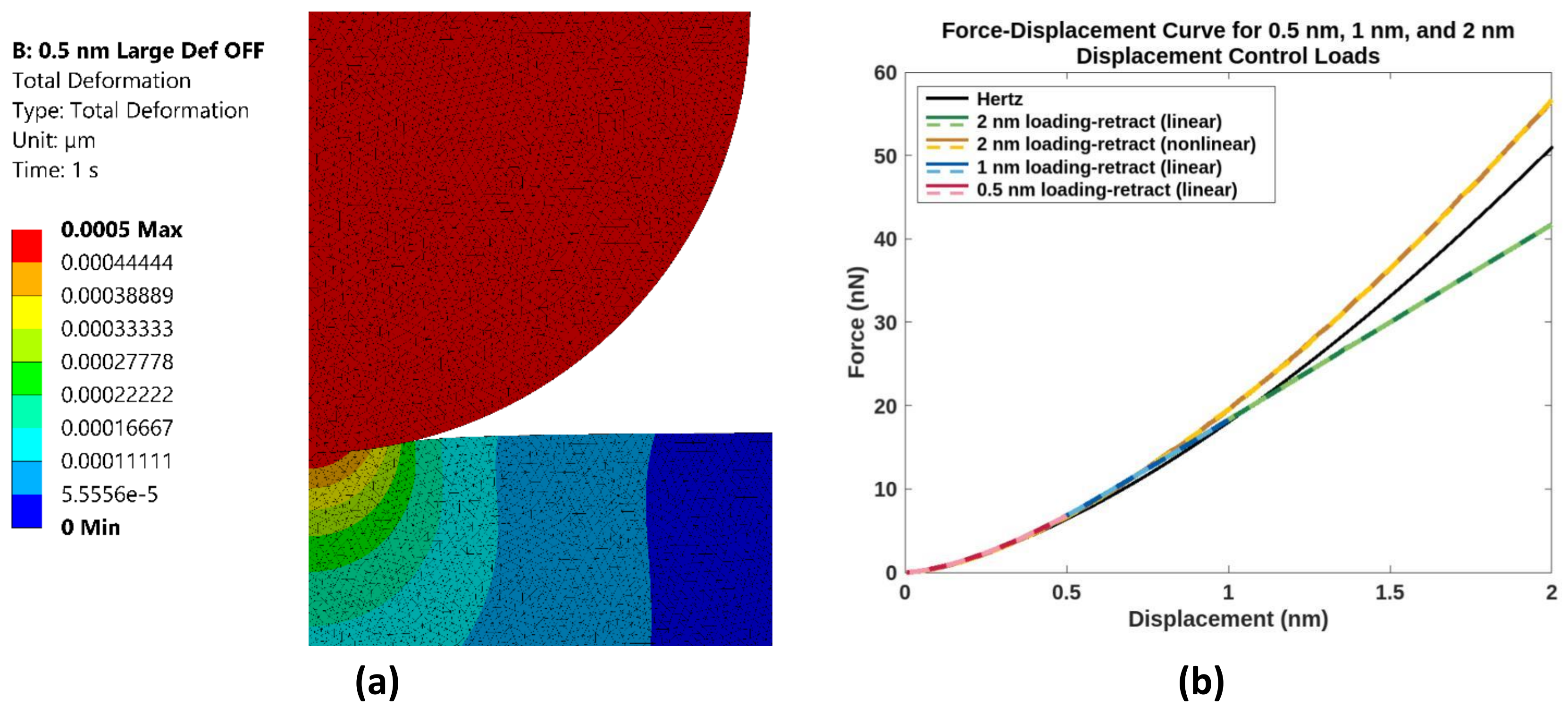
- **AFM** Peak Force Quantitative Nanomechanics Mapping (**PFQNM**) on multi-walled carbon nanotubes (MWCNT) and CNT buckypaper to obtain property data
- **Finite Element Analysis (FEA)**
    - Simulate quasi-static AFM indentation at varying depths on 2D axisymmetric FE polymer-matrix model to study the effects of 1) destructive indentation and 2) rigid body motion of particles on force-displacement data
- **Models/Equations**
    - Derjaguin-Muller-Toporov (DMT) contact theory

$$E_r = \frac{3(F_{con} + F_{disp})}{4r^{0.5}\delta^{1.5}} \quad E_r^{-1} = \frac{1 - v_{mat}^2}{E_{mat}} + \frac{1 - v_{tip}^2}{E_{tip}}$$

    - Microscopic yield strength based on Hertz and Tresca (Ikeshima et al., 2019)

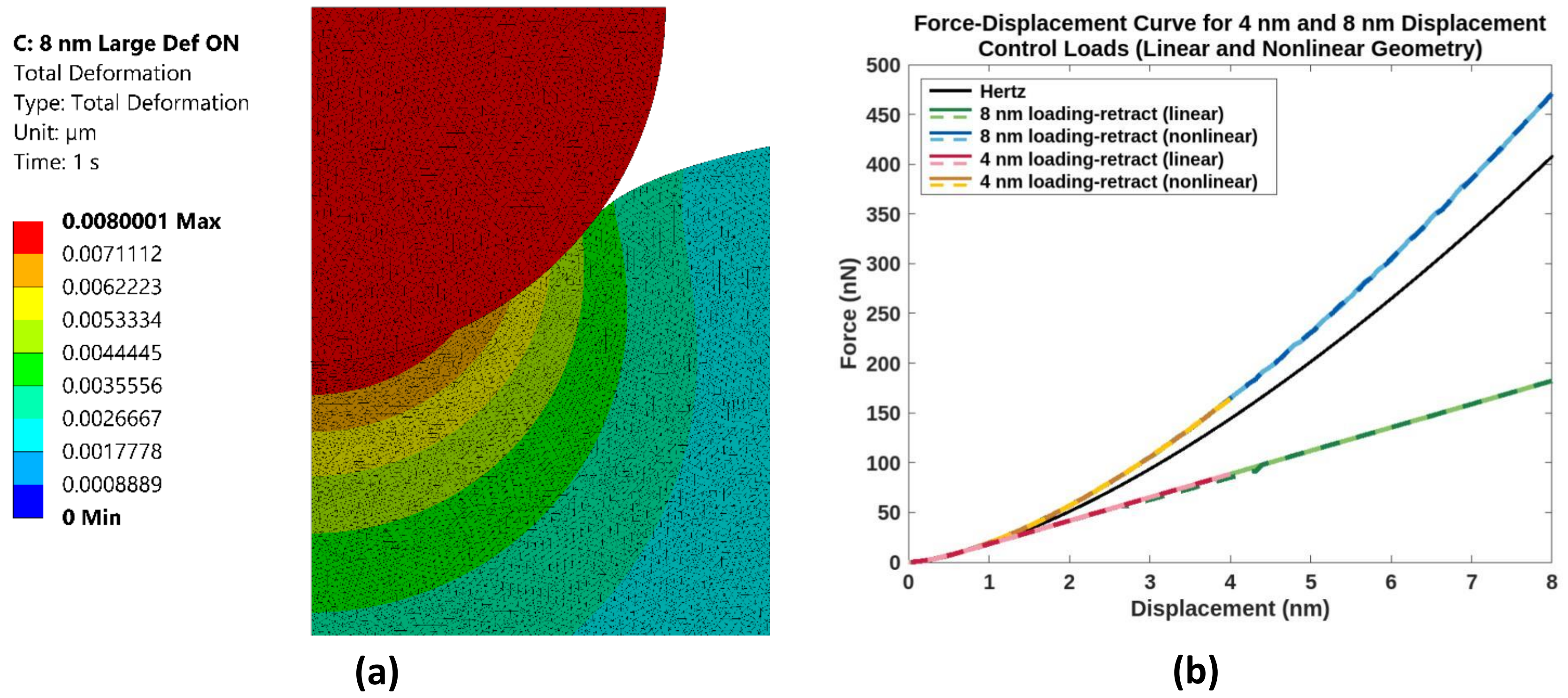
$$S_y = 1.09\left(\frac{F_y E_r^2}{\pi^3 r^2}\right)^{\frac{1}{3}}$$

Results



(a) (b)

Figure 2 (a) FEA displacement contour for 0.5 nm indentation displacement control load (at time *t* = 1 s) and **(b)** force-displacement curves (loading and retract) for 0.5 nm, 1 nm, and 2 nm (linear and nonlinear geometry) indentation loads alongside the Hertzian force-displacement curve



(a) (b)

Figure 3 (a) FEA displacement contour for 8 nm indentation displacement control load (nonlinear geometry at time *t* = 1 s) and **(b)** linear and nonlinear geometry force-displacement curves for 4 nm and 8 nm indentation loads alongside the Hertzian force-displacement curve

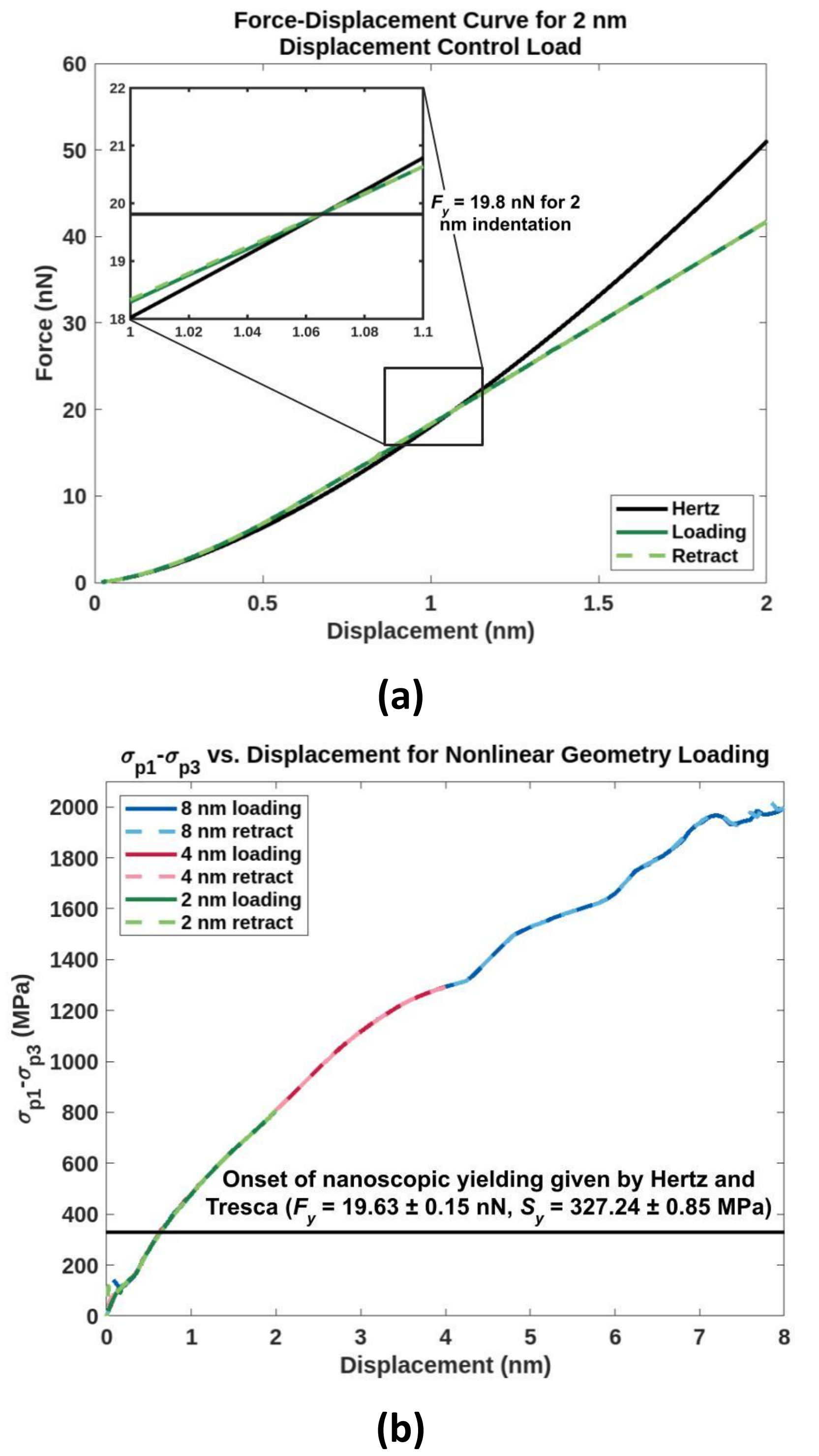


Figure 4 (a) Onset of nanoscopic yielding indicated by the deviation of the simulated force-displacement curve (linear geometry) from Hertzian contact theory at ~1 nm indentation depth and indentation force $F_y = 19.8$ nN and **(b)** threshold for nanoscopic yielding based on Tresca's yield criterion and Hertzian contact theory ($S_{y,avg} = 327.25 \pm 0.85$ MPa)

- Force-displacement data obtained for 0.5, 1, 2, 4, and 8 nm indentations, plotted alongside Hertzian curve
- Identified micro(nano)scopic yield threshold, $S_{y,avg} = 327.25 \pm 0.85$ MPa
- Simulated force-displacement data for linear and nonlinear geometry analyses deviate as indentation depth increases
- Higher indentation forces for nonlinear geometry
- FE model poorly described by Hertz and DMT at high indentation depth (small strain/small deformation assumption no longer applies)

Challenges Faced/Overcome

- Computational limitations
    - Inaccurate stress solution from linear geometry FEA simulation caused by mesh distortion at higher indentation depths
    - Lack of detail at highest indentation depths (4-8 nm) due to inadequate number of time steps ($\Delta t = 0.01$ s)

Future Direction

- Perform FEA for subsequent indentations including particles with varying contact conditions
- Provide AFM scientists with a technique to deconvolute AFM data
- Future of AFM
    - Combine AFM techniques with artificial intelligence to characterize unknown materials using a library of properties
    - Quantify material subsurface with advances in AFM methods and computing power
    - Apply new contact models to study/quantify hyperelastic and viscoelastic materials

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References

- Scan for full list of references

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