3.032 Mechanical Behavior of Materials

Fall 2007

Using U(r):

Measure parameters for U(r) in physical model to predict stresses that are high enough for elastic instabilities to occur (e.g., nucleation of defects in crystals).

Raft of soap bubbles with interbubble potential similar to interatomic potential of fcc metals, under distributed force of an indenter.

How does stress to move atoms depend on size of grains in polycrystalline metals?

σ_{ii} or τ_{ij} ~ dU/dr

Van Vliet et al., Nature (2002); Phys Rev B (2003); Phil Mag A (2003)

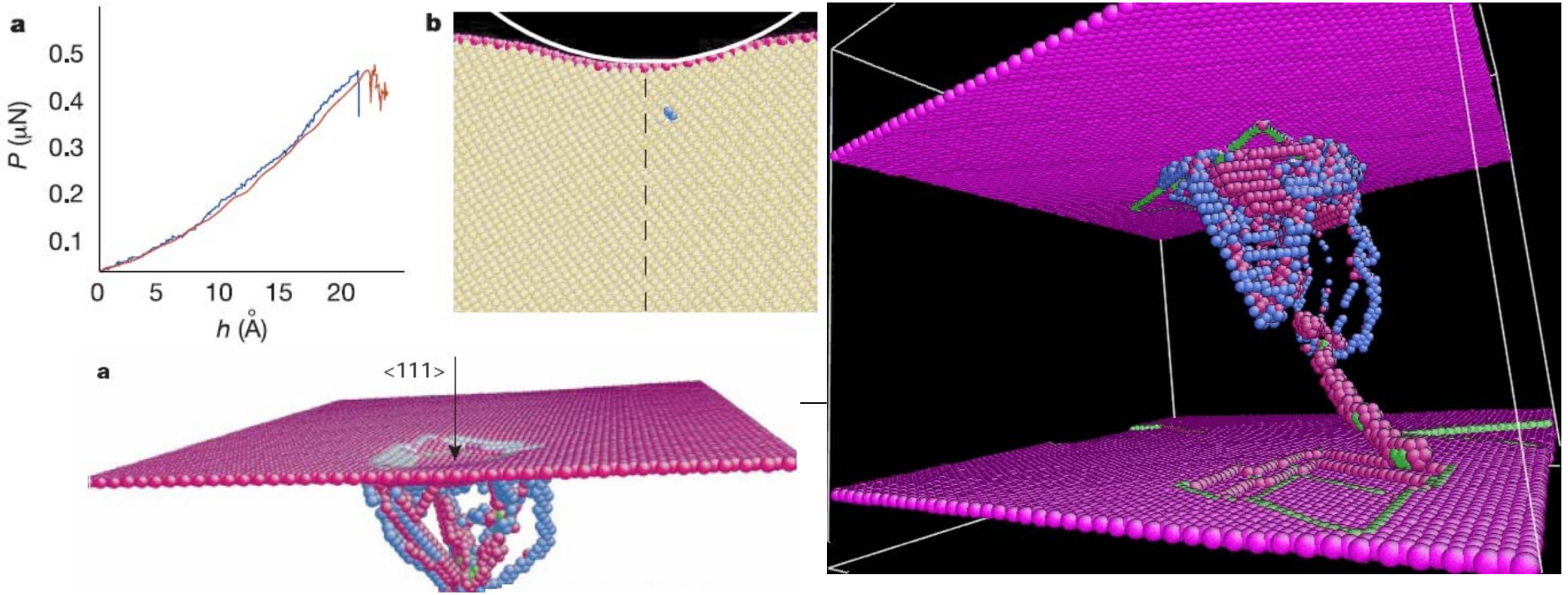
3.032 Mechanical Behavior of Materials

Fall 2007

Using U(r):

Molecular dynamics simulations move atoms according to Newton's Law, F = ma
where F = dU/dr and U = interatomic potential such as L-J potential.

Courtesy of Sidney Yip. Used with permission.



Thin film of aluminum, moving atoms according to U(r) under distributed load of spherical indenter. Atom color = atomic coordination number.

Li, Van Vliet et al., Nature (2003); Phys Rev B (2004)

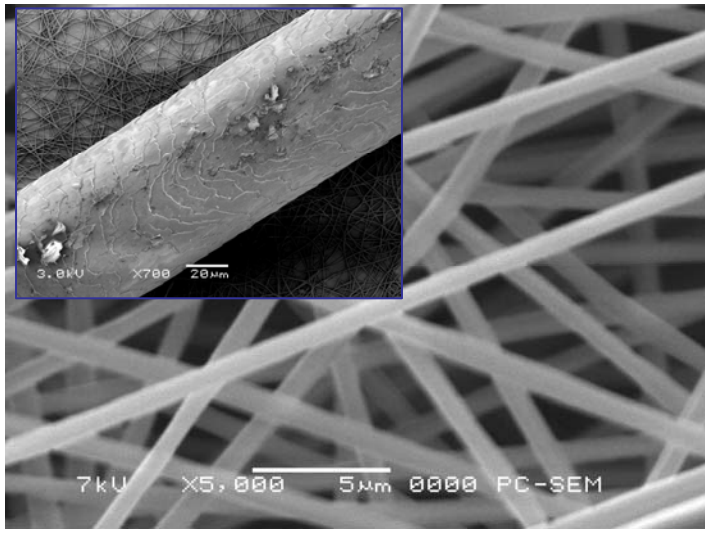
3.032 Mechanical Behavior of Materials

Fall 2007

Using U(r):

Polymer nanofibers: Do physical and mechanical properties differ from bulk polymers?

Courtesy Gregory Rutledge. Used with permission.



Electrospun PEO could be used for filters, composites, fuel cells, drug delivery, cell scaffolds, etc. [Rutledge Group, MIT]

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Please see Fig. 1 and 4 in Curgul, Sezen, et al. "Molecular Dynamics Simulation of Size-Dependent Structural and Thermal Properties of Polymer Nanofibers." *Macromolecules* 40 (2007): 8483-8489.

Internal energy inside polymer nanofiber increases for fibers of R < 5 nm.

Curgul, Rutledge and Van Vliet, Macromolecules (2007, in press)

3.032 Mechanical Behavior of Materials

Fall 2007

Using U(r):
Polymer nanofibers exhibit lower glass transition temperature and elastic deformation up to 5% normal strain.

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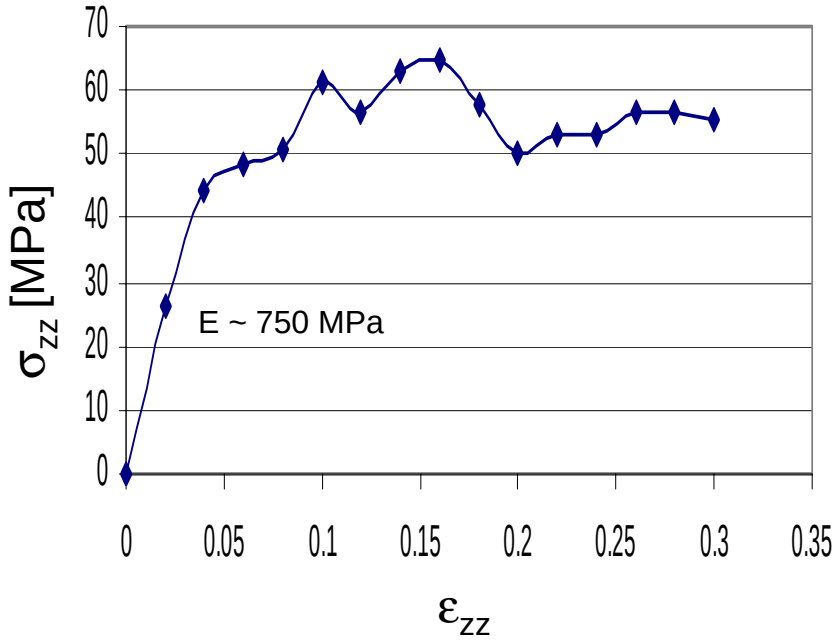
Please see Fig. 7 and 10, and Eqn. 1 in Curgul, Sezen, et al. "Molecular Dynamics Simulation of Size-Dependent Structural and Thermal Properties of Polymer Nanofibers." *Macromolecules* 40 (2007): 8483-8489.



Curgul, Rutledge and Van Vliet, Macromolecules (2007, in press)