Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

All-atom molecular dynamics simulations of amorphous, crosslinked PDMS PHILIP T. SHEMELLA, TEODORO LAINO, IBM Research - Zurich, OLIVER FRITZ, ABB Corporate Research - Switzerland, ALESSANDRO CURIONI, IBM Research - Zurich — The structure, dynamics, and self-diffusion properties of an amorphous, binary mixture of large poly(dimethylsiloxane) (PDMS) and small poly(hydromethylsiloxane) (PHMS) are characterized with atomic-level molecular dynamics simulations. Molar masses and mixing properties are comparable and relevant to commerical products, and simulations require massively parallel molecular dynamics simulations. The system consists of 100 vinyl-terminated PDMS molecules (∼72,500 g/mol) and 200 crosslinker PHMS molecules (∼1960 g/mol), for a total of more than 1 million atoms. Molecular diffusion is studied as a function of temperature, electric field, and end-crosslinking density. Simulation results provide an atomic-level description for molecular motion and an understanding of the local structure that contributes to molecular self-diffusion.

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Date submitted: 06 Jan 2010 Electronic form version 1.4