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.

II. Methods
- Parameters and potentials for interatomic interactions were taken from previous simulations of PDMS\textsuperscript{1,2}, and from the Universal Force Field for the Ni-Mn-Ga\textsuperscript{3}.
- 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.

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.
- Temporal 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.

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.
- Increasing 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.

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

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

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

Figure 5. Ni-Mn-Ga Unit Cell

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

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

Table 1. Potentials for PDMS used in simulations

<table>
<thead>
<tr>
<th>Potential</th>
<th>Energy (kJ/mol)</th>
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<tbody>
<tr>
<td>C-E</td>
<td>3.786</td>
</tr>
<tr>
<td>Si</td>
<td>3.383</td>
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<tr>
<td>O</td>
<td>0.8493</td>
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