Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Multiscale Modeling of Biomimetic Self-Healing Materials GERMAN KOLMAKOV, AMY SCARBROUGH, CHET GNEGY, ISAAC SALIB, Chemical Engineering Department, University of Pittsburgh, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, ANNA BALAZS, Chemical Engineering Department, University of Pittsburgh — We use a hybrid computational approach to examine the self-healing behavior of polymeric materials composed of soft nanogel particles crosslinked by a network of both stable and labile bonds. The latter are highly reactive and therefore, can break and readily reform. To capture the multiscale structure of the material, we take advantage of the multi-level Hierarchical Bell Model (mHBM) where the labile crosslinks are organized into M levels of interconnected elements, each of them represents a number of bonds that lie in parallel and is described by a single-level HBM. We vary the number of hierarchical levels M and the number of labile bonds in each element to determine optimal conditions for improving strength and toughness of the material. We also compare the properties of the multiscale material with those for the gel, in which only single-level interconnections are presented. This study takes its inspiration from biological systems that show remarkable resilience in response to mechanical deformation.

German Kolmakov
Chemical Engineering Department, University of Pittsburgh

Date submitted: 19 Nov 2010 Electronic form version 1.4