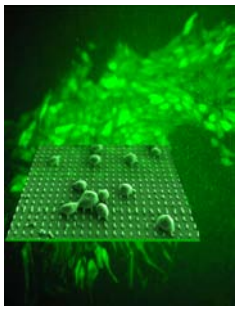
CNMS DISCOVERY SEMINAR SERIES

Thursday, February 17, 2011
2:00 pm
Iran Thomas Auditorium, 8600

Field-Based Simulations for the Design of Polymer Nanostructures



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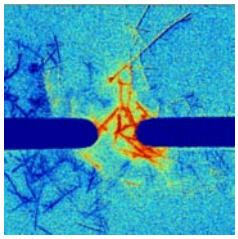
Abstract:

Plastic materials and solution-borne polymer formulations prove challenging to design because they often contain many components and can exhibit self-assembly and phase behavior of daunting complexity. I will describe a suite of new modeling tools that is well suited to this class of soft material design problems. Rather than applying conventional computer simulation techniques to "particle-based" models of polymeric fluids, we have developed "field-theoretic computer simulation" schemes for numerically sampling functional integrals comprising statistical field-theory models of complex fluid systems. Such simulation methods are particularly advantaged for studying dense polymer systems of high molecular weight. I will discuss applications to nanostructured block copolymers as advanced elastomers, thin copolymer films for patterning microelectronic devices, and polyelectrolyte-based coatings and adhesives.



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Center for Nanophase Materials Sciences