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Molecular Interactions of Polydimethylsiloxane and Ni-Mn-Ga

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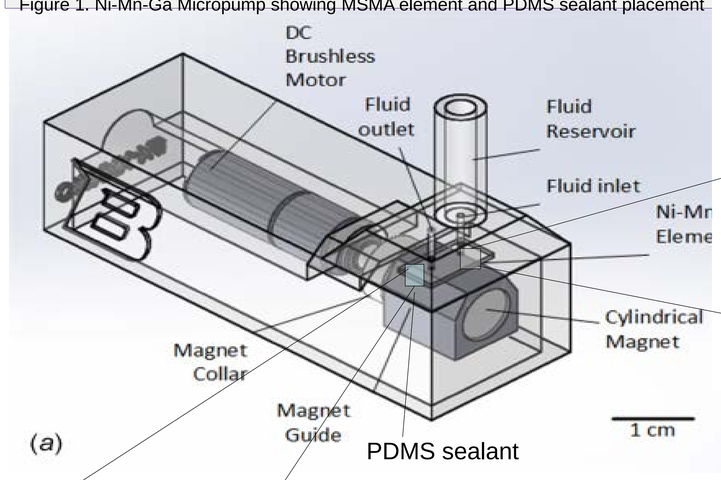
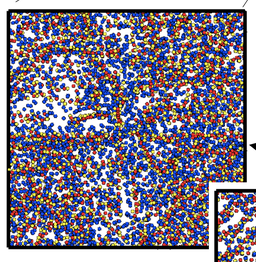
I. Introduction

- 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





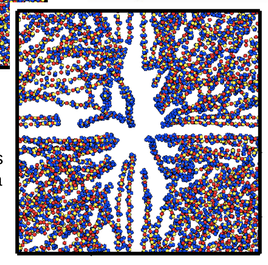


Figure 3. Volume of 80 20-mer chains of PDMS in its initial time step (top). Same volume in its final time step (right) at a temperature of 294.7 K (~21.7 Celsius. Total number of atoms: 7120)

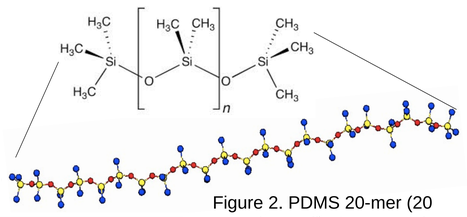


Figure 2. PDMS 20-mer (20 repeating cell) chain, and its formula[2]. The longer chain configuration provides a more rigid PDMS

II. Methods

- Parameters and potentials for interatomic interactions were taken from previous simulations of PDMS[2], and from other lists of potentials
- PDMS was constructed to be of chains twenty repeating cells long (i.e. a 20-mer), with the main volume being comprised of these chains being replicated 80 times
- Ni-Mn-Ga was constructed using its Martensitic unit cell (Figure 5) and replicating the unit cell ten times in both X and Y, with a height, Z, of 5 Angstroms
- 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
- All scripts were written by Jaime Guevara

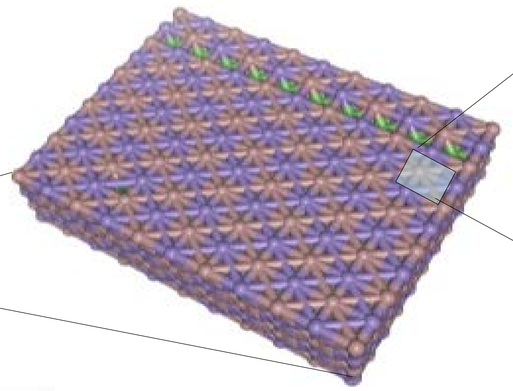


Figure 4. Crystal slab of Ni-Mn-Ga

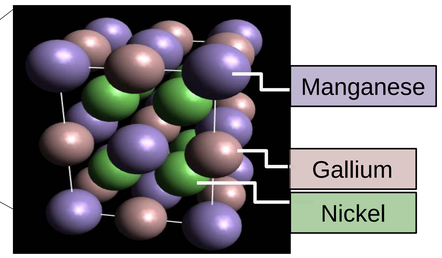


Figure 5. Unit cell of Ni-Mn-Ga

Bond	Length (Å)
O–Si	1.647
CH3–Si	1.866
Angle	**θ (Degrees)**
Si–O–Si	146.9
Si(O)(O)	119.0
Si(CH3)(CH3)	105.7
Si(O)(CH3)	107.5

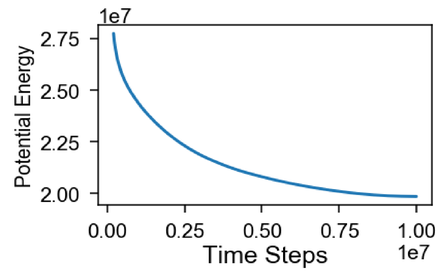
Dihedrals	Degrees
Si–O–O–Si	-114.9
Si–O–Si–CH3	123.4

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

Table 1: Potentials for PDMS bonds, angles, dihedrals, and atom pairs used in simulations

III. Results

- The PDMS particles at room temperature seem to attract each other to contract into a tighter version of our unit
  - Makes sense that a hardening gel would contract
- By examining the outputs, and graphs (Figure 6), there is an initial peak (not shown) that indicates a drastic increase in energy, which comes from needing an initial surge of energy
- The volume of PDMS was simulated at 294.7 K, 884.15 K, and 1768.2 K
- Next steps will be to run the PDMS side-by-side with the alloy
- Efficiency of the system is ~3500 TPS (time-steps per second) which equilibrates in 45 minutes of run-time



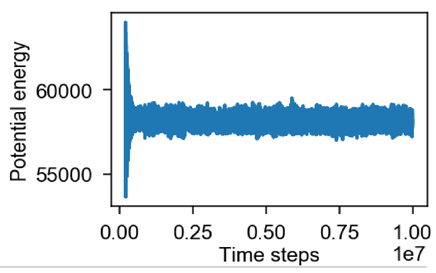


Figure 6. Difference in potential energy stabilization in PDMS based on temperature: 294.7K (top), 884.15K (bottom). Time step Range: 2000 – 1e7

IV. Conclusions and Follow-ups

- So far the PDMS stabilized energy shows that our use of the HOOMD toolkit and the Blue Waters system can represent the materials for understanding pump/seal interfaces
- Ni-Mn-Ga surfaces simulated in contact with the PDMS is the next step to calculating binding energies
- 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

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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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