SAND2007-0351P

Elucidating the Mysteries of Wetting

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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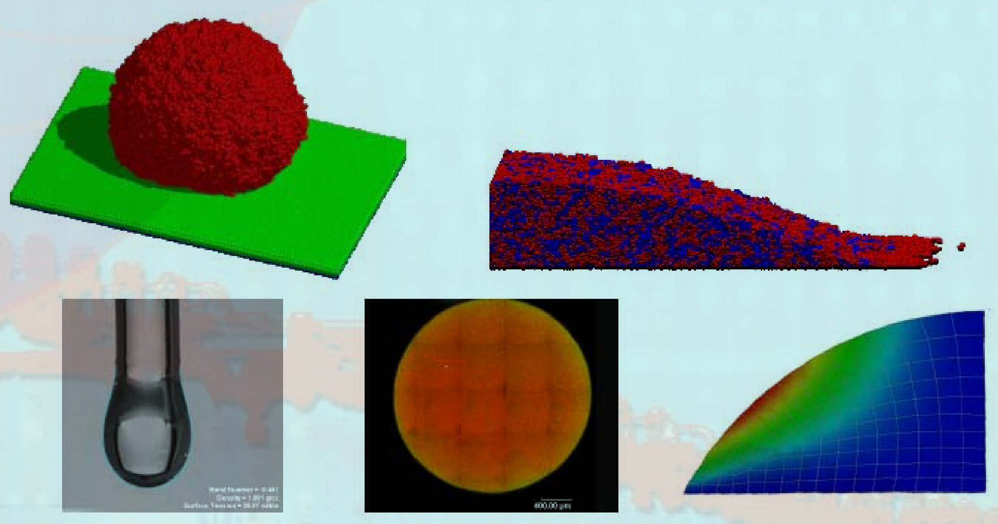
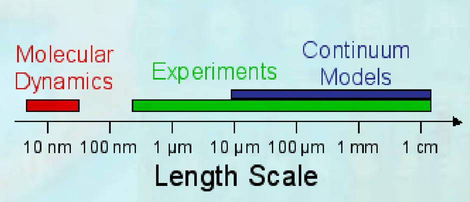


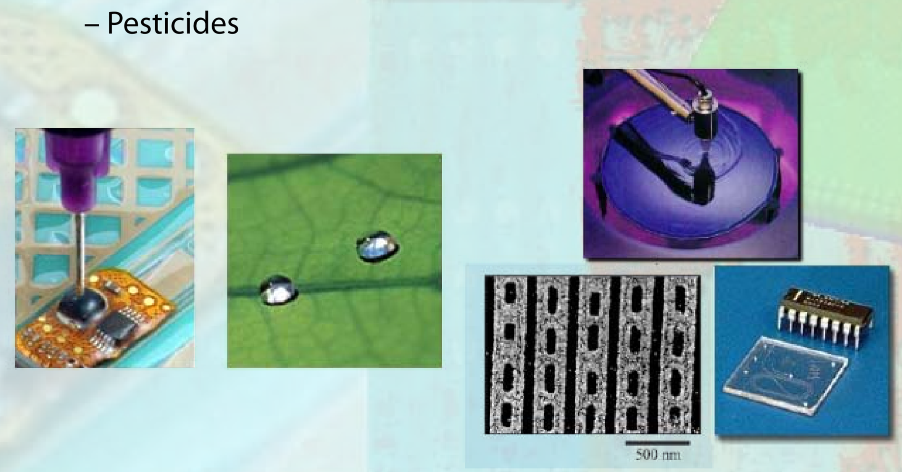
Problem/Approach

- Establish a multi-scale competence for characterizing and predicting wetting behavior of blends by combining atomistic and continuum level modeling with experiment
- Science-based engineering of manufacturing processes dominated by capillary hydrodynamics
  - Devise pertinent experimental diagnostics to characterize wetting dynamics and real-time composition variation
  - Develop atomistic molecular simulation capability to study interfacial wetting properties of multi-component blends
  - Investigate dynamic wetting models and validate for drop spreading
  - Advance micro-systems development by providing new theoretical and computational tools for modeling multi-phase micro-flows



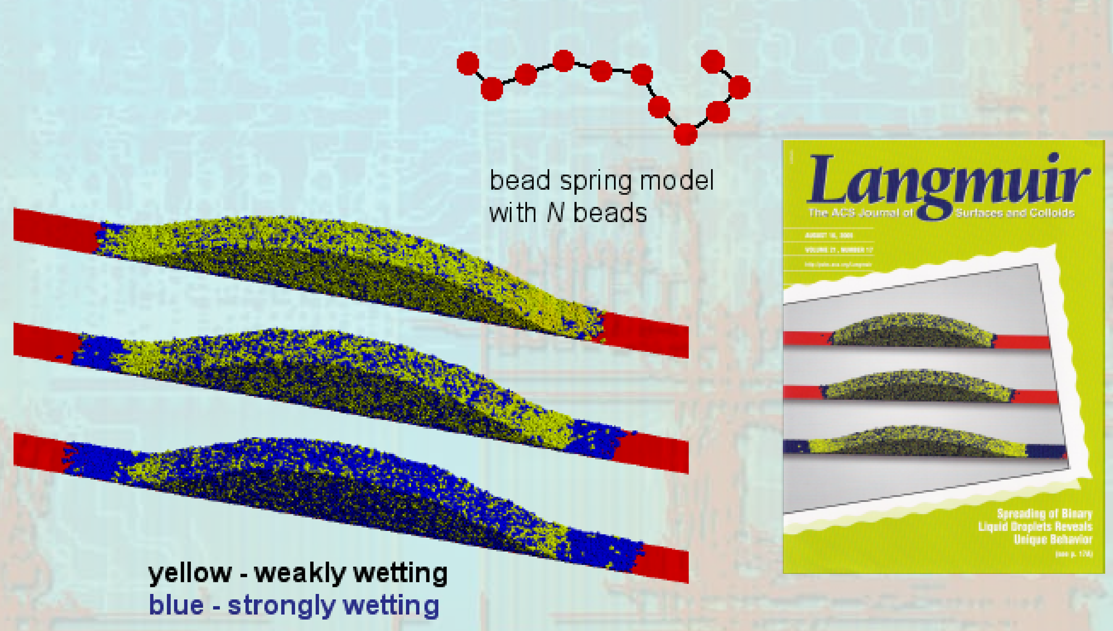
Applications

- Classical
  - Adhesion
  - Encapsulants
  - Lubrication
  - Pesticides
- Modern
  - Photolithograpghy
  - Microcontact printing
  - Microfluidics



Molecular Dynamics Simulations of Wetting

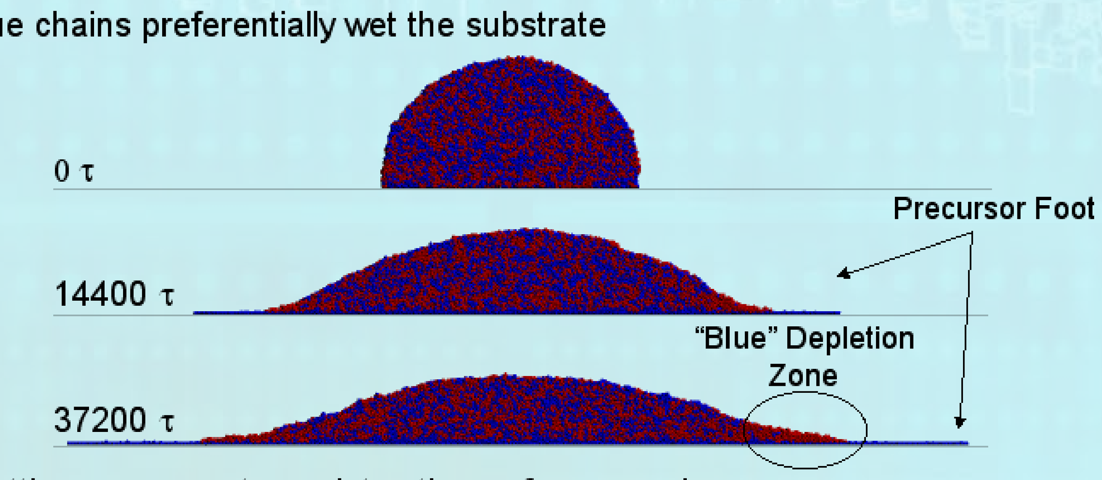
- Simulations of spreading polymer drops
- Extract physical parameters for continuum models
  - surface tension, viscosity, diffusivity
- Mixture of wetting molecules (vary concentration of more strongly wetting component)



Wetting Segregation

$N_{red} = 10$, $N_{blue} = 10$ (equal concentration)

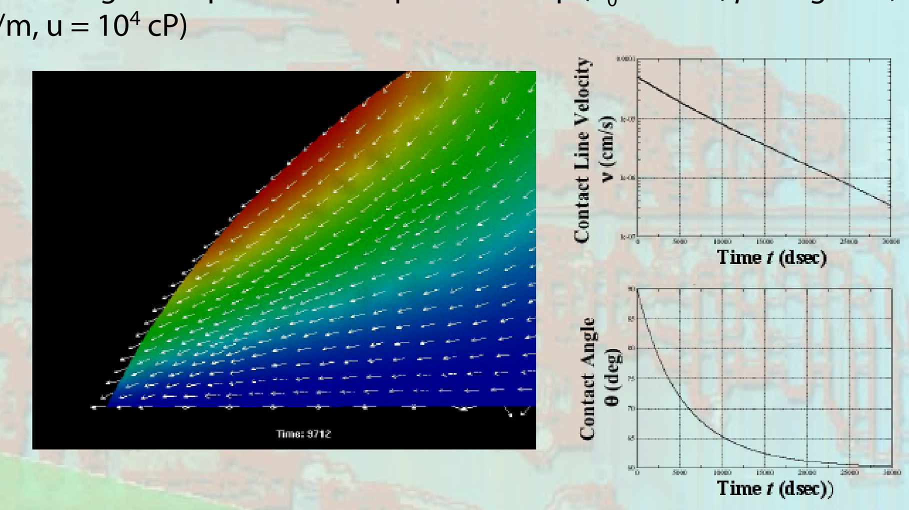
Blue chains preferentially wet the substrate



Wetting component populates the surface monolayer
Depletion zone forms at the edge of the drop

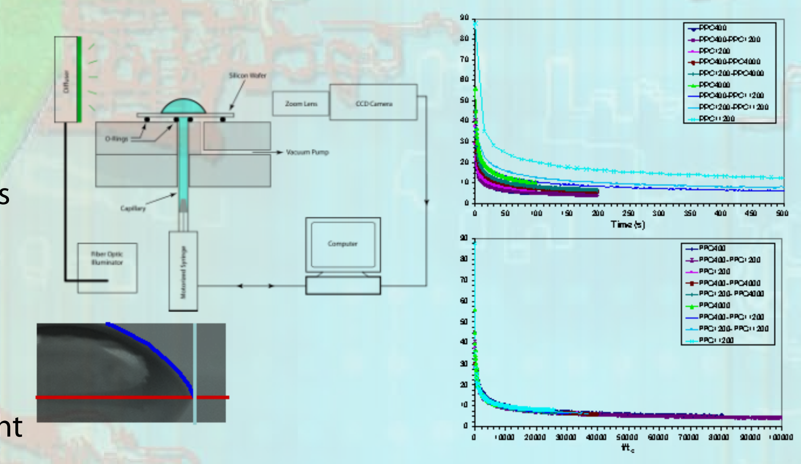
Continuum Simulations of Wetting

- Simultaneously solve fully coupled problem for flow and drop shape
- Starting from a single component hemispherical drop (R_0 = 1mm, p = 1 g/cm^3, y = 40 mN/m, u = 10^4 cP)

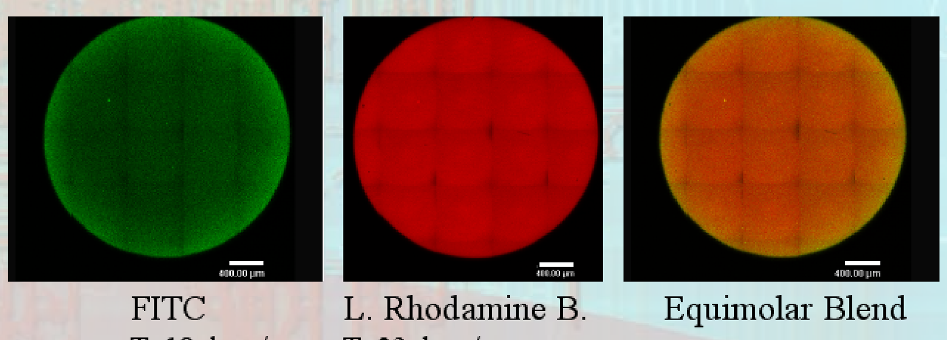


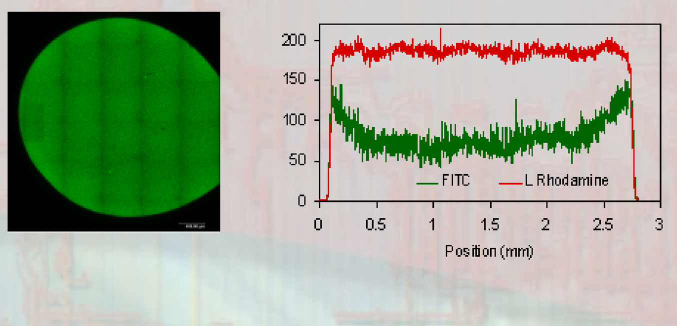
Wetting Experiments

- Feed Through Goniometer:
  - enables experimental analysis of dynamic wetting behavior of viscous multi-component liquids
- Correct time-viscosity scaling collapses dynamic wetting response of pure polymers and polymer blends over two orders of magnitude in molecular weight



Confocal Microscopy - Segregation of a Multi-Component Drop





Summary

- Several experimental methods have been developed to characterize wetting properties of blends, including Wilhelmy fiber tensiometry and the feed through goniometer
  - Wetting dynamics of pure polymers and blends analyzed to produce time-viscosity scaling rules for blends
- Fluorescence microscopy demonstrated be a powerful tool to investigate concentration segregation during spreading
- Large scale molecular dynamics simulations have been performed on single polymers and binary blends
  - Spreading of single component drops was found to obey molecular kinetic, dynamic wetting model
  - Wetting induced concentration segregation in binary systems driven by differences in the surface interaction potential whereas surface tension differences caused equilibrium segregation at the liquid/vapor interface
- Continuum finite element modeling of a pure drop demonstrates enhanced velocities in surface flow near the 3-phase contact line

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