ATOMISTIC SIMULATION STUDY OF INDENTATION OF METALLIC NANOWIRES

A Thesis
Presented to the Faculty of the
College of Engineering and Mathematical Sciences
and Honors College of the
University of Vermont
in Partial Fulfillment of the Requirements for the Graduation of the
Honors College

by
Trevor Avant
April 2011

Background

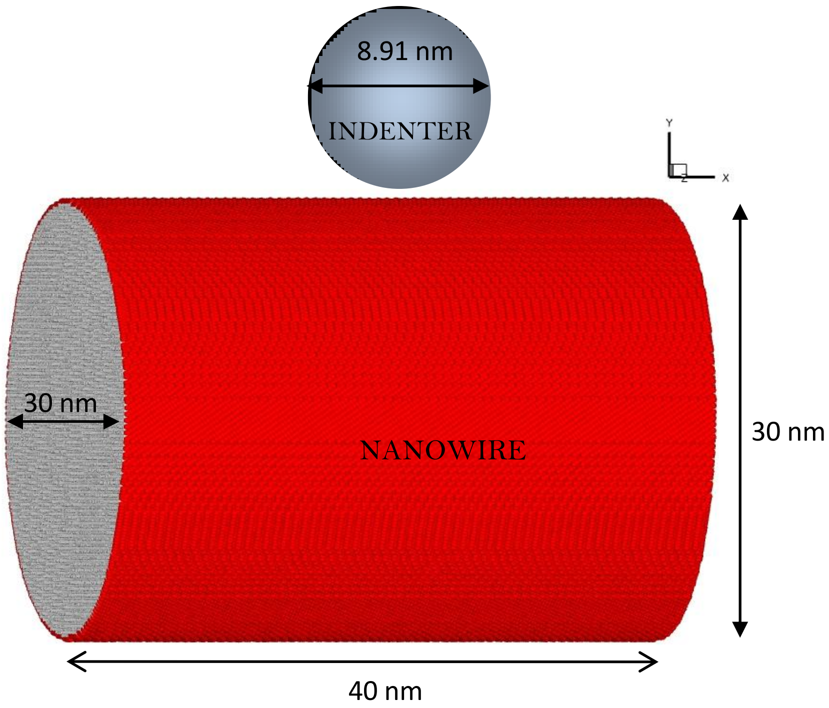
- Nanomaterials study materials on a scale less than 100 nm
- Two common methods to determine hardness: indentation tests and compression tests
- Nanoindentation is difficult, and does not allow us to completely understand deformation mechanisms
- Molecular Dynamics simulates individual atoms
  - LAMMPS
- Nanowires: promises in biology, photonics, electromechanics
- Five different face-centered cubic (FCC), nickel nanowires
- Orientation along the axis of the wire (x-direction) was the same for all wires, [1 1 1]

Objectives

- Use molecular dynamics simulations to simulate the indentation of [1 1 1]-oriented nickel nanowires
- Model different rotations of nanowires (all still having a [1 1 1] orientation)
- Calculate and characterize the differences in hardness of the nanowires, due to the effect of rotation

The Models

- All models: 30 nm in diameter, 40 nm in length
- Spherical indenter with a radius of 8.91 nm
- 400,000 timesteps of length 5 fs (2 ns total)
- Bottom layer of atoms fixed
- Angles: 0°, 10.893°, 30°, 49.107°, 60°
- Ackland #’s



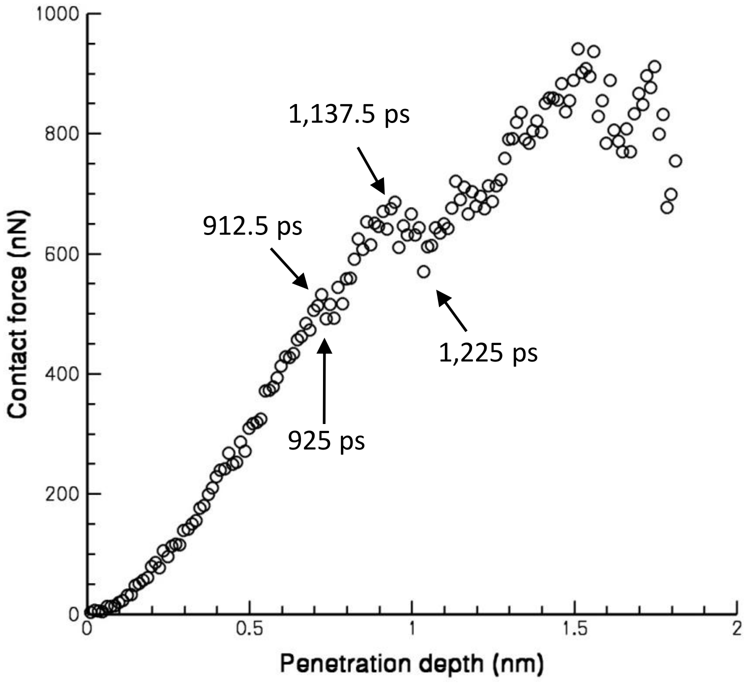
Calculations

- Mean contact pressure $p_m = \frac{P}{A}$
- Max pressure is largest p_m (occurs at yield point)
- Hardness (all p_m beyond 1 nm of penetration depth)
- Young's modulus found through best fit line

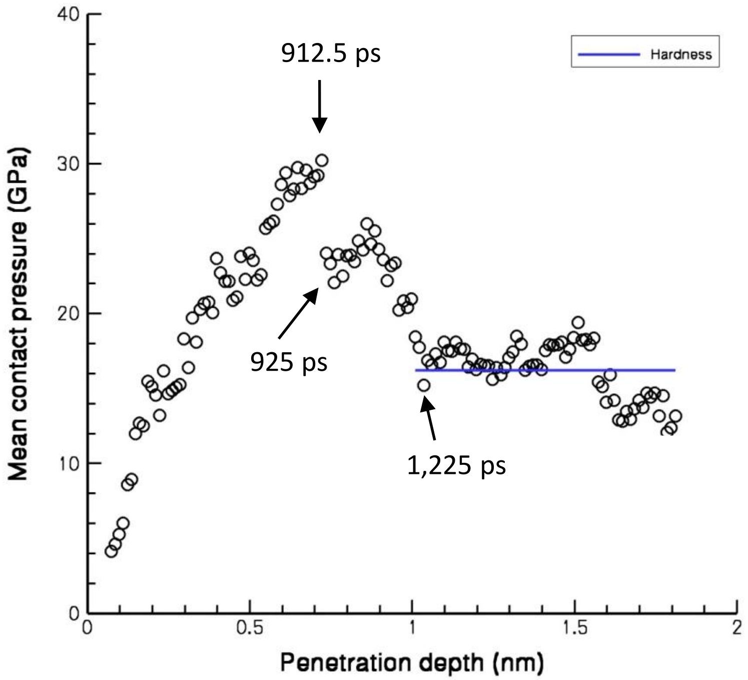
$$P = \frac{4}{3}\sqrt{R\frac{E}{1-v^2}}\,\delta^{3/2} \longrightarrow P = C\delta^{3/2}$$

$$E = \frac{3(1-v^2)}{4\sqrt{R}}C$$

10.893° Model: Force & Pressure



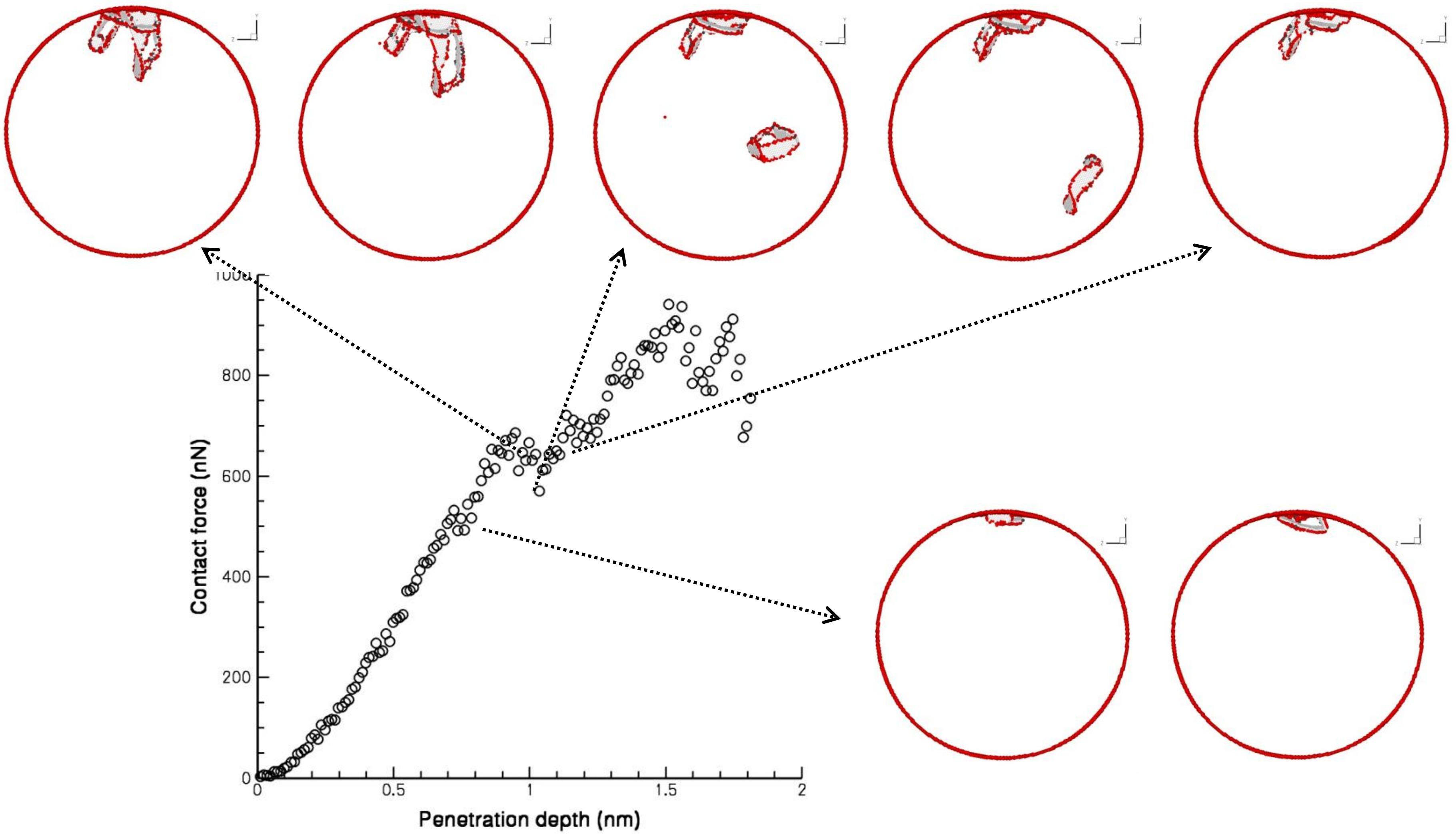
Contact Force



Mean Contact Pressure

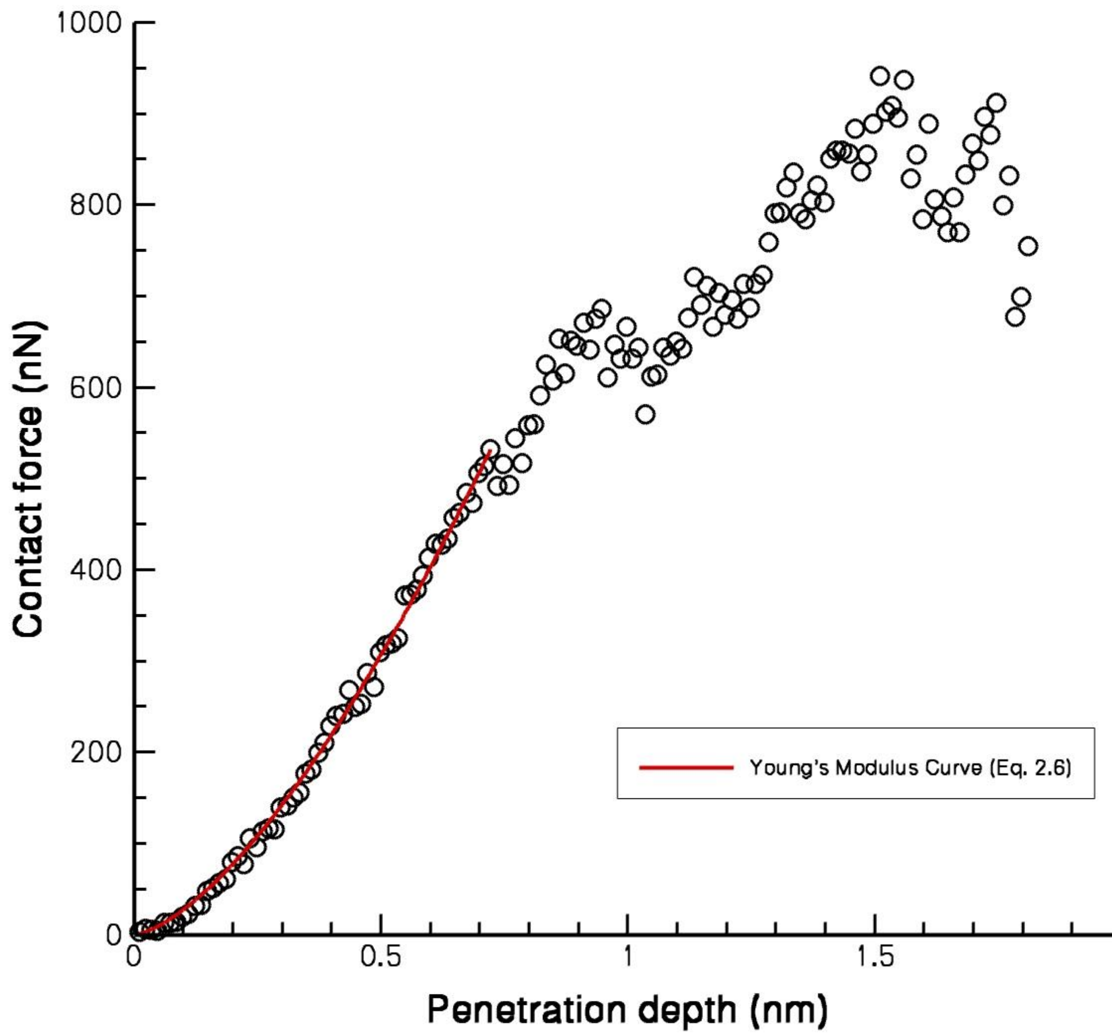
(Hardness = 16.2 GPa)

10.893° Model: Nucleation & Emission of Loops



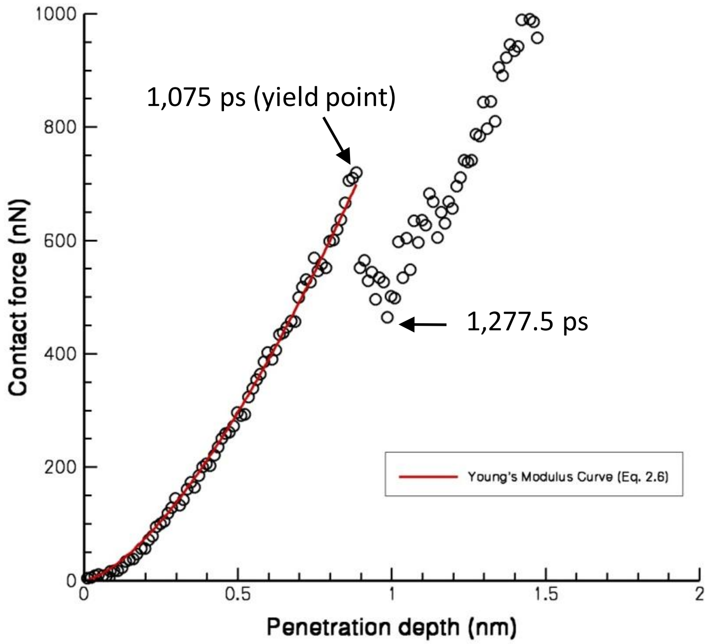
10.893° Model: Young's Modulus

- Young's modulus found through best fit line
- E= 240 GPa

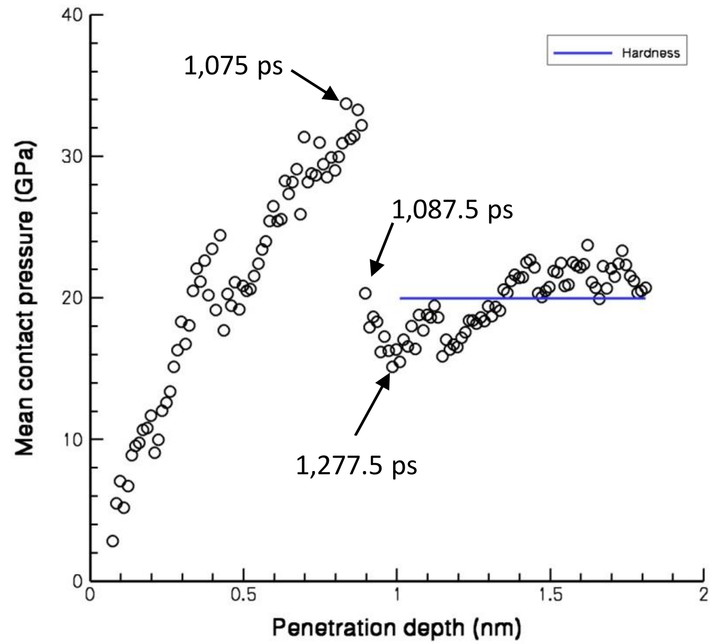


0° Model: Force & Pressure

Contact Force

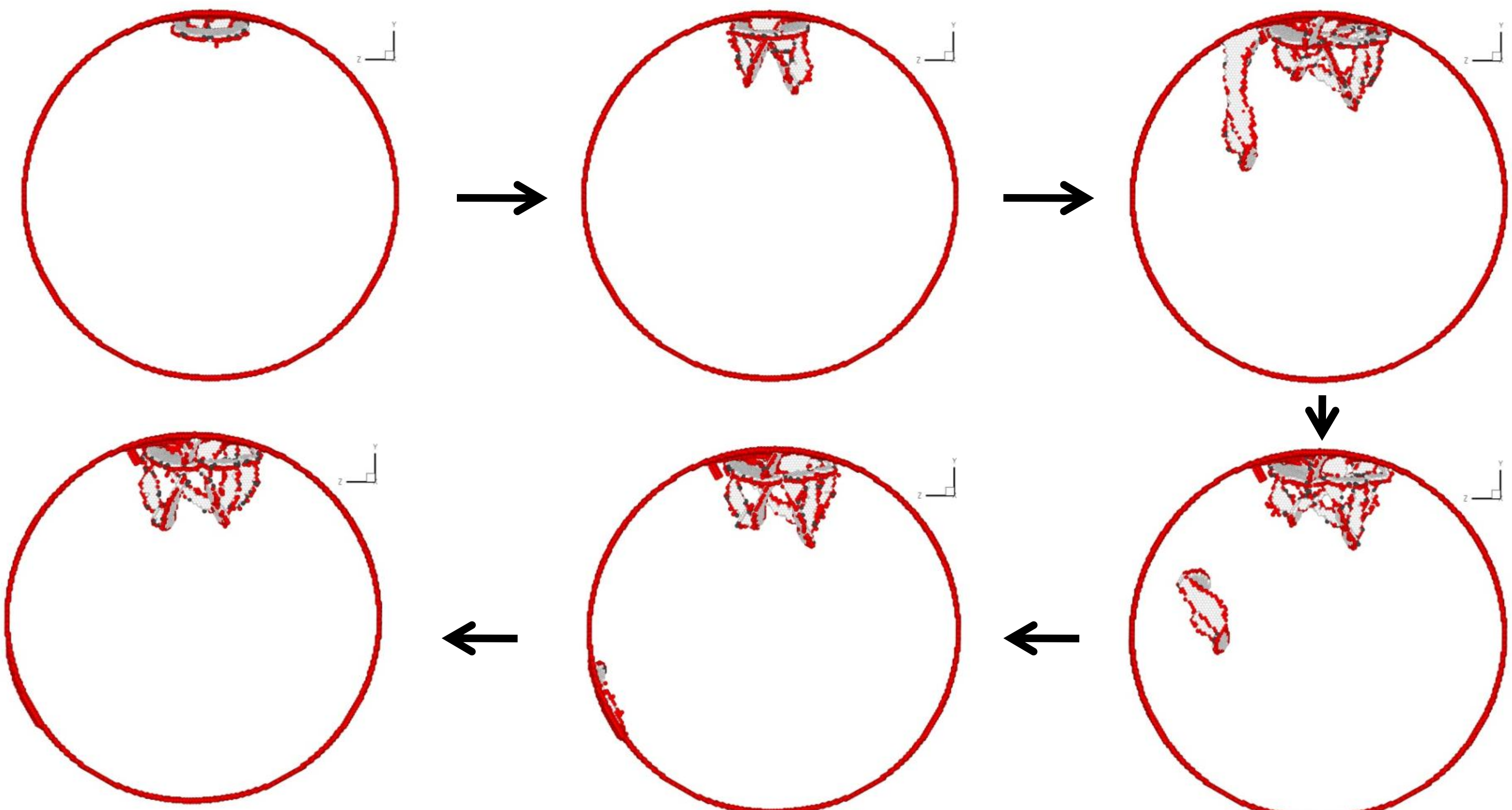


Mean Contact Pressure

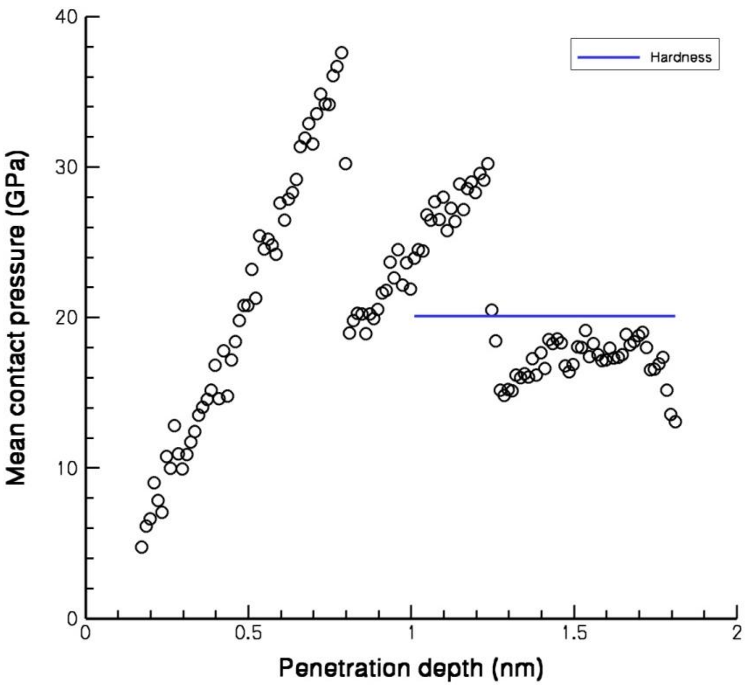


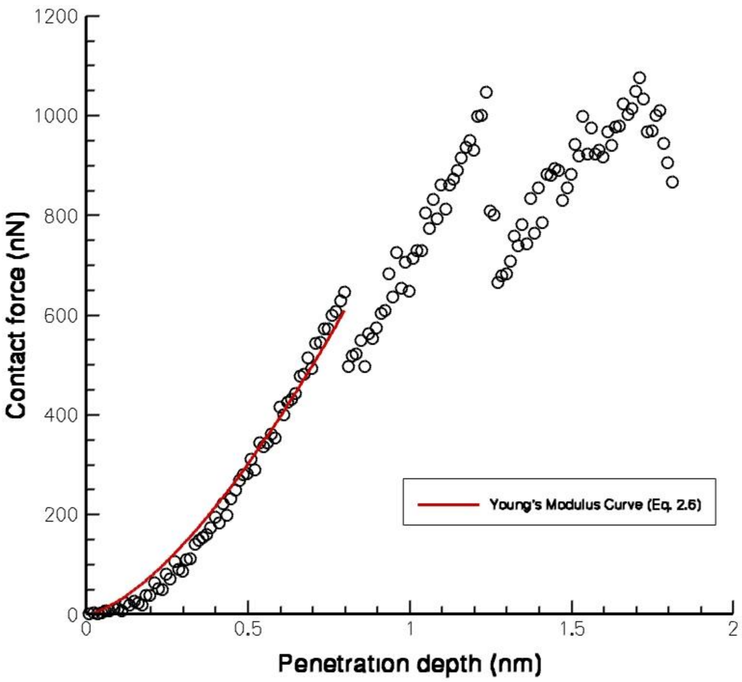
0° Model: Prismatic Loops

- Nucleation & emission takes place in "one fell swoop"



30° Model: Pressure & Force





Mean Contact Pressure

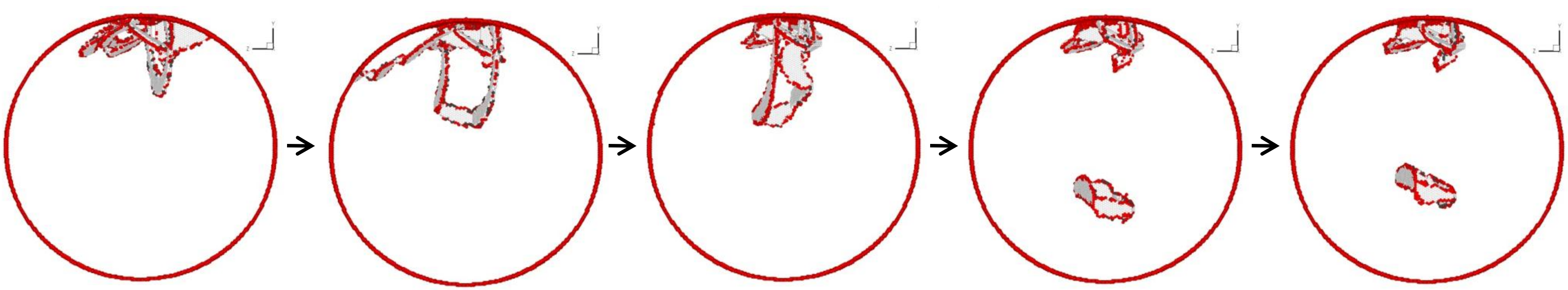
- (Hardness = 20.1 GPa)

Contact Force

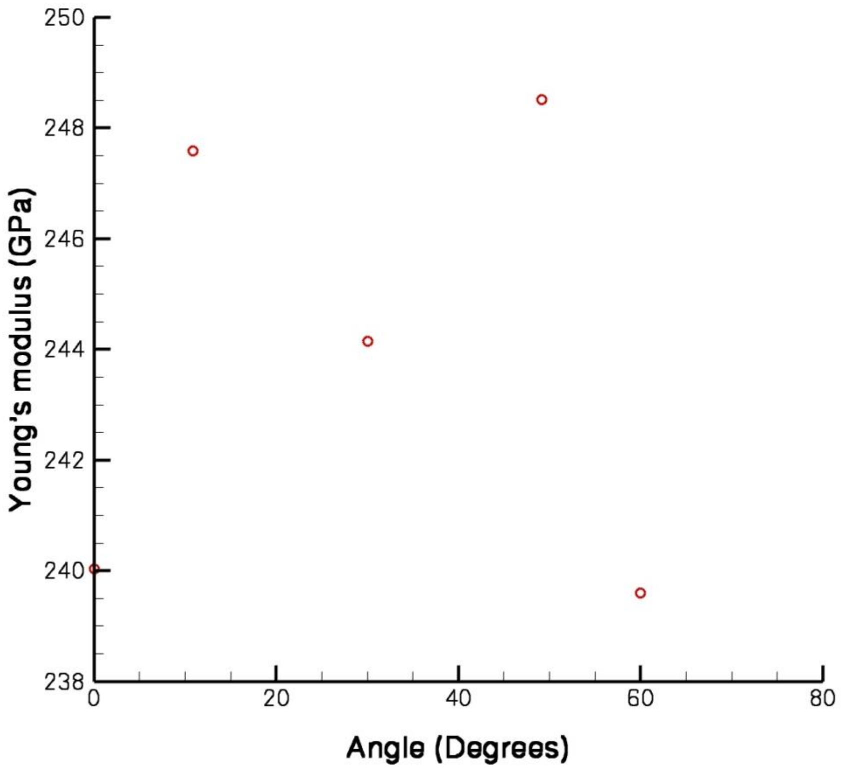
- w/ best fit function?

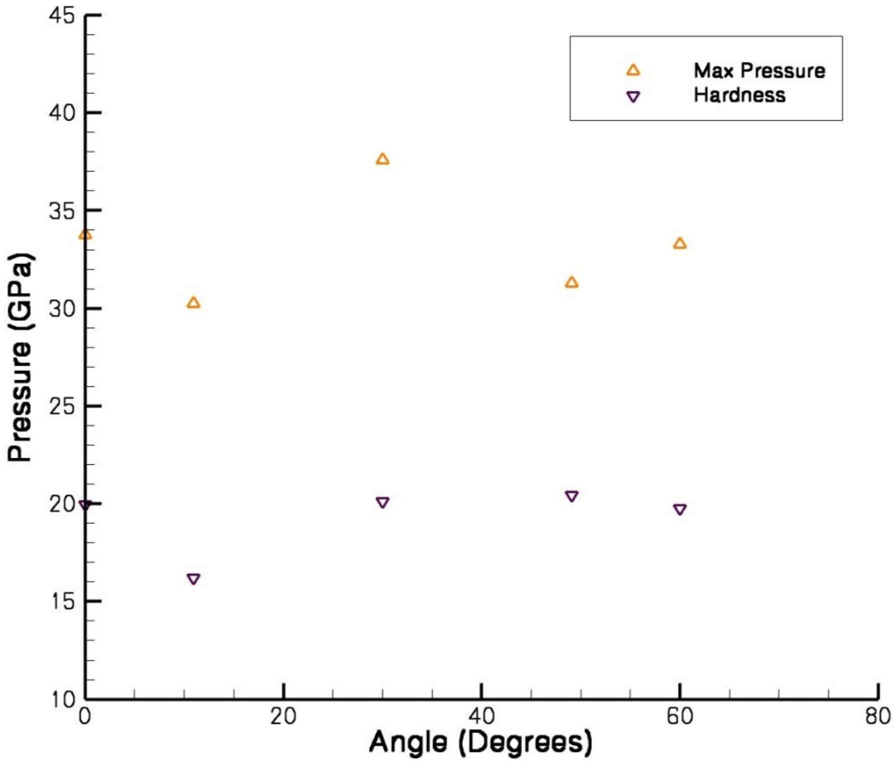
30° Model: Unabsorbed Loops Error

- Loops nucleate, are emitted, but aren't absorbed by free surface
- Due to the fixed atoms at the bottom
- Loops aren't absorbed, so remain in the wire
- Probably explains the poor fit of Young's modulus function



Results





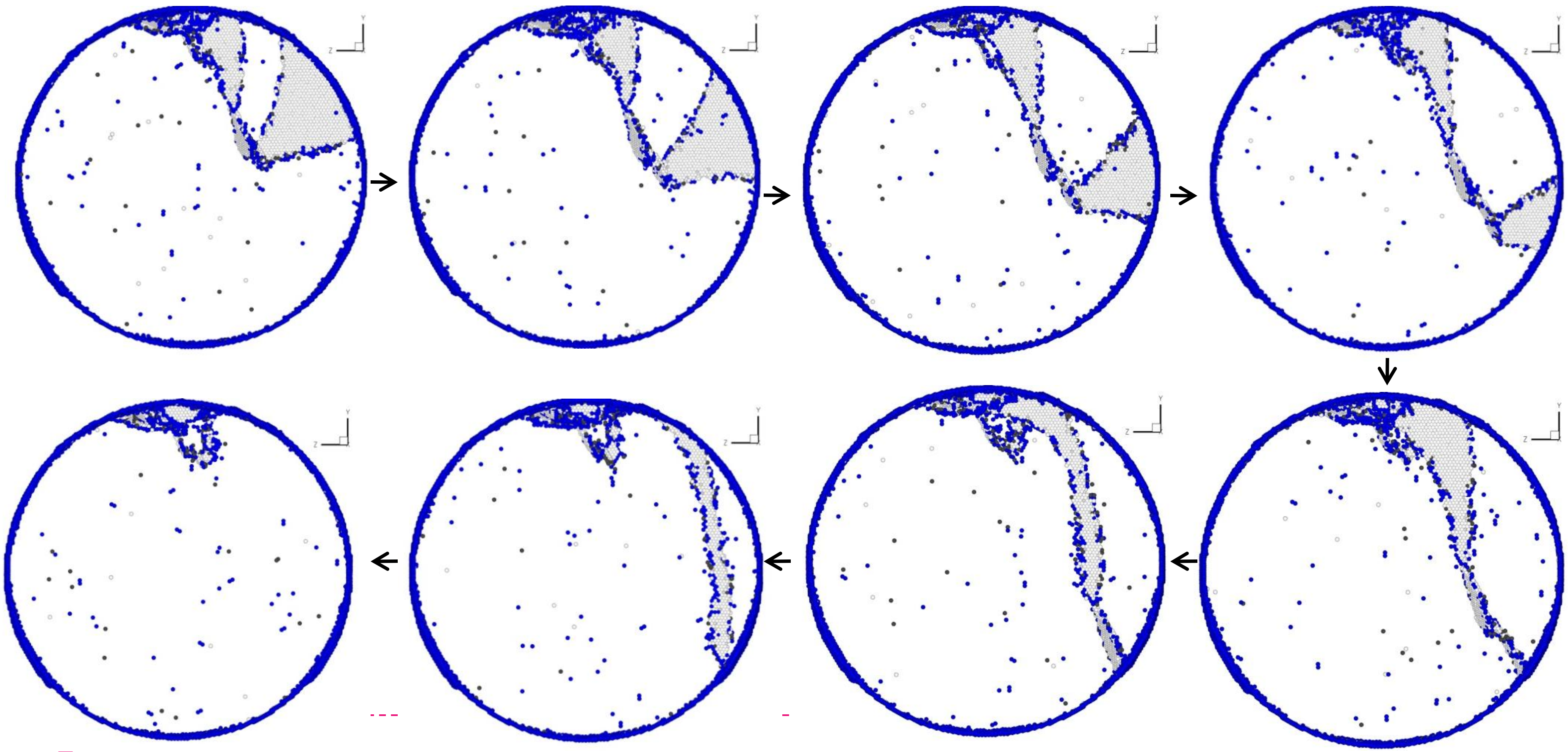
- Trends?
- Angle Sets: 0° & 60°, 10.893° & 49.107°

Conclusions & Future Work

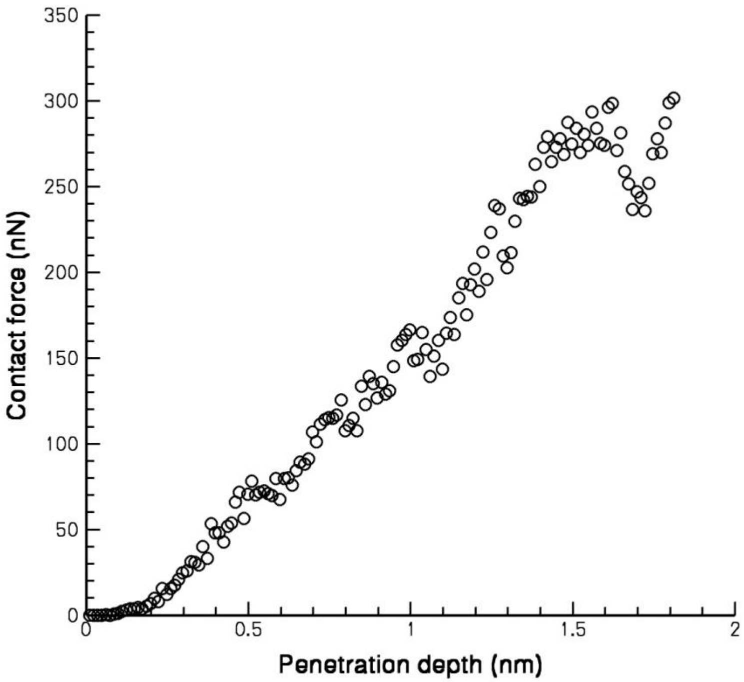
- There is a variation in Young’s modulus, max pressure and hardness based on angle
  - Difficult to tell exact trend, since confidence only in four models
  - Similarity found between some angle sets
- Ideas to Extend Research
  - Develop better means to restrain wire
  - Gather more angles to fill in curve
  - Fit curve with periodic function
  - Test other metals…

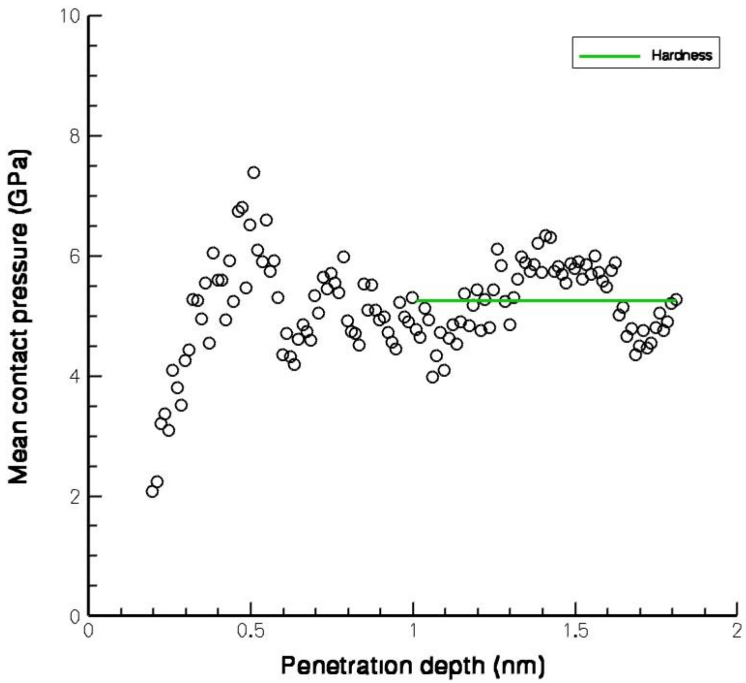
Gold Nanowires: Loops

- Prismatic dislocation loops have much larger radii
- Loops larger than wire radius, thus cannot fully form



Gold Nanowires: Force & Pressure Curves





Contact Force

- Not as smooth as nickel, harder to fit curve
- More loops nucleate more readily

Mean Contact Pressure

- (Hardness ≈ 5 GPa)

References

- J.J. Mock, S.J. Oldenburg. D.R. Smith, D.A. Schultz, and S. Schultz: Composite plasmon resonant nanowires. *Nano Lett.* **2**, 465 (2002).
- A. Husain, J. Hone, H.W. Ch. Postma, X.M.H. Huang, T. Drake, M. Barbic, A. Scherer, and M.L. Roukes: Nanowire-based very-high-frequency electromechanical resonator. *Appl. Phys. Lett.* **83**, 1240 (2003).
- L.A. Bauer, N.S. Birenbaum, and G.J. Meyer: Biological applications of high aspect ratio nanoparticles. *J. Mater. Chem.* **14**, 517 (2004).
- C.J. Barrelet, A.B. Greytak, and C.M. Lieber: Nanowire photonic circuit elements. *Nano Lett.***4**, 1981 (2004).
- Dupont, V. & Sansoz, F. (2009). *Molecular dynamics study of crystal plasticity during nanoindentation in Ni nanowires*.
- C. Deng and F. Sansoz, "Near-Ideal Strength in Gold Nanowires Achieved through Microstructural Design", *ACS Nano*, **3**, 3001-3008 (2009).
- C. Deng and F. Sansoz, "Fundamental Differences in the Plasticity of Periodically Twinned Nanowires in Au, Ag, Al, Cu, Pb and Ni", *Acta Materialia*, **57**, 6090-6101 (2009).
- C. Deng and F. Sansoz, "Enabling Ultrahigh Plastic Flow and Work Hardening in Twinned Gold Nanowires", *Nano Letters*, **9** (4), 1517-1522 (2009).
- Y. Mishin, D. Farkas, M.J. Mehl, D.A. Papaconstantopoulos, *Phys. Rev. B* **59**, 3393 (1999).
- G.J. Ackland and A.P. Jones: Applications of local crystal structure measures in experiment and simulation. *Phys. Rev. B: Condens. Matter* **73**, 054104 (2006).
- G. Feng, W.D. Nix, Y. Yoon, and C.J. Lee: A study of the mechanical properties of nanowires using nanoindentation. *J. Appl. Phys.* **99**, 074303 (2006).
- K.L. Johnson: *Contact Mechanics* (Cambridge University Press, Cambridge, UK, 1985).
- M.A. Meyers and K.K. Chawla: Mechanical Behaviors of Materials (Prentice Hall, Upper Saddle River, NJ, 1999).