Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Predicting Themomechanical Responses of Polymer Thin Films and Nanocomposites via an Innovative Coarse-grained Approach WENJIE XIA, DAVID HSU, SINAN KETEN, Northwestern University — Understanding and predicting the thermomechanical responses of nanoscale polymer systems are very challenging as their responses are greatly influenced by many factors, such as interfacial energy, filler volume fraction and molecule weight, giving rise to the presence of nanoscale interface and free surface. To overcome these issues, here we employ a novel atomistically informed coarse-grained computational technique, called thermomechanically consistent coarse graining (TCCG), to investigate how the nanoscale interface and free surface influence the elastic modulus (E) and glass transition temperature (Tg) of polymer films and nanocomposites. By performing tensile tests and nanoindentation simulations, we are able to predict the size dependent elastic properties of polymer films and quantify the length scale of the local mechanical interphase. Finally, taking cellulose nanocrystal (CNC) and poly(methylmethacrylate) (PMMA) nanocomposites as a relevant model system, we present a multi-scale framework built upon our CG approach to allow the prediction of Tg of nanocomposite as a function of interfacial energy and filler volume fractions by drawing the analogy between thin film and nanocomposites. Our established multi-scale framework is validated by recent experiments and breaks new ground in predicting, without any empirical parameters, key structure-property relationships for polymer nanomaterials.

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Date submitted: 04 Nov 2015 Electronic form version 1.4