Nanomanufacturing: Nano-Structured Materials Made Layer-by-Layer

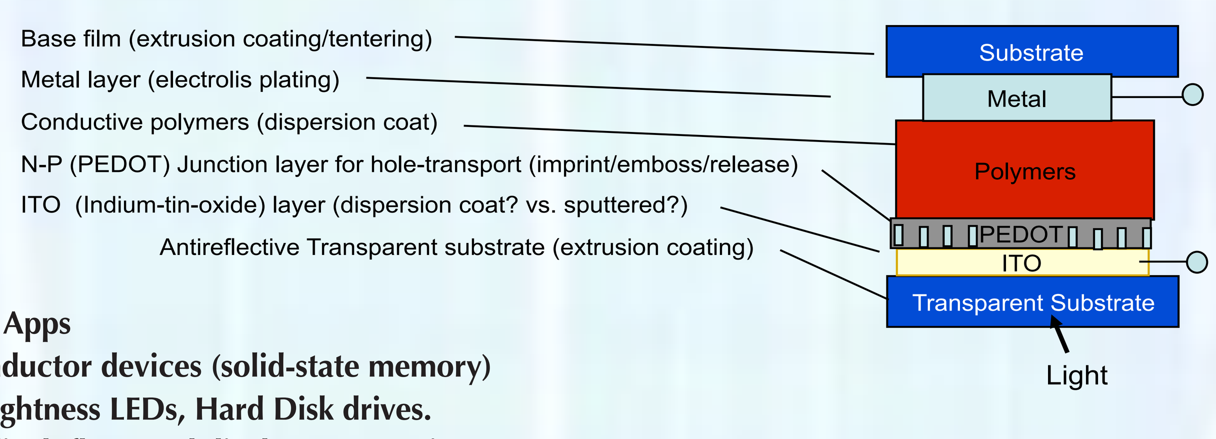
Sandia National Laboratories

P. Randall Schunk, J. B. Lechman, M. E. Chandross, L. Musson, E. D. Reedy, J. V. Cox, G. S. Grest, H. Fan

Problem

Nanomanufacturing Unit Operations — high-throughput, nanostructured films in layers

- Series of dispersion coating, nano-imprinting/embossing, in a layer-by-layer way (e.g., photovoltaic)

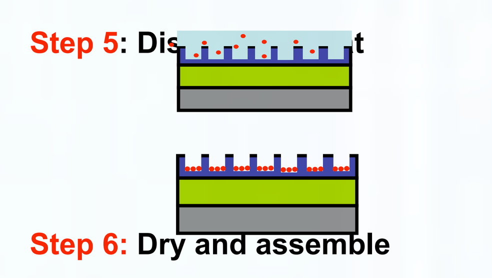


- Additional Apps
  - Semiconductor devices (solid-state memory)
  - High-brightness LEDs, Hard Disk drives.
  - Bio-Medical, flat panel displays, CMOS image sensors
  - Thermoelectric and photovoltaics
- Nanomanufacturing projected to be $1T by 2015 (NSF)
- Breakthroughs in clean, affordable, abundant energy will require volume manufacturing
- Materials design and manufacturing must be considered (designed) together!

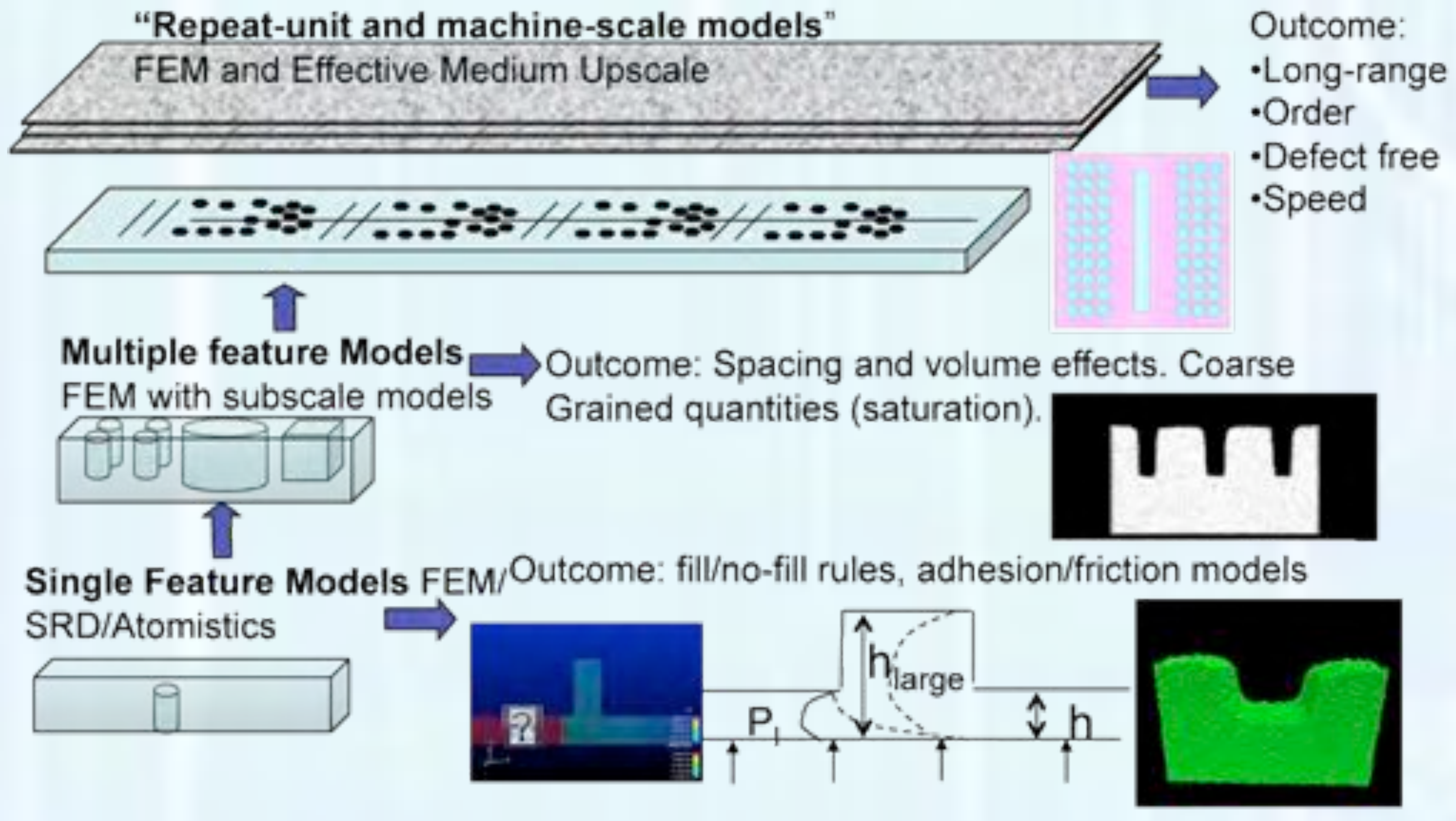
Approach

- **SFIL Prototype: Step-and-Flash Imprint Lithography — K,** SFIL Epitomizes Nanomanufacturing. Our UT partner and NIL/dispersion coating labs provide the capability.
  - Liquid-based coating, molding, imprinting/release
  - How fast? Long range order (We can make 10 trillion dots for 50 cents! That's cheap!)
- **Goal:** Produce mod/sim capabilities, validated and up-scaled so as to impact machine design (viz., emboss pressures, imprint rates, feature density, defect reduction, etc.). Produce experimental capability for high-throughput convective assembly.
- FY09:
  - Feature scale models aimed at materials and physics issues (e.g., wetting, speed, throughput, etc.)
  - Upscaling to multiple features (monodisperse and polydisperse)
  - Proposed methodologies for large-area template and machine-level models.

Focus on emboss/imprint and release
  - Prototype multilayered prototype material (embossed and coat-ed?). What defects dominate in pushing to larger throughput?
- FY10/FY11:
  - Completion of feature and multi-feature cabilities and models (including validation)
  - Prototype upscale models for fluid and solid-phase based top-down. (effective medium)
  - Validation with experimental effort



Vision and Motivation — Multiscale From Feature to Machine

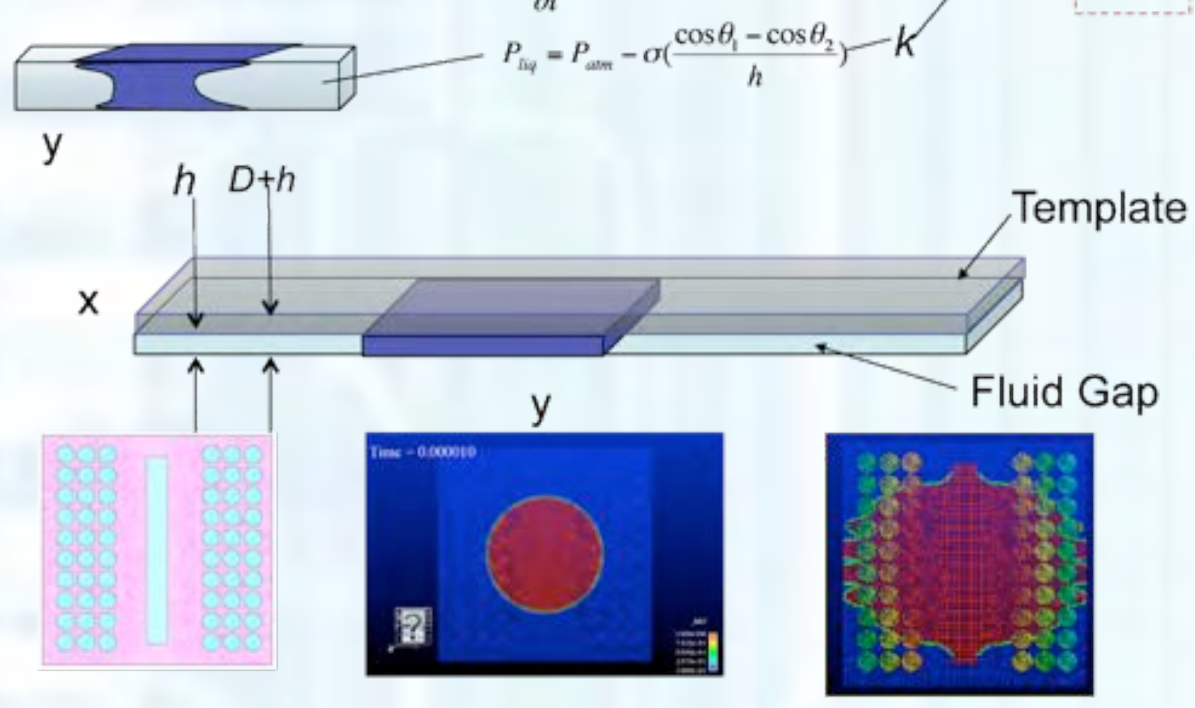


Results

Sample Results: Large Area Analysis using Lubrication

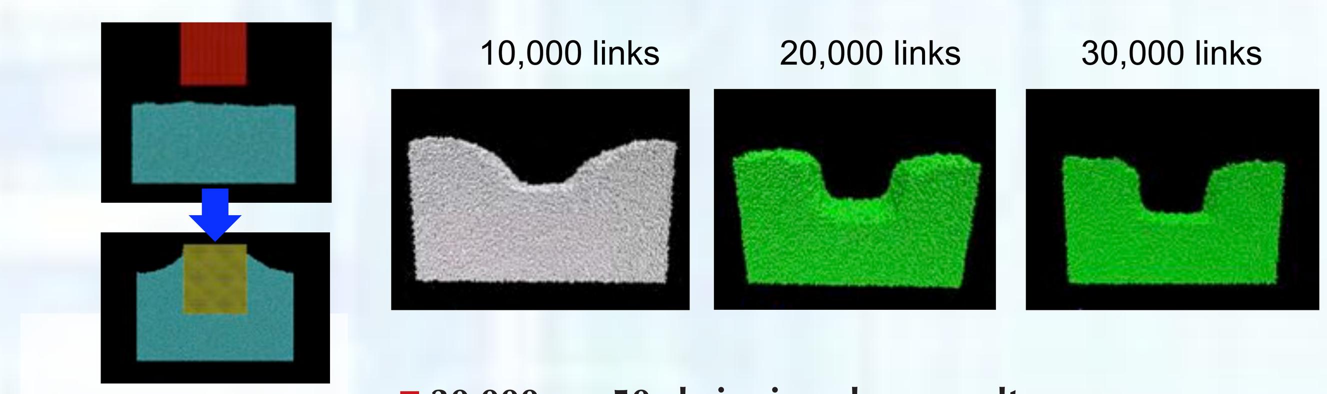
$$\nabla\{[D(x,y,t)+h(x,y)]^3\nabla P\} = -12\mu(\phi)\frac{\partial D}{\partial t} + \nabla\cdot[(D(x,y,t)+h(x,y))^3\sigma k n\delta(\phi)] - \rho v_{porous}$$

$$P_{liq} = P_{atm} - \sigma\left(\frac{\cos\theta_1 - \cos\theta_2}{h}\right) \quad k$$



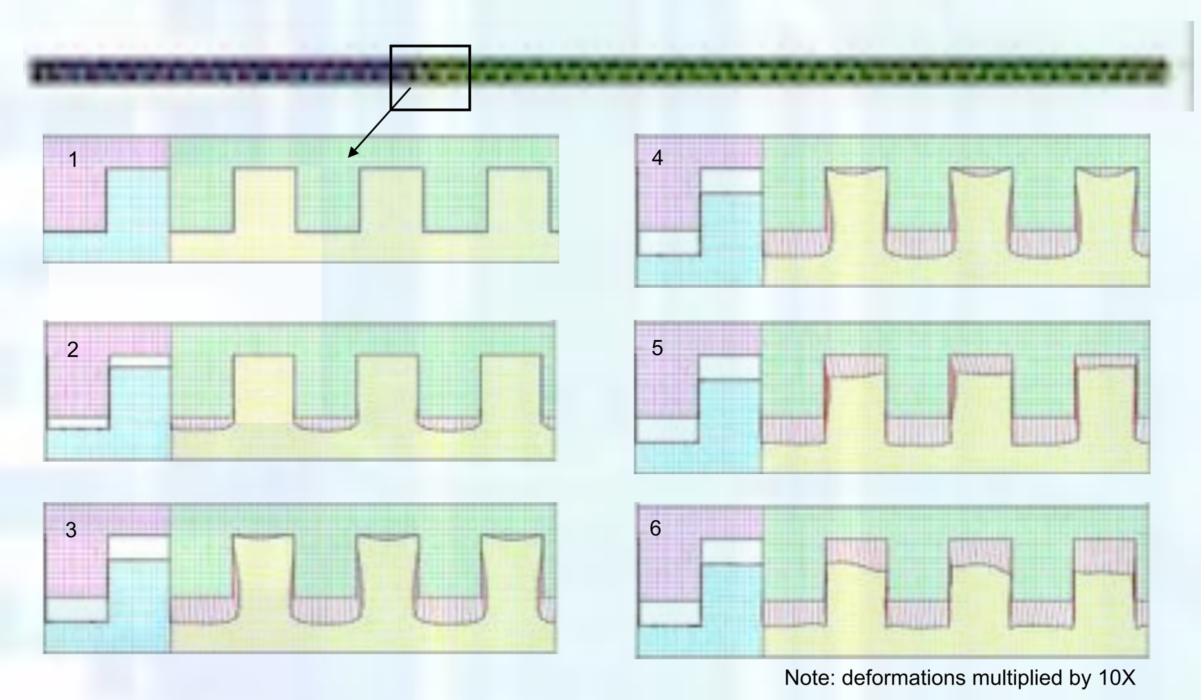
Atomistic Simulations of Release after Crosslinking:

Goal to produce Effective Toughness model



- 30,000 n = 50 chains in polymer melt
  - Low viscosity
  - unentangled
- too many crosslinks necessary!

Sample Results: FEM Model Nano-Fabrication Release Step



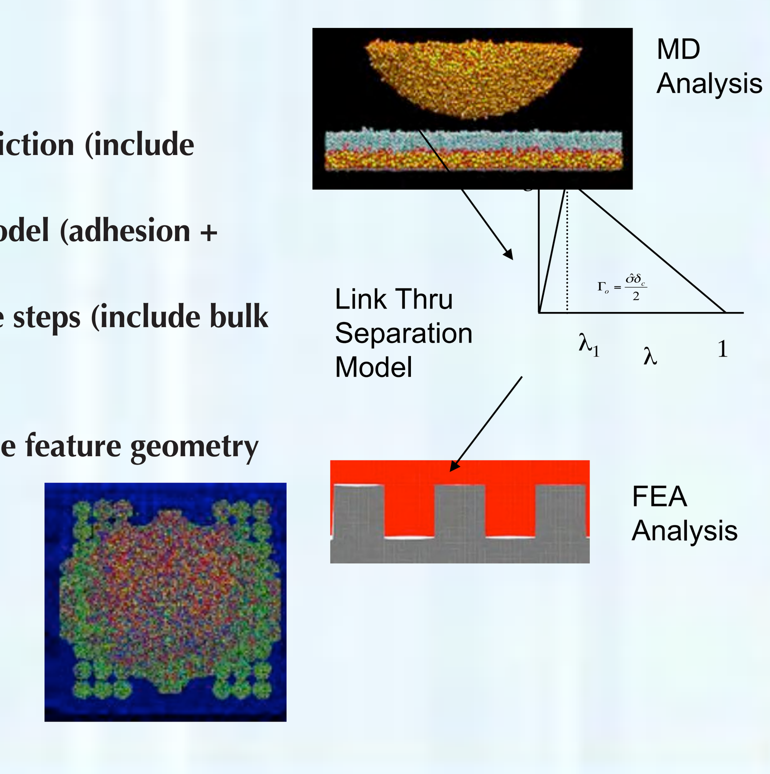
Rigid mold and substrate, elastic polymer layer (E= 3 GPa, ν = 0.4)
Interfacial toughness Γ = 0.05 J/m^2

Significance

Ongoing Work

Solid Phase

1) Use MD to determine atomistics of adhesion and friction (include coatings)
2) Link to FEA with an effective traction-separation model (adhesion + atomistic friction)
3) Use FE to calculate macroscale molding and release steps (include bulk yield and failure)
4) Validate FE results with large-scale MD simulations
5) Define an effective toughness that reflects nanoscale feature geometry and properties



Liquid Phase

1) Upscaling with effective medium approach
2) Structural shell for template
3) Porous shell for fluid gap and features

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2009-5135P