Molecular Dynamics Simulations Require Sophisticated Software - Molecular Dynamics Studio is Delivering

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NanoEngineer-1[2]

- NanoEngineer-1 provides molecular CAD capabilities for molecular and biological systems – See Figure 2
- NanoEngineer-1 Modifications allow the user to draw and type atoms to create a molecule
- Molecule is saved in a Molecular Machine Part File now readable by PACKMOL.

PACKMOL[3]

- PACKMOL provides a capability to pack molecules into a space without creating large repulsive forces between atoms – See Figure 1
- PACKMOL Modifications allow atom types to be carried into the MD cell.
- PACKMOL MD cell is saved in a Molecular Machine Part File readable by MSI2LMP

MSI2LMP[4]

- MSI2LMP converts the PACKMOL MD cell into a LAMMPS MD Cell
- LAMMPS is used create the final MD cell through energy minimization and simulated annealing – See Figure 3

Cross-linker

- A dynamic cross-linker is needed
- The new software could generate a pseudo-random spatial distribution of monomers and curing molecules
- LAMMPS would be executed to change atom positions
- Curing and monomer molecules close enough could be bonded together using a cutoff radius
- The number of molecules decreases as bonds are created
- Atom types change as bonds are deleted/created.
- Cross-linking is repeated to the desired percentage of cross-linking.

References

1. Molecular Dynamics Studio: http://sourceforge.net/projects/moleculardynami/
2. NanoEngineer-1: http://www.nanoengineer-1.net
3. PACKMOL: http://www.ime.unicamp.br/~martinez/packmol/
4. LAMMPS: http://lammps.sandia.gov/
5. Ismail, A., Grest, G. S., Heine, D. R., & Stevens, M. J. (2009). Interfacial Structure and Dynamics of Siloxane Systems: PDMS-Vapor and PDMS-Water. *Macromolecules , 42*, 3186-3194.
6. Chang, K.-S., Chung, Y.-C., Yang, T.-H., Lue, S. J., Tung, K.-L., & Lin, Y.-F. (2012). Free volume and alcohol transport properties of PDMS membranes: Insights of nano-structure and interfacial affinity from molecular modeling. *Journal of Polymer Science , 417* (418), 119-130.

Project/Research Objectives

- **Continue my open source software development**
- **Leverage the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)**
- **Model RTV compounds in an electric field**
- **Create cross-linker software**
- **Create realistic MD cells for simulation**
- **Generate system properties (Elastic, Shear and Bulk Modulus) comparable to laboratory experiment**
- **Add new software capabilities**
- **Opportunity to add magnetic field capability to LAMMPS**

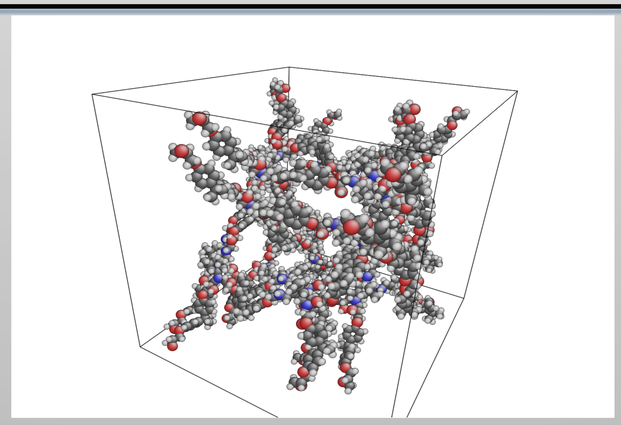

Figure 1. PACKMOL created MD cell

RTV Simulations

- An operational cross-linker is critical to RTV molecular dynamics simulations
- Existing software could be modified to use the Buckingham force field and perhaps additional force fields
- Modeling could include the following:
  - Diffusion of low molecular weight materials (LMW) materials
  - Behavior of Graphene in a PDMS matrix
  - Diffusion of water
  - How the presence of an electric field affects diffusion
  - Simulation of surface hydrophobicity
- Development of a reaction module for LAMMPS to simulate physical and chemical damage

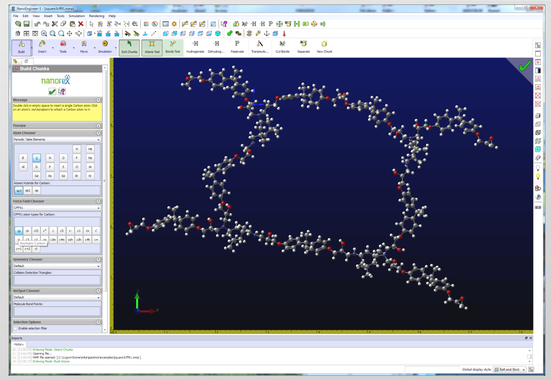

Figure 2. NanoEngineer-1 created oligomer

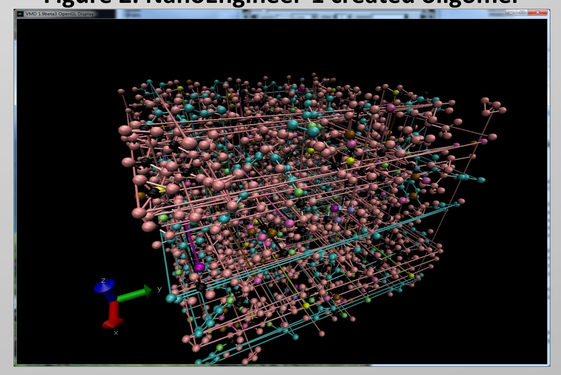

Figure 3. LAMMPS MD cell after annealing

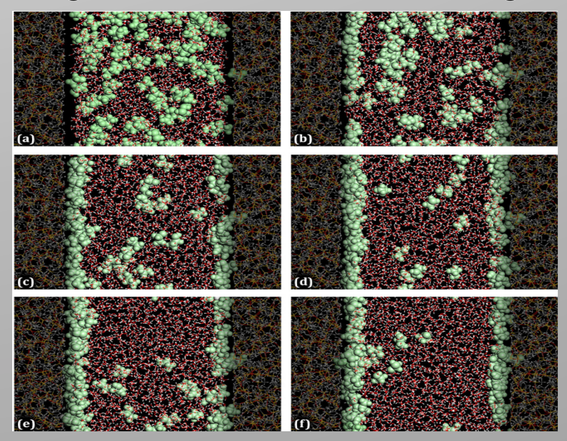

Figure 4. PDMS matrix, alcohol/water diffusion[6]

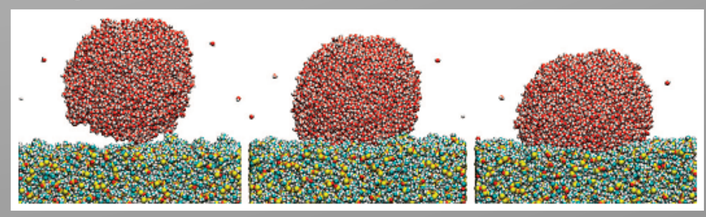

Figure 5. Hydrophobicity via molecular dynamics[5]