Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Using Mesoscopic Models to Design Strong and Tough Biomimetic Polymer ISAAC G. SALIB, University of Pittsburgh, Pittsburgh, PA 15261, USA , GERMAN V. KOLMAKOV, New York City College of Technology, CUNY, New York, NY 11201, USA, BENJAMIN J. BUCIOR, University of Pittsburgh, Pittsburgh, PA 15261, USA, ORIT PELEG, MARTIN KROGER, THIERRY SAVIN, VIOLA VOGEL, ETH Zurich, CH-8093 Zurich, Switzerland, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon University, Pittsburgh, PA 15213, USA, ANNA C. BALAZS , University of Pittsburgh, Pittsburgh, PA 15261, USA — Using computational modeling, we investigate the mechanical properties of polymeric materials composed of coiled chains, or globules, which encompass a folded secondary structure and are crosslinked by labile bonds to form a network. In the presence of an applied force, the globules can unfold into linear. Our goal is to determine how to tailor the labile intra- and inter-molecular bonds within the network to produce material exhibiting both toughness and strength. We use the lattice spring model (LSM) to simulate the globules and the crosslinked network. We utilize our modified Hierarchical Bell model (MHBM) to simulate the rupture and reforming of N parallel bonds. We demonstrate that the mechanical properties of the system are sensitive to the values of N_{in} and N_{out}, the respective values of N for the intra- and inter-molecular bonds. We find that the strength of the material is mainly controlled by the value of N_{out}, with the higher value of N_{out} providing a stronger material. We also find that if N_{in} is smaller than N_{out}, the globules can unfold under the tensile load before the sample fractures and thus, can increase the ductility of the sample.

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Date submitted: 09 Nov 2011 Electronic form version 1.4