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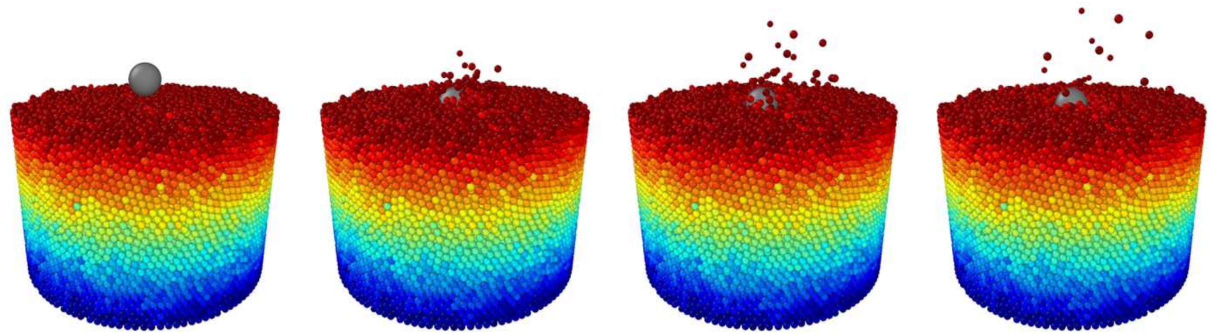

Implementation and Validation of an Analytic Elastic-Plastic Contact Model with Strain Hardening in LAMMPS

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LAMMPS Granular Package

- LAMMPS:
  - Large-scale Atomic/Molecular Massively Parallel Simulator
  - Takes position, mass, force/energy functions for a set of atoms
  - Integrates Newton's equations of motion over many timesteps to predict material behavior
- Granular package:
  - Assigns each particle a radius, density, angular momentum, friction
  - Detects particle collisions, relative tangential motion
  - Applies repulsive force (Hookean or Hertzian), frictional force, damping forces

[S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J Comp Phys, 117, 1-19 (1995).
http://lammps.sandia.gov]

LAMMPS Granular Package

- Normal force on point of contact:

$$F_n = F_{n(elas)} + F_{n(damp)}$$

- For Hertzian case:

$$F_{n(elas)} = \sqrt{\delta r_{eff}}\left(k_n \delta \mathbf{n}_{ij}\right), \quad F_{n(damp)} = -\sqrt{\delta r_{eff}} m_{eff} \gamma_n \mathbf{v}_n,$$

- Tangential force on point of impact:

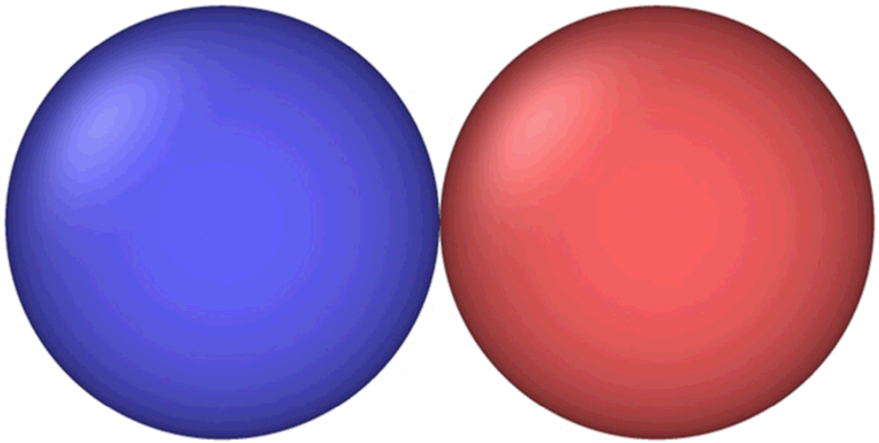
$$F_t = F_{(fric)} + F_{t(damp)}$$

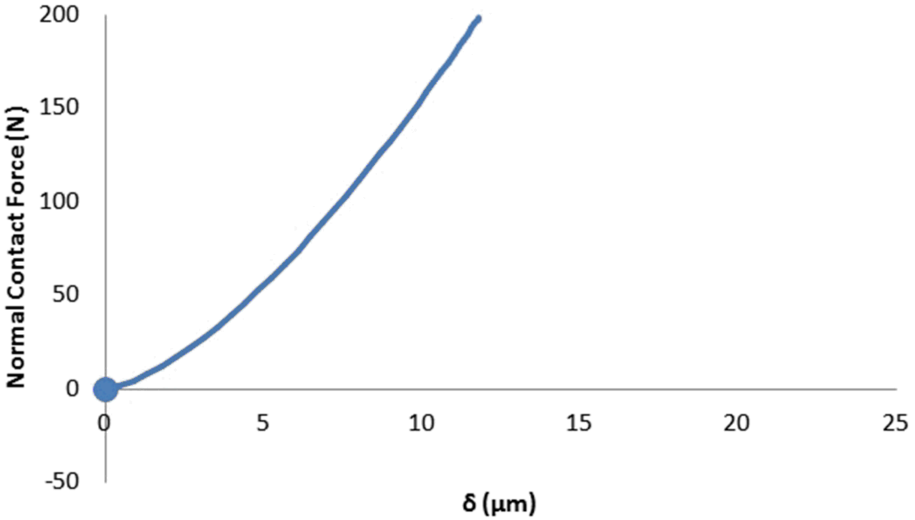
- For Hertzian case:

$$F_{t(fric)} = \begin{cases} -\sqrt{\delta r_{eff}} k_t \Delta s_t & \sqrt{\delta r_{eff}} |k_t \Delta s_t| < \mu \|F_n\| \\ -\mu \|F_n\| \widehat{v_t} & \sqrt{\delta r_{eff}} |k_t \Delta s_t| \geq \mu \|F_n\| \end{cases}, \quad F_{t(damp)} = -\sqrt{\delta r_{eff}} m_{eff} \gamma_t \mathbf{v}_t$$

Normal Contact Force Demo

Hertzian Solution:



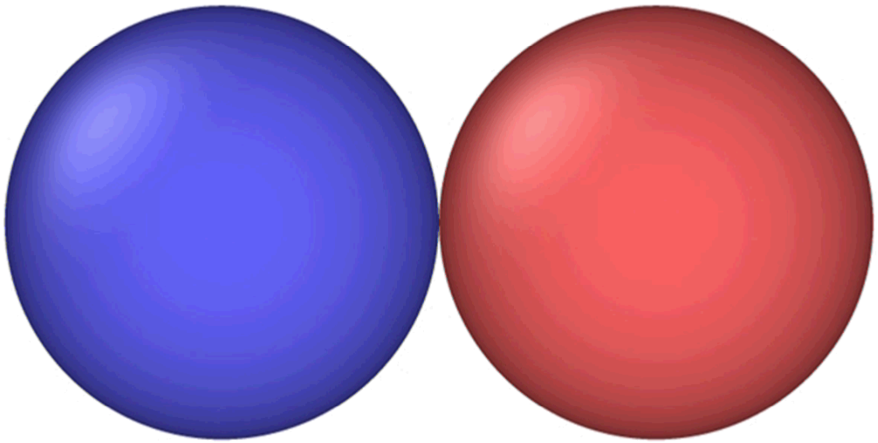


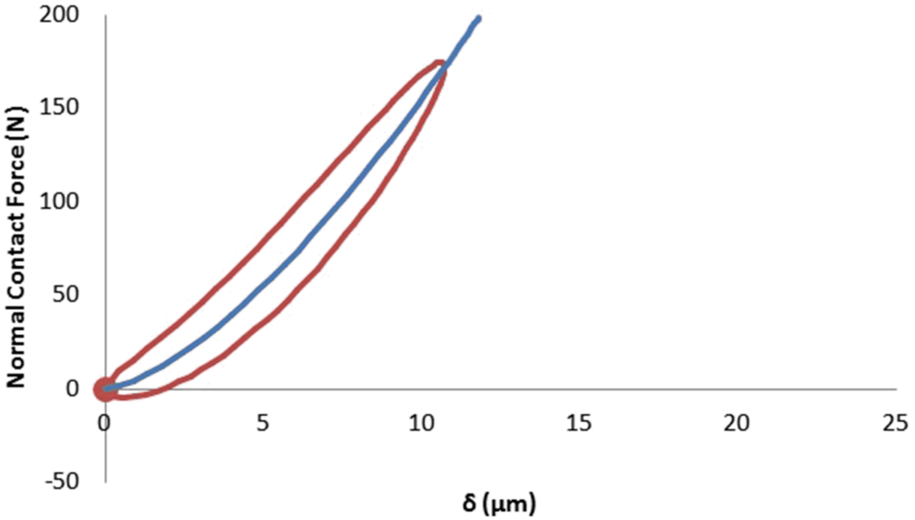
1/8" Ni and WC spheres

Visualized in OVITO [A. Stukowski, Modelling Simul. Mater. Sci. Eng. 18 (2010), 015012, http://ovito.org/]

Normal Contact Force Demo

Hertzian Solution with damping:





1/8" Ni and WC spheres, γ_n=1e8/s-m

Brake Elastic Plastic Contact Model

- Hertzian elastic behavior until point of yield:
  - Same as LAMMPS model

$$F_{n(elas)} = \sqrt{\delta r_{eff}}\left(k_n \delta \mathbf{n}_{ij}\right)$$

- Mixed elastic/plastic behavior after point of yield
  - Plastic force response defined as

$$F_{n(plas)} = p_0 \pi \frac{a^n}{a_p^{n-2}} \mathbf{n}_{ij}$$

  - Contribution from each mechanism defined by

$$F_{n(Brake)} = \phi_1(\delta) F_{n(elas)} + \phi_2(\delta) F_{n(plas)}$$

$$\phi_1(\delta) = \begin{cases} \operatorname{sech}\left((1+\xi)\dfrac{\delta - \delta_y}{\delta_p - \delta_y}\right) & \delta > \delta_y \\ 1 & \delta \leq \delta_y \end{cases}$$

$$\phi_2(\delta) = \begin{cases} 1 - \operatorname{sech}\left((1-\xi)\frac{\delta - \delta_y}{\delta_p - \delta_y}\right) & \delta > \delta_y \\ 0 & \delta \leq \delta_y \end{cases}$$

Brake Contact Model Cont.

- Restitution completely elastic
  - Force response:

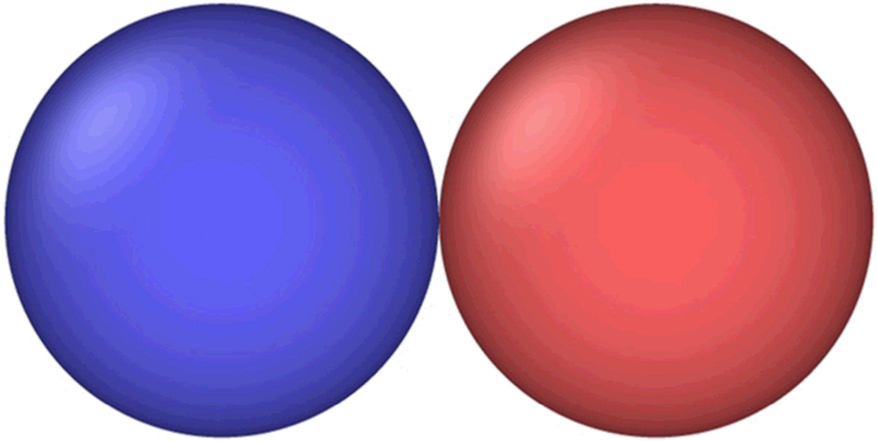
$$F_{n(rest)} = \begin{cases} k_n\sqrt{\bar{r}_{eff}}\left(\delta - \bar{\delta}\right)^{3/2} & \partial > \bar{\partial} \\ 0 & \partial \leq \bar{\partial} \end{cases}$$

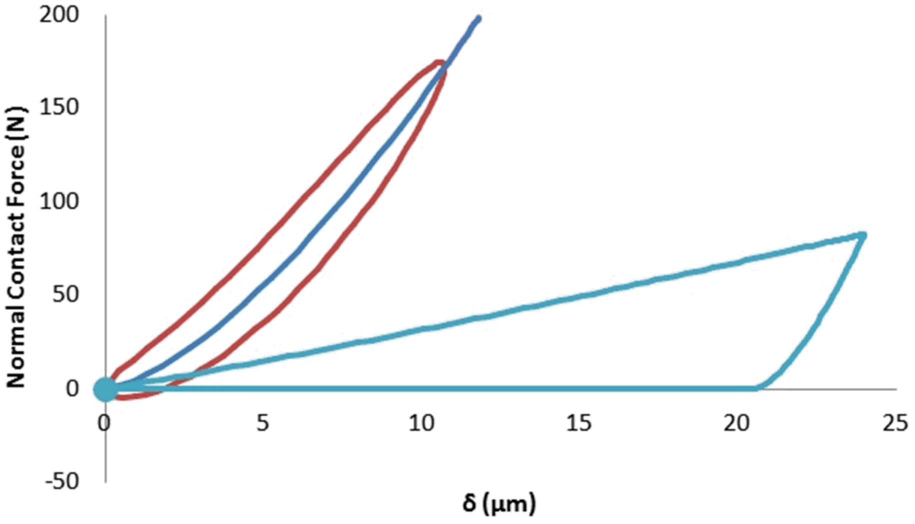
$$\bar{\delta} = \delta_m\left(1 - \frac{F_m}{k_n\sqrt{r_{eff}}\delta_m^{3/2}}\right)$$

Complete model available in [M. R. Brake, An analytical elastic-perfectly plastic contact model, International Journal of Solids and Structures, Volume 49, Issue 22, 1 November 2010, p. 3129-3141.]

Brake Contact Force Demo

Brake Elastic/Plastic Response:





1/8" Ni and WC spheres

LAMMPS Implementation

- Pair style gran/ep/history
  - Normal force calculated by

$$F_n = \begin{cases} \phi_1(\delta)\left(F_{n(elas)} + F_{n(damp)}\right) + \phi_2(\delta)F_{n(plas)} & \delta > \delta_m \\ F_{n(rest)} + F_{n(damp)} & \delta \leq \delta_m \end{cases}$$

  - Tangential force not changed
  - Inputs:
    - $k_n, k_t, \gamma_n, \gamma_t, \mu$ (for Hertzian, friction, damping calculations)
    - c_y (δ_y/r_{eff}), c_p (δ_p/r_{eff}), n, ξ, p_0 (for plasticity calculations)
- Initiation script
  - Calculates appropriate LAMMPS input parameters from material properties
  - Inputs: E, ν, σ, n, HB
  - Outputs: k_n, c_y, c_p, n, ξ, p_0

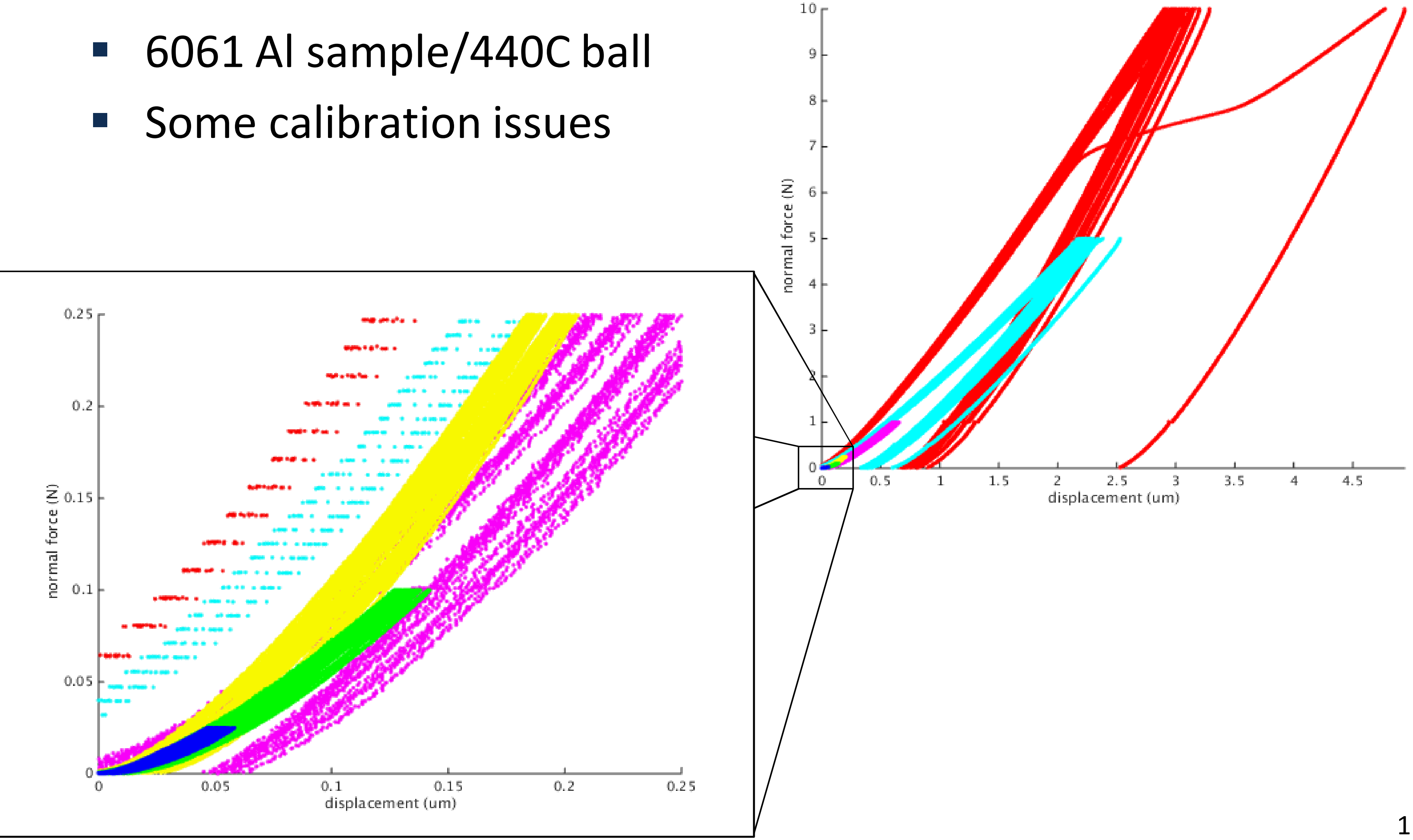
Experimental Data

- 8 metals indented
  - Al 6061, Annealed Cu, Phosphor Bronze, Cu, Hiperco Steel, Nitronic Steel, 304 Stainless Steel, Ti
- 2 indenters
  - 0.125in radius 440C Steel, 3.155mm Sapphire
- 6 load levels
  - 25 mN, 100 mN, 250 mN, 1 N, 5 N, 10 N
- 9 indentations on each of 2 samples for each material/indenter/load combination
- Displacement controlled indentations with
  - 30s load/unload time
  - 5s dwell at max load
  - 30s dwell at 90% unload (for thermal drift correction)

Nanoindentation Data taken by Jon-Eric Mogonye [J.-E.~Mogonye and S.~V.~Prasad, Novel Nano-Impact Techniques for Determining the onset of Fracture in Brittle Films, International Conference on Metallurgical Coatings and Thin Films, April 2014, San Diego, CA]

Raw Experimental Data

- 6061 Al sample/440C ball
- Some calibration issues

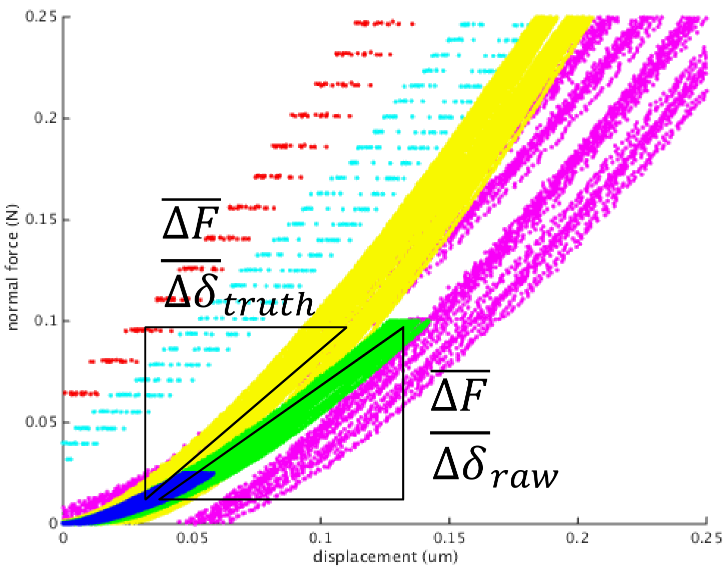


Accounting for Fixture Compliance

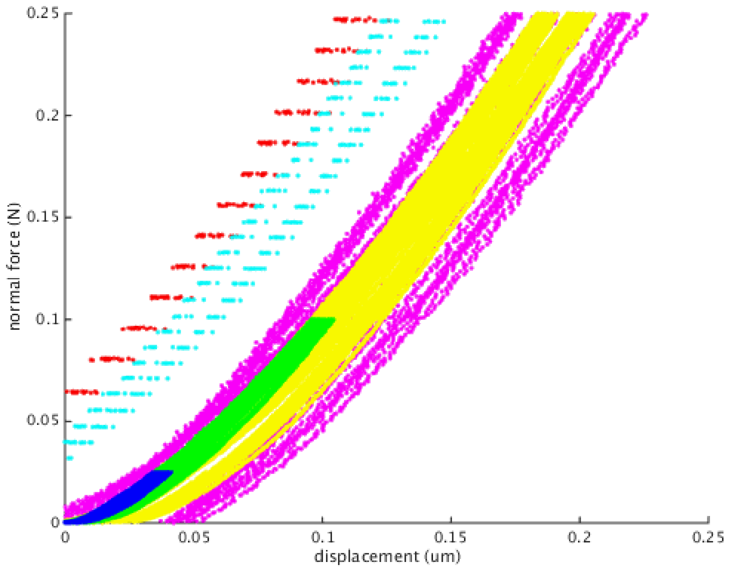
- Outliers eliminated
- Shifted to 0,0
- To correct calibration problems, data was scaled to 250mN load runs with

$$\delta_{new} = \delta_{raw}\left(\frac{\overline{\Delta F}}{\overline{\Delta\delta}_{truth}} \Big/ \frac{\overline{\Delta F}}{\overline{\Delta\delta}_{raw}}\right)$$

Raw Data

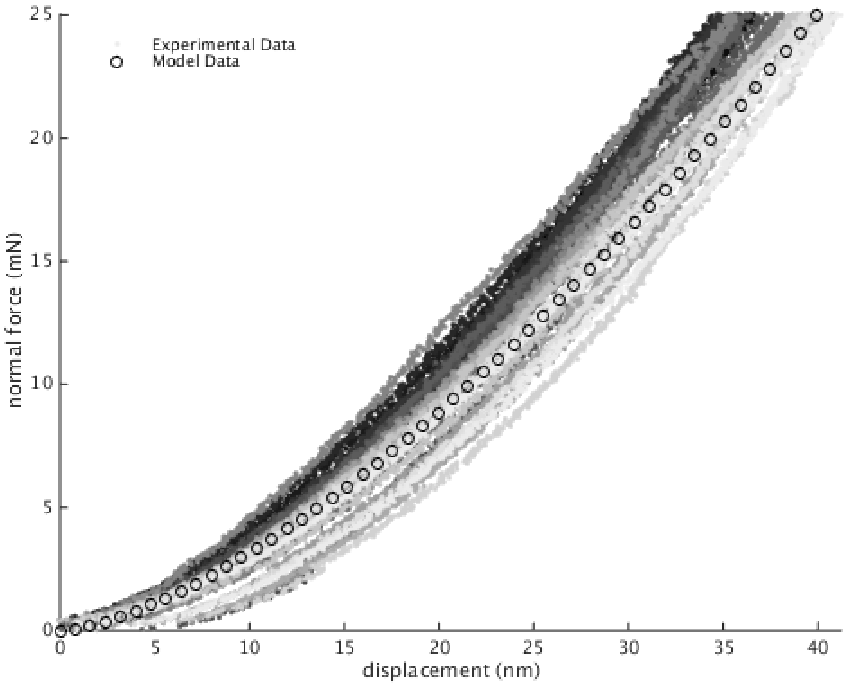


Scaled Data



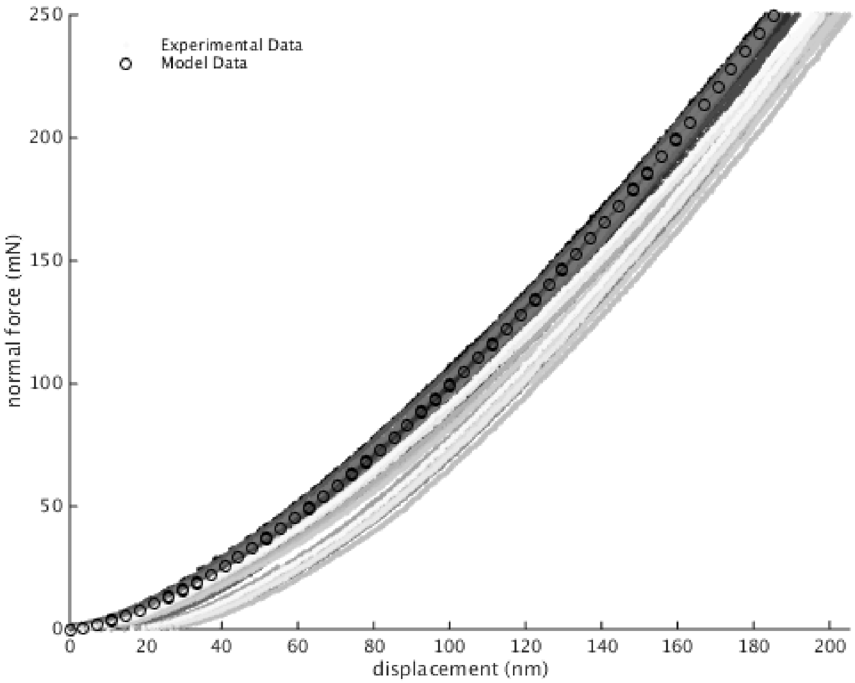
Model Comparison

- 6061 sample/440C ball/25mN load
- Modeled loading curve is within experimental error
- Model predicts zero plastic deformation at this load (onset occurs at 103nm)
- Confirmed by lack of hysteresis



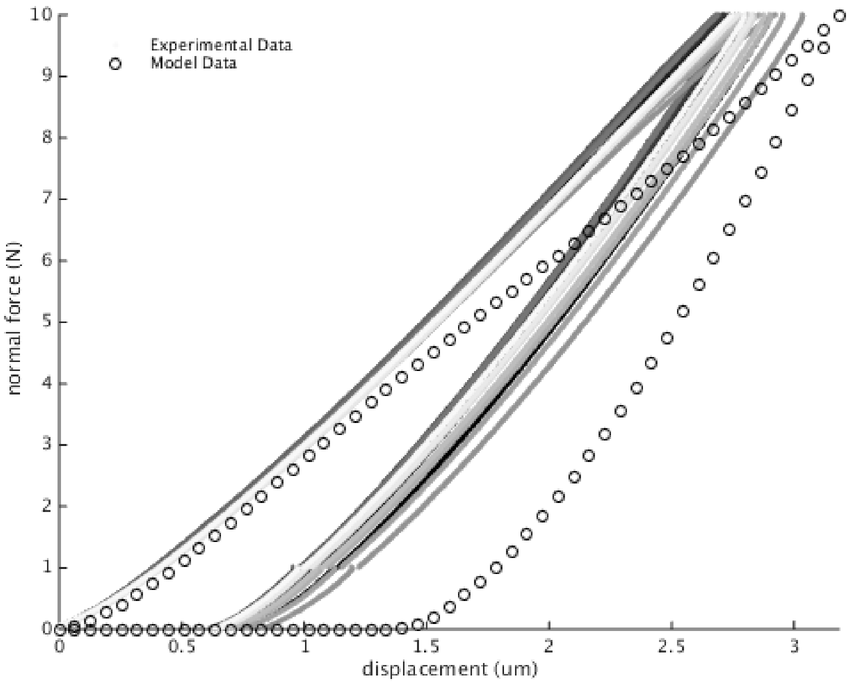
Model Comparison

- 6061 sample/440C ball/250mN load
- Loading curve is accurately modeled
- Model predicts minimal plastic deformation at this load (model restitution curve is indistinguishable)
- Hysteresis is minimal



Model Comparison

- 6061 sample/440C ball/10N load
- Loading curve is less accurately modeled
- Model predicts significant plastic deformation at this load
- Predicted hysteresis is too high



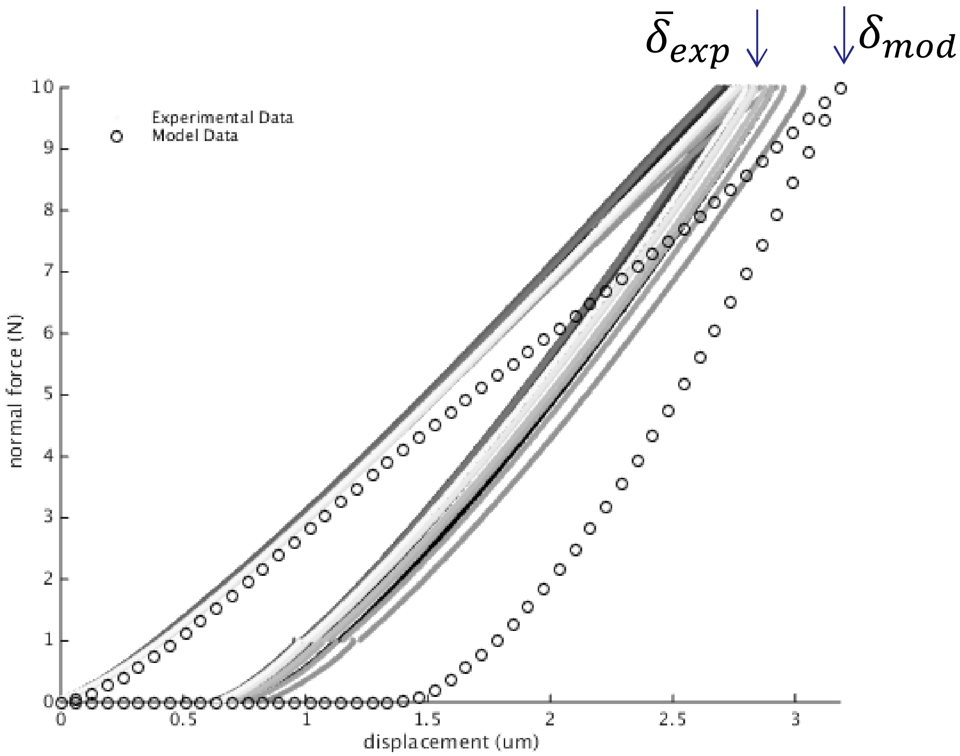
Model Comparison

- % error between model and experiment calculated for each ball/sample/load combination using

$$\%error \pm 95\%CI = \frac{\delta_{mod} - \bar{\delta}_{exp}}{\delta_{mod}} \pm 1.96\frac{\sigma_\delta}{\sqrt{n}}$$

- In this case

  13.20 ± 1.07%

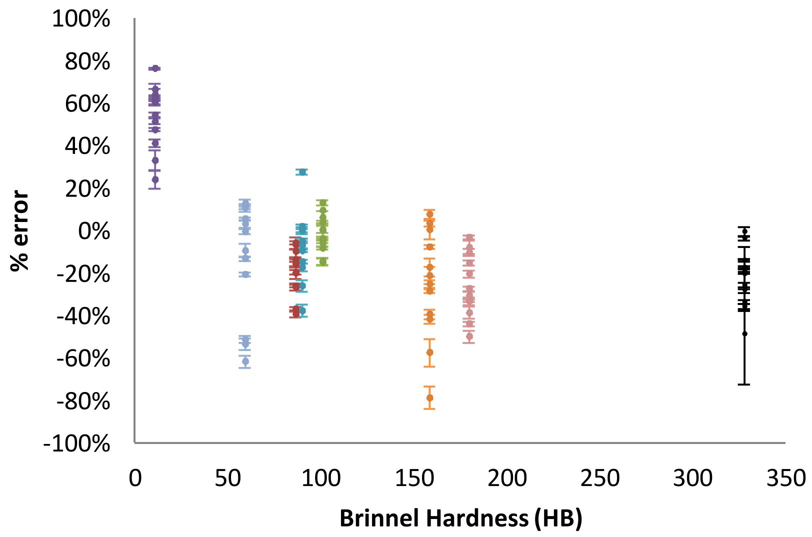


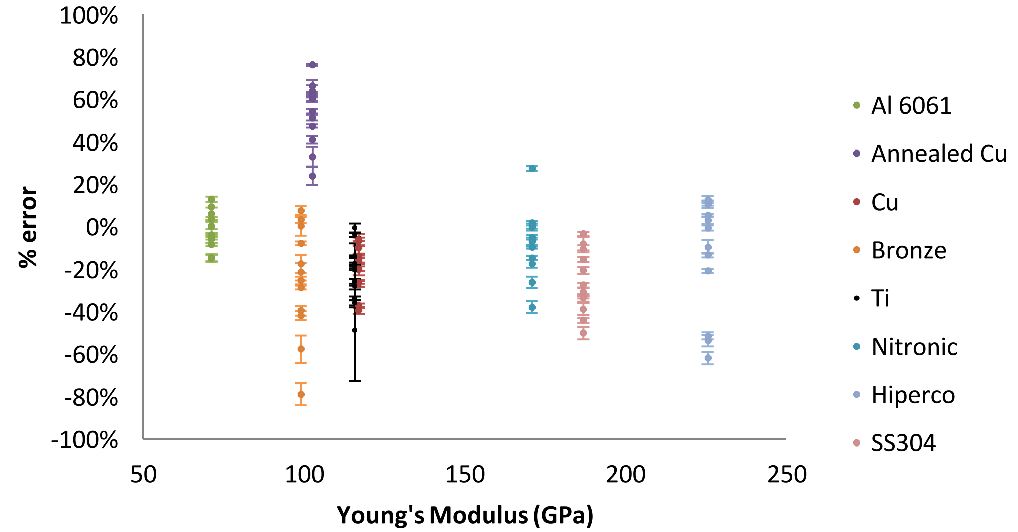
% Error at max load

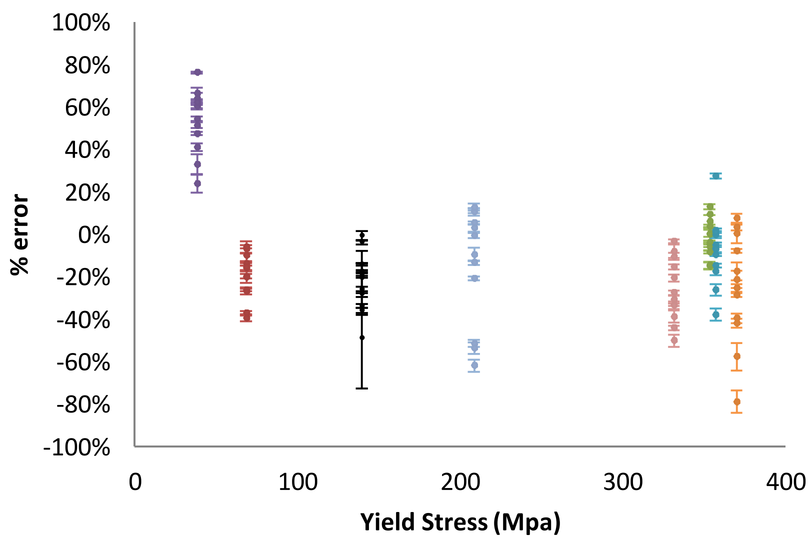
	25mN	100mN	250mN	1N	5N	10N
	440C Ball					
Al 6061	6.26 ± 3.17%	0.60 ± 1.64%	-3.78 ± 1.66%	-8.22 ± 1.73%	-4.76 ± 1.00%	13.20 ± 1.07%
Annealed Cu	24.07 ± 4.36%	41.05 ± 1.76%	51.43 ± 1.32%	62.19 ± 1.01%	64.15 ± 2.51%	66.43 ± 2.75%
Bronze	-57.51 ± 6.39%	-78.69 ± 5.23%	-39.37 ± 2.26%	-28.58 ± 0.87%	-41.73 ± 1.99%	-21.12 ± 4.12%
Cu	-5.95 ± 5.92%	-6.86 ± 1.82%	-13.60 ± 1.22%	-26.05 ± 1.50%	-37.03 ± 6.26%	-15.84 ± 4.74%
Hiperco	-61.75 ± 8.63%	-51.28 ± 4.06%	-20.72 ± 2.55%	5.61 ± 1.08%	-13.19 ± 3.71%	-0.37 ± 2.69%
Nitronic	-37.76 ± 5.31%	-17.26 ± 2.76%	-14.61 ± 1.56%	-9.54 ± 1.09%	-4.89 ± 3.77%	27.65 ± 4.76%
SS304	-38.66 ± 6.50%	-33.23 ± 0.94%	-27.41 ± 0.59%	-33.01 ± 0.45%	-43.92 ± 0.51%	-15.12 ± 0.45%
Ti	-48.58 ± 24.02%	-25.77 ± 12.07%	-20.40 ± 7.02%	-17.42 ± 0.70%	-33.63 ± 0.85%	-18.53 ± 0.83%
	Sapphire Ball					
Al 6061	9.45 ± 2.88%	0.21 ± 1.76%	-5.84 ± 0.96%	-14.35 ± 0.59%	-14.83 ± 1.11%	3.74 ± 1.16%
Annealed Cu	33.04 ± 4.80%	47.61 ± 0.84%	54.43 ± 1.07%	76.30 ± 0.49%	60.50 ± 1.58%	60.86 ± 1.31%
Bronze	0.31 ± 4.23%	7.57 ± 2.11%	3.35 ± 1.48%	-7.58 ± 0.86%	-25.21 ± 1.78%	-17.39 ± 4.24%
Cu	-20.00 ± 9.06%	-9.77 ± 2.40%	-15.15 ± 2.40%	-26.53 ± 1.00%	-39.2 ± 2.74%	-19.67 ± 2.69%
Hiperco	-53.52 ± 20.62%	-9.46 ± 2.56%	12.94 ± 1.70%	10.70 ± 0.81%	3.05 ± 1.63%	11.15 ± 3.79%
Nitronic	-26.14 ± 4.42%	-6.88 ± 3.45%	-6.55 ± 2.14%	1.06 ± 0.57%	0.00 ± 0.97%	1.90 ± 2.92%
SS304	-50.00 ± 26.68%	-7.87 ± 2.77%	-10.28 ± 1.63%	-20.36 ± 2.18%	-30.62 ± 3.05%	-3.12 ± 2.33%
Ti	-14.03 ± 6.25%	-0.55 ± 2.27%	-3.55 ± 1.10%	-13.98 ± 0.65%	-35.71 ± 1.07%	-27.92 ± 1.39%

Presented as %error ± 95%CI (< |10%|, > |30%|)

Trends With Material Properties

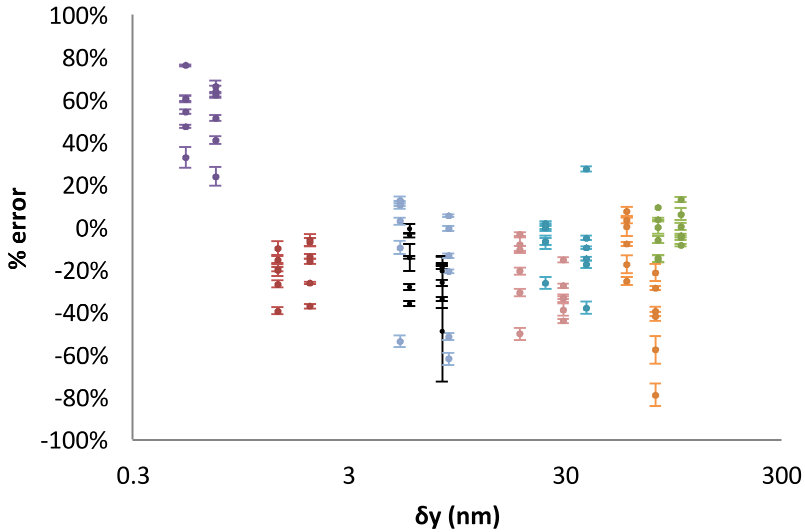


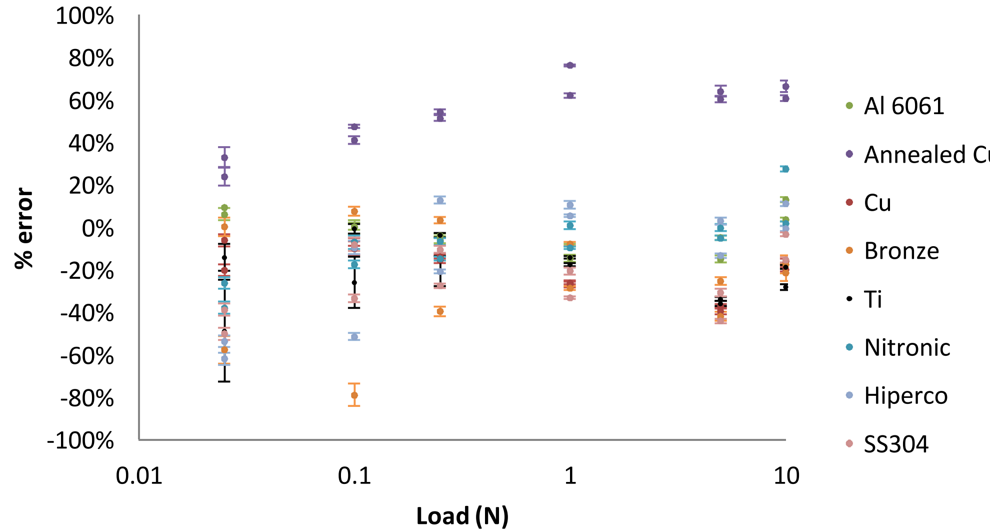


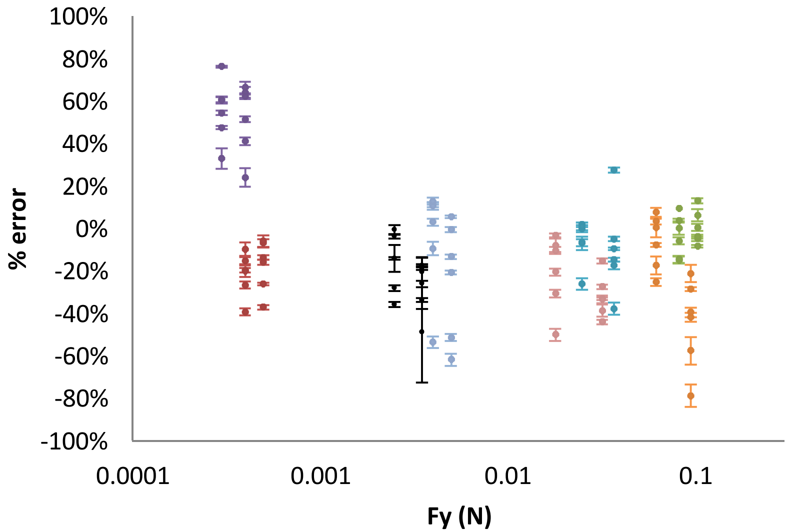


- Error increases with decreasing strength, hardness
- Negative error values indicate the sample was more compliant than expected

Trends with Model Parameters, Load







- At low loads, model overpredicts stiffness
- At high loads, model slightly underpredicts stiffness
- Overall error magnitude decreases as load increases
- Trend starts to emerge

Trends with Normalized Load

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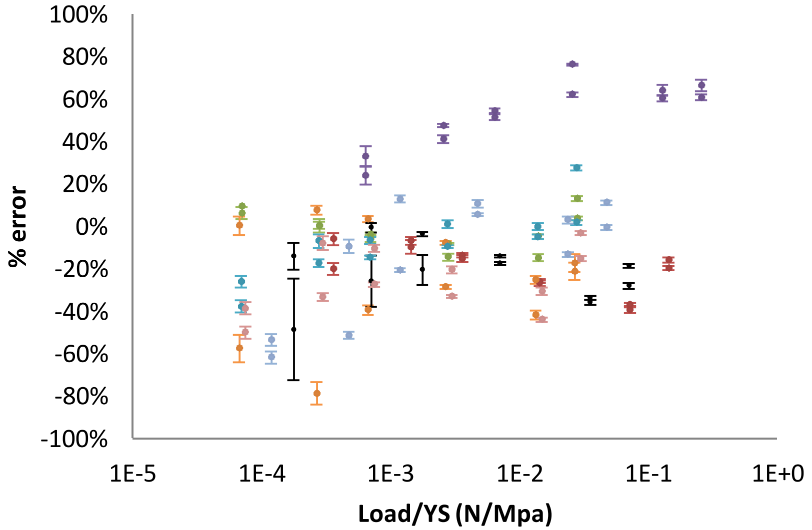

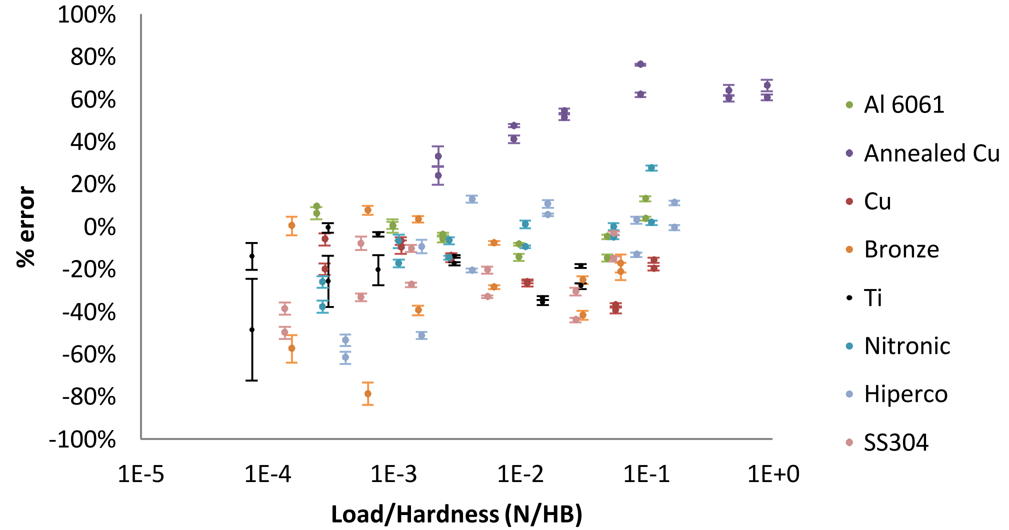

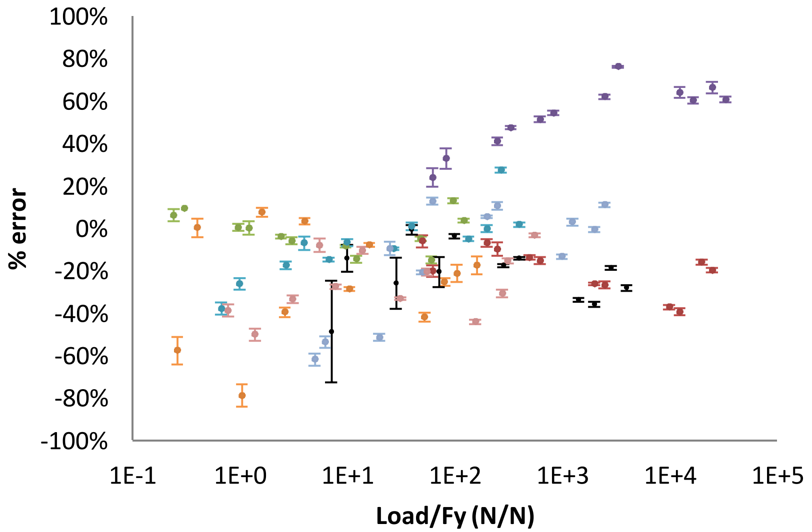

- Trend begins to emerge when load is corrected for material hardness
- Large error bars at low load levels
  - Indicates high scatter, room for improvement in transition
  - Less reliable data
- Smaller scatter at high loads indicate room for improvement with more precise calibration

Conclusions

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- A LAMMPS pair style was developed to incorporated strain hardening effects in a particle dynamics simulator
- The model gives an improved picture of hysteresis for strain-hardening metals
- Validation of the model using high-resolution indentation data showed varying degrees of accuracy depending on force levels and material properties
- Future work on this project includes refining calibration steps and defining the limits of its accuracy