Molecular Interactions of Polydimethylsiloxane and Ni-Mn-Ga

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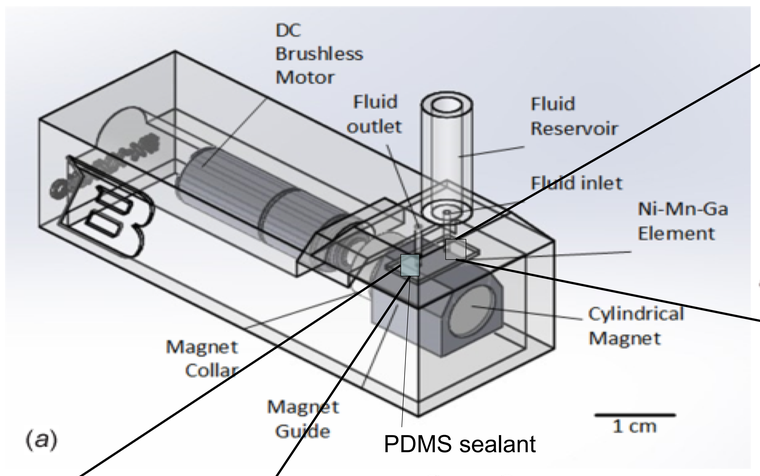
I. Introduction

- Ni-Mn-Ga can deform in the presence of a magnetic field, and still return to its original state
- Due to its deformation properties Ni-Mn-Ga has been used to make micropumps here at Boise State University
- Since the Ni-Mn-Ga plays all the roles needed for the micropump to function, typical O-rings can't be used to provide a seal to maintain proper pressure
- Polydimethylsiloxane (PDMS), has been found to be a good sealant solution
- Understanding how the polymer/metal interface sticks and delaminates is central for engineering better pumps. We use simulations here to improve this understanding

Figure 1. Ni-Mn-Ga Micropump showing MSMA element and PDMS sealant placement



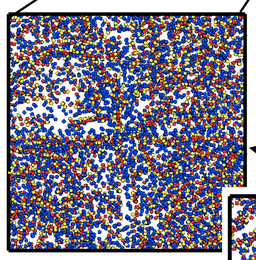


Figure 3. Volume of 80 20-mer chains of PDMS in its initial time step (top). Same volume in its final time step (right) at a temperature of 294.7 K (~21.7 Celsius. Total number of atoms: 7120)

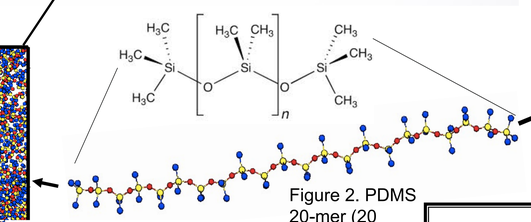


Figure 2. PDMS 20-mer (20 repeating cell) chain, and its formula[2]. The longer chain configuration provides a more rigid PDMS

II. Methods

- Parameters and potentials for interatomic interactions were taken from previous simulations of PDMS[1,3], and from the Universal Force Field for the Ni-Mn-Ga[4]
- PDMS chains of 20 repeat units are constructed, and volumes with 80 or 100 chains are initialized. Ni-Mn-Ga is constructed using its unit cell (Figure 5) and replicating the unit cell 20x20x1
- Simulations of the materials required the use of the National Center for Supercomputing Applications' Blue Waters supercomputer
- HOOMD-blue, a molecular simulation toolkit, was utilized to equilibrate the materials as well as to observe their interactions
- The volume of PDMS was simulated at 294.7 K, 884.15 K, and 1768.2 K
- The interaction of the PDMS & MSM has been simulated at 294K and 500K

Figure 4. 20 x 20 x 1 Ni-Mn-Ga surface

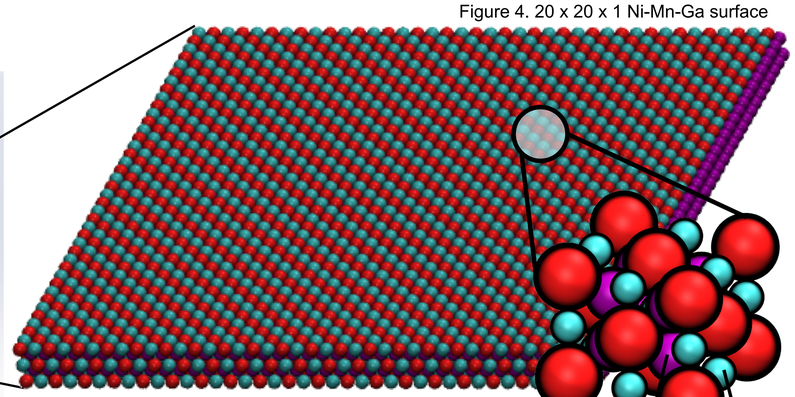


Figure 5. Ni-Mn-Ga Unit Cell

Bond	Length (Å)
	1.647
	1.866
Angle	**θ (degrees)**
	146.9
	119.0
	105.7
	107.5
Dihedrals	**θ (degrees)**
	-114.9
	123.4

Non-bonded	σ	ε
CH3	3.786	0.7532
Si	3.385	2.4480
O	0.8493	2.955

Table 1. Potentials for PDMS used in simulations

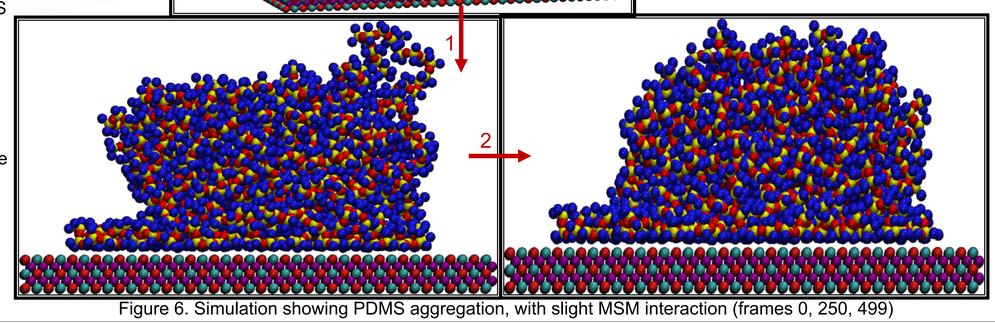


Figure 6. Simulation showing PDMS aggregation, with slight MSM interaction (frames 0, 250, 499)

III. Results

- We observe PDMS chains to self-aggregate at room temperature prior to binding to the Ni-Mn-Ga
- By examining the outputs, and graphs (Figure 7. A & B), there is an initial peak (not shown) that indicates a drastic increase in energy, which comes from needing an initial surge of energy to get the particles in motion
- Temperature profiles (Figure 7. C & D) show interface stabilization
- Efficiency of the system is ~3500 TPS (time-steps per second) which equilibrates in 45 minutes of run-time
- PDMS seems to aggregate first above the surface, then binds quickly to the surface

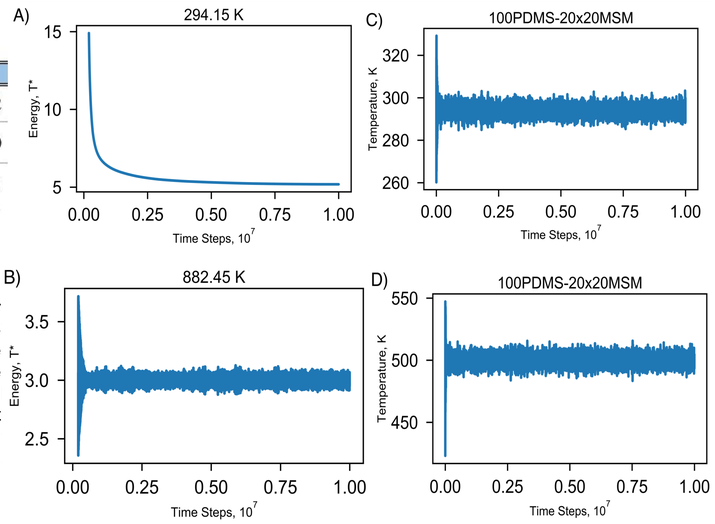


Figure 7. Difference in potential energy stabilization in PDMS based on temperature (A & B). Temperature profiles of PDMS-MSM interface (C & D) at different simulation temperatures.

IV. Conclusions and Follow-ups

- Stable energy in the system points towards a stable simulation system that can continue to be expanded
- PDMS if far enough away tends to keep to itself in the simulations, and sticks to surface otherwise
- Using GPUs in parallel cuts down the time needed to process large volumes of data that would otherwise be prohibitive if limited to CPU processing
- Incrementing chain counts, may help PDMS to not clump together in the simulation
- The individual materials can be used in conjunction with Rhaco on different clusters to investigate polymer-surface interactions in more depth

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Sources: 1. Frischknecht, A. L., & Curro, J. G. (2003). Improved United Atom Force Field for Poly(dimethylsiloxane). *Macromolecules, 36*(6), 2122-2129.
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