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Molecular Interactions of Polydimethylsiloxane and Ni-Mn-Ga

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Abstract

With the recent advent of magnetic shape memory alloys (MSMA), such as martensitic Ni-Mn-Ga, researchers focused studies about these materials on properties such as magnetic-field-induced deformation. Currently, some of the properties of interest include, but are not limited to: twin boundary deformation, strain, stress, magnetic and thermal activation, operating temperatures, magnetic permeability, and electric resistivity. Given some of these properties, materials such as Ni-Mn-Ga have been used as actuators, channels, and membranes in pumps. While these pumps are currently at the stage of sub-microliter medical application, they have also been shown to possess great accuracy in delivery as well as strength in pumping against relatively high back pressures. In this system, given the small size of the pump, a typical O-ring cannot provide the same effective seal as it would in a regular impeller pump. However, using a Polydimethylsiloxane (PDMS) gel has proven to be a useful sealant for these MSMA pumps. The interaction of the sealant against the Ni-Mn-Ga itself, in particular adhesion and detachment, take on a critical role in the pumping process. That is to say that as the "channel", created by the twin boundary shift, moves, the PDMS must adhere to the alloy up to a specific limit and then detach. This adhesion-detachment must be controlled and repeatable. This simulation study aims to quantify the interaction of PDMS and Ni-Mn-Ga, as it pertains to the adhesivity of the former to the latter, in order to better determine how best to cure PDMS for optimal adhesion and separation. In order to study these PDMS-MSMA surfaces, GPUs in the XK nodes of the Blue Waters Supercomputer, at the University of Illinois, Urbana-Champaign, were used in conjunction with the HOOMD-blue particle simulation kit to render them and study the molecular dynamics between these two materials. The PDMS models for this simulation were based on a united atom (UA), Lennard-Jones potential modified from previous studies[(1)] , utilizing 20-mer chains. While the Ni-Mn-Ga surface was based on an M1 matrix developed at Boise State. The MSMA surface his modeled as a rigid lattice structure without twin boundary movement, the motion is instead replaced by simulating a pulling force on the PDMS surface up to where it detaches from the MSM surface. By utilizing these constraints we can begin to study the effects that the curing time of PDMS has on this interaction with Ni-Mn-Ga, how the MSMA's lattice structure reacts in this scenario, and how best to continue incorporating further constraints into these simulation studies, such as simulated twin boundary movement.

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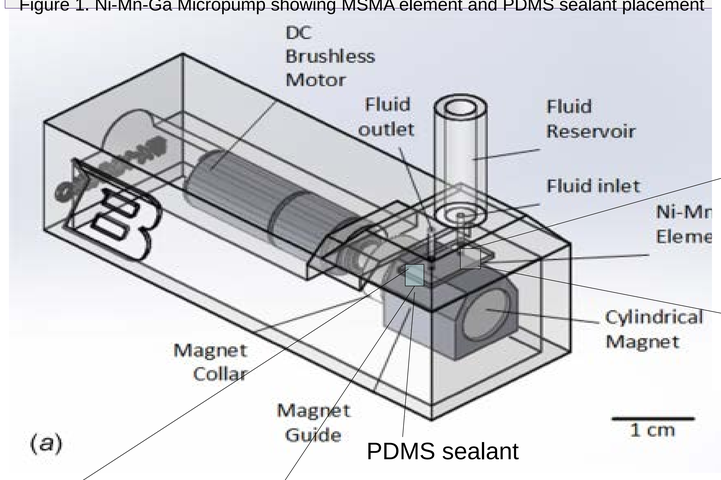
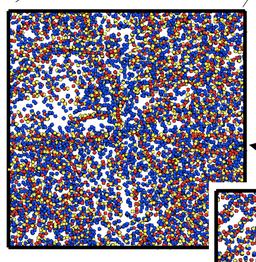
I. Introduction

- 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





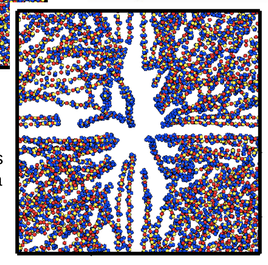


Figure 3. Volume of 80 20-mer chains of PDMS in its initial time step (top). Same volume in its final time step (right) at a temperature of 294.7 K (~21.7 Celsius. Total number of atoms: 7120)

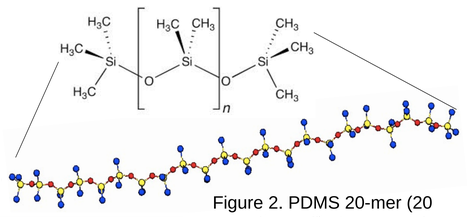


Figure 2. PDMS 20-mer (20 repeating cell) chain, and its formula[2]. The longer chain configuration provides a more rigid PDMS

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

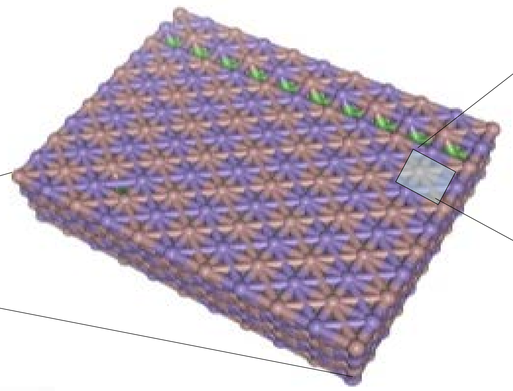


Figure 4. Crystal slab of Ni-Mn-Ga

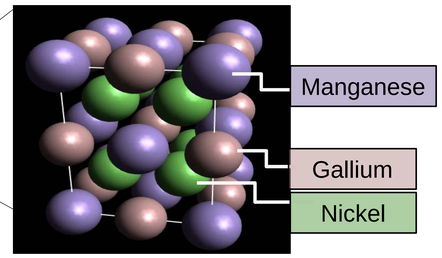


Figure 5. Unit cell of Ni-Mn-Ga

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

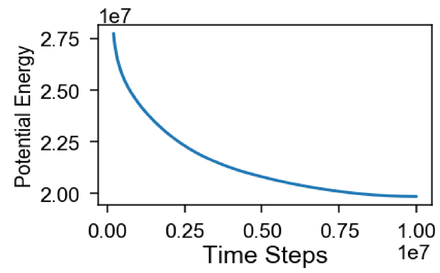
Dihedrals	Degrees
Si–O–O–Si	-114.9
Si–O–Si–CH3	123.4

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



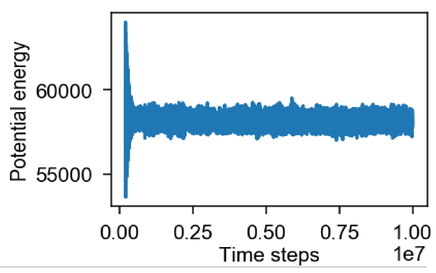


Figure 6. Difference in potential energy stabilization in PDMS based on temperature: 294.7K (top), 884.15K (bottom). Time step Range: 2000 – 1e7

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.
2. **Pdms: A Review.** https://www.elveflow.com/microfluidic-tutorials/microfluidic-reviews-and-tutorials/the-poly-di-methyl-siloxane-pdms-and-microfluidics/
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