Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Simulating the Oxidation of Polypropylene Using a Reactive Forcefield[1] JOANNE BUDZIEN, AIDAN THOMPSON, Sandia National Laboratories — Oxidation of organic materials is a problem for seals and membranes in many environments. Any particular instance of a chemical reaction is fast with purely local effects. Over longer times, the cumulative effect of many reactions results in large changes in average stress, strain, and other macroscopic properties of the sample. We have had some success in developing constitutive models for rubber, which connect the topology of the network with the observed stress during aging under strain. As the next phase of the project, we have performed simulations using a reactive forcefield to examine the atomistic changes during oxidation. Results will be presented for polypropylene and compared with experimental data for labeled samples undergoing oxidation.

[1]Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Joanne Budzien
Sandia National Laboratories

Date submitted: 13 Nov 2006 Electronic form version 1.4