Quantification of uncertainty of the yield stress of nanocrystalline Nickel

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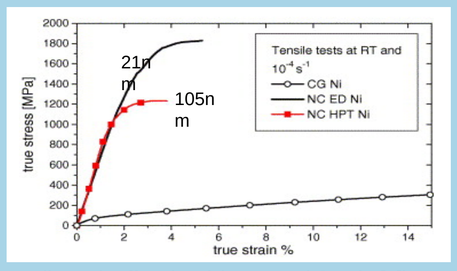
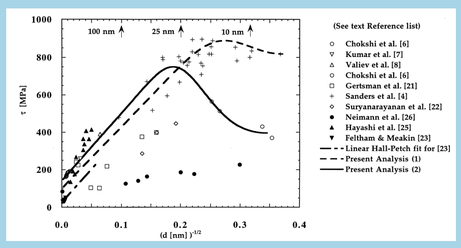
Motivation

- In nanocrystalline (nc) materials, deformation mechanisms are affected by
  - large volume fraction of grain boundaries [1]
  - confinement of dislocations in small grains [2].
- The mechanical response of polycrystalline materials is usually described in terms of the average grain size.
- Experiments [3] and simulations [4] show that the average grain size is not enough to characterize the mechanical response of nc materials.
- The goal of this work is to quantify the effects of
  - grain size distribution
  - initial dislocation density

on the yield stress of nc Nickel.



Hall Petch effect in Ni (Torre and Spatig [5])



Large scatter for Cu (Musumura et all [3])

Phase Field Dislocation Dynamics (PFDD) Model

Model Formulation and Numerical Implementation

- The plastic distortion is related to the phase field variable by

$$\beta^p_{ij}(x) = \frac{1}{w}\sum_\alpha b^\alpha \zeta(\alpha, x)\, s^\alpha_i m^\alpha_j$$

- Strain energy is the sum of elastic interaction energy and misfit energy

$$E = E^{elastic} + E^{misfit}$$

$$E^{misfit} = \int \left[\sum_\alpha A_1 \sin^2(\pi\zeta(\alpha, x))\right] d^3x$$

$$E^{elast} = \frac{1}{2}\oint \hat{A}_{mnuv}(\mathbf{k})\hat{\beta}^p_{mn}(\mathbf{k})\hat{\beta}^{p*}_{uv}(\mathbf{k})\frac{d^3k}{(2\pi)^3} - \int \sigma^{appl}_{ij}\beta^p_{ij} d^3x$$

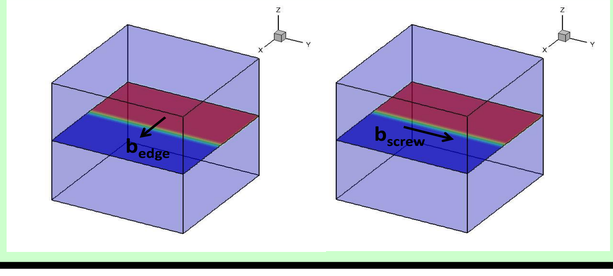
- The temporal evolution of the phase field is driven by the Ginzburg-Landau kinetic equation,

$$\frac{\partial \zeta(\alpha, x, t)}{\partial t} = -L\frac{\delta E}{\delta \zeta(\alpha, x, t)}$$

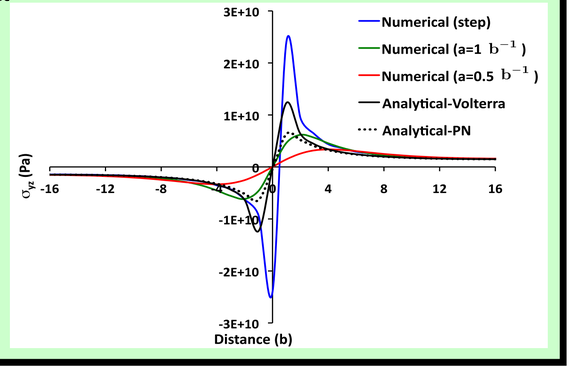
- The simulation cell has more than 100 million grid points (a grain size of 128 nm).
- Grain boundaries are impenetrable barriers to dislocations.
- Active slip systems consist of (111) planes and three <110> directions.
- Simulations are run with 256 processors on Steele, Coates and Hansen, RCAC, Purdue University.

Verification

- We can verify the stress and strain implementation by comparing with the Volterra analytical model for a infinitely long, straight dislocation.



Stress (σ_{yz}) in a Screw Dislocation

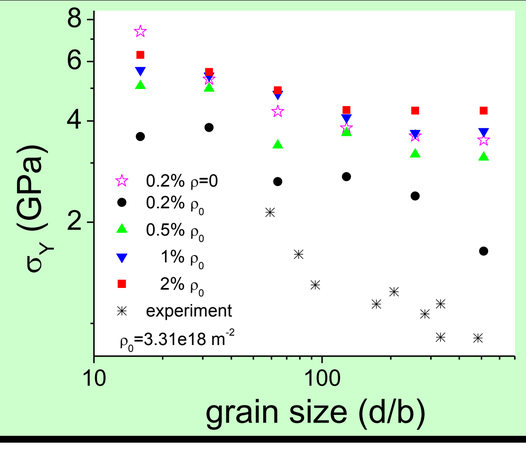


Validation

- Our simulation results are consistent with the experiment by Meyers et al. [2] qualitatively – both exhibit size effect,

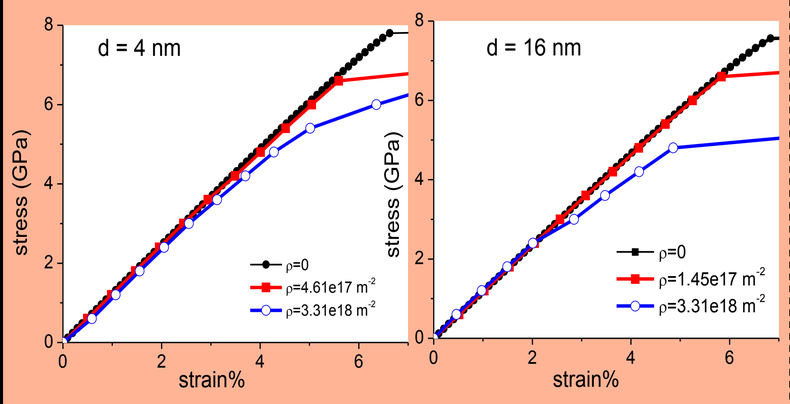
$$\sigma_y = A\mu\left(\frac{d}{b}\right)^{-B}$$

d grain size;
b (=0.249 nm) the Burgers vector in Nickel.

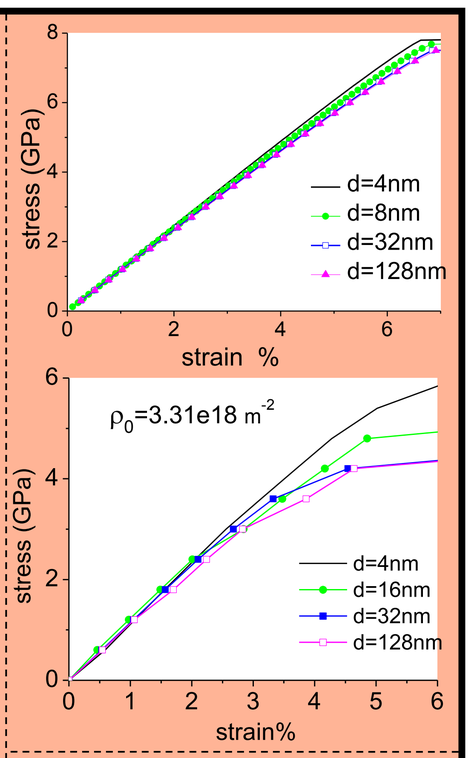


UQ analysis in yield stress prediction

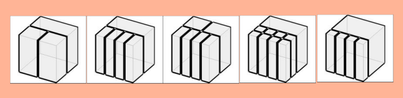
Initial dislocation density



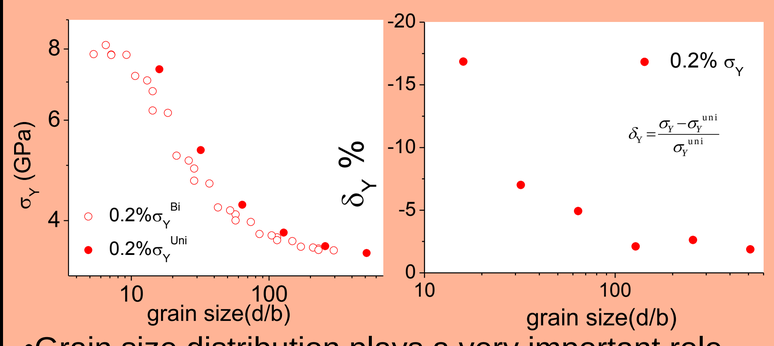
- Smaller initial dislocation density results in harder material.



Grain size distribution

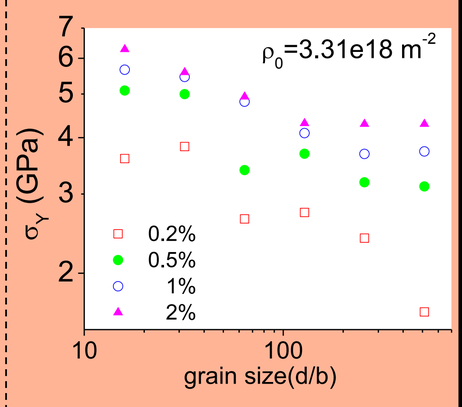


Bimodal grain configurations

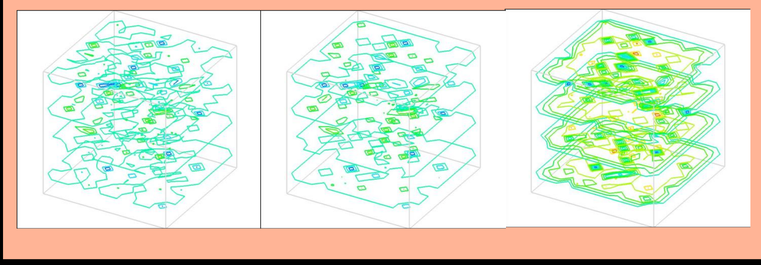


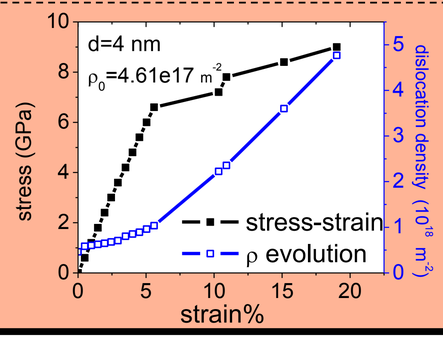
- Grain size distribution plays a very important role in the mechanical response of materials at grain size smaller than 8 nm.

Yield stress definition



Dislocation evolution





Meshless PFDD Modeling of Microstructure

- 2D (middle) and 3D (right) polycrystalline microstructure reconstruction based on the TEM image (left) for nc Ni [2]

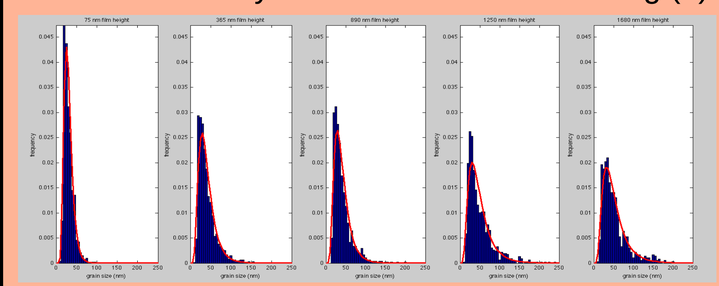
PDF of the Yield Stress of Ni Membranes

- PDFs of grain distributions at different depth of the Ni film of the PRISM device (1)
- Extrapolated Hall-Petch equation relating the average grain size to yield stress (2)
- The PDF of the yield stress is obtained using (3)

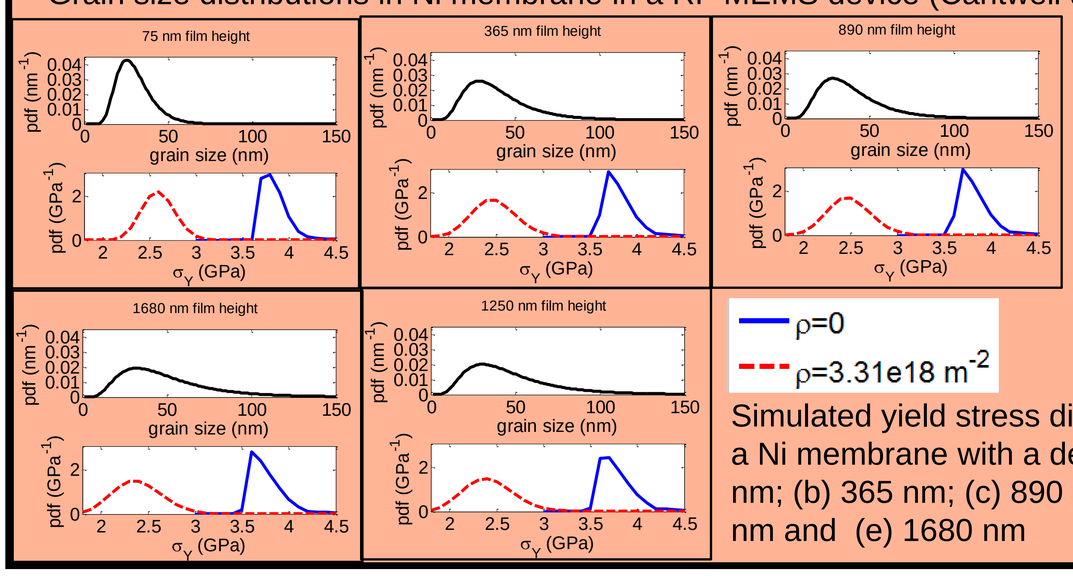
$$f_X(x;\mu,\sigma) = \frac{1}{x\sigma\sqrt{2\pi}} e^{-\frac{(\ln x-\mu)^2}{2\sigma^2}} \quad (1)$$

$$\sigma_y = g(d) = A\mu\left(\frac{d}{b}\right)^{-B} \quad (2)$$

$$f_Y(y) = \frac{f_X(g^{-1}(y))}{\left|g'(g^{-1}(y))\right|} \quad (3)$$



Grain size distributions in Ni membrane in a RF MEMS device (Cantwell and Stach)



Simulated yield stress distribution of a Ni membrane with a depth of (a) 75 nm; (b) 365 nm; (c) 890 nm; (d) 1250 nm and (e) 1680 nm

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References
[1] E. Arzt, *Acta Mater.* 1998
[2] M. A. Meyers, *Progress in Materials Science*.2006
[3] R. A. Masumurael all, *Acta Materialia*, 46(13):4527 – 4534, 1998. M.
[4] M. Koslowski, *Physical Review B* 2010
[5] F. Dalla Torre, *Acta Mater.* 2005

Collaborators
Materials Characterization, P. Cantwell and Eric Stach, School of Materials Engineering, Purdue University.

Atomistic Simulations: Hojin Kim and Alejandro Strachan, School of Materials Engineering, Purdue University,