

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Multiscale Modeling of Deformation of Glassy Polymers THOMAS ROSCH, JOHN BRENNAN, SERGEI IZVEKOV, JAN ANDZELM, Army Research Lab — We examine the ability of chemically informed coarse-grained (CG) models to quantitatively describe correct mechanical properties of glassy polymer systems. The force-matching and the structure-matching procedures were used to obtain CG potentials at different levels of resolution. Equilibrium molecular dynamics simulations of amorphous polymers modeled at the all-atom level provided the necessary reference data. This work explores what characteristics are necessary for quantitative agreement of stress-strain curves between scales. For large coarse-graining (17 atoms per CG site of polystyrene) the force-matching procedure produces a potential that does not contain enough attraction to predict the correct elastic properties. Systematic methods were employed to match mechanical properties and their effects on polymer structure were examined. Higher resolution coarse-graining (5-11 atoms per CG site) is better able to reproduce atomistic mechanical data.

Thomas Rosch
Army Research Lab

Date submitted: 15 Nov 2012

Electronic form version 1.4