Discovery at the Interface of Science and Engineering: **Science Matters!**

Materials Science and Technology
Wetting

Snapshots at two different times from simulations of binary component polymer nano-droplets. The wetting constituent (blue) forms a monolayer on the surface (red) and spreads outward. Subsequently, the non-wetting constituent (yellow) spreads on top of the wetting monolayer.

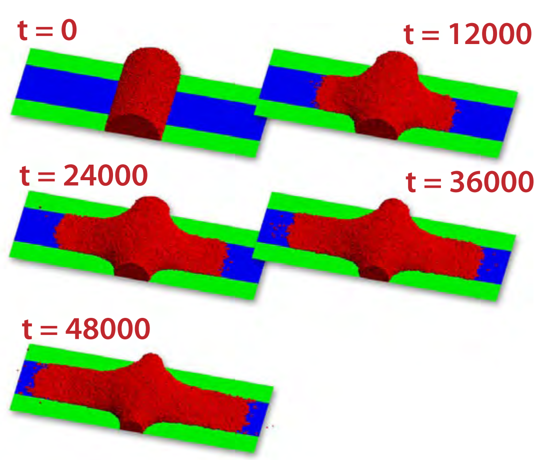
Modeling and simulation takes coating technology to the next level

The challenge becomes greater as we advance engineered devices into ever diminishing length scales.

Ensuring that a substrate material is evenly and securely coated, or wetted, by a wetting agent has long been the challenge in coating technology. Failure to develop a complete wetting of a substrate often leads to coating failure. For epoxy systems, for instance, this can lead to sealant failure and, in turn, device failure if the coating is not uniformly distributed on the surfaces to be joined. The challenge becomes greater as we advance engineered devices into ever diminishing length scales.

Understanding coating failure requires molecular level descriptions of the coating constituents as well as the coating/solid interface—a level of resolution unattainable by existing experimental techniques. Molecular scale simulations have been used to study wetting phenomena, but until recently computational resources did not exist to study chemically realistic coating materials. Sandia National Laboratories researchers, using Sandia's Institutional Computational Clusters (high performance, large-scale, parallel processing computers), have developed numerical simulations of multi-component polymer nano-droplets being applied to substrates. Simulations were performed of binary component droplets and conditions were revealed under which a non-wetting coating constituent was made to wet the substrate by carefully controlling the interaction between coating constituents. With sufficient interaction strength between the polymer components, the non-wetting substance spread on top of a molecular layer of the wetting substance. Such work revealed previously unavailable molecular scale information about phenomena controlling wetting (coating) behavior.

The model can address constituents of arbitrary molecular structure and interaction strength, permitting broad applicability across coating engineering science. In addition, complexities such as introducing a chemical pattern on the substrate surface have been studied. Results are helping coatings scientists to develop stable multi-component wetting formulations that allow the use of required wetting agents even when those substances would not otherwise coat the substrate.



Snapshots from simulations of a polymer nano-droplet (red) spreading on a chemically patterned surface. The pattern consists of parallel strips of alternating wetting (blue) and non-wetting (green) regions. The droplet spreads on the wetting strip by removing material from on top of the non-wetting region. Understanding wetting on complex patterns will guide the way to engineering material delivery to specified device areas.

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NNSA National Nuclear Security Administration

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G.S. Grest, D.R. Heine, E.B. Webb III, "Liquid Nanodroplets Spreading on Chemically Patterned Surfaces," *Langmuir*; May 9, 2006; **v.22, no.10**, p.4745-4749

D.R. Heine, G.S. Grest, E.B. Webb III, "Surface Wetting of Liquid Nanodroplets: Droplet-size Effects," *Physical Review Letters;* September 2, 2005; **vol.95, no.10**, p.107801/1-4

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D.R. Heine, G.S. Grest, E.B. Webb III, "Spreading Dynamics of Polymer Nanodroplets In Cylindrical Geometries," *Physical Review E* (Statistical, Nonlinear, and Soft Matter Physics); July 2004; **vol.70, no.1**, p.11606-1-10

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E.B. Webb III, G.S. Grest, D.R. Heine, J.J. Hoyt, "Dissolutive Wetting of Ag on Cu: A Molecular Dynamics Simulation Study," *Acta Materialia*; June 2005; **vol.53, no.11**, p.3163-77

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