Malcolm Baldrige National Quality Award
2009 Award Recipient
Honeywell FM&T

Utilization of LAMMPS in a Rapid-Response Production Environment to Solve Manufacturing Challenges

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NNSA

Honeywell

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Outline

- **About NSC**
- **Simulation Technology**
- **Molecular Dynamics Concepts**
- **Molecular Dynamics**
- **Origination of need for molecular dynamics**
  - Choosing how to implement
  - Rapid response to production issue
- **Summary**

If we have time, we will show additional applications where we used molecular dynamics in rapid response to production issues

National Security Campus

-60 Years of Continuous Service to Dept. of Energy
-Associates ~ 2500
-Area ~1.5 million sq. ft.
-Kansas City, Missouri

ELECTRICAL/ ELECTRONIC

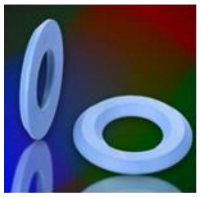
- Microelectronics
- Arming, Fusing and Firing Systems
- Embedded Software
- Fiber Optics
- Fire sets / Initiators
- Optics and Initiators
- Radars
- Secure Electronics
- Sensors
- RF / Antenna Design
- Telemetry
- RF / Microwave
- Film Deposition
- Systems Integrator

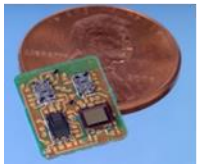
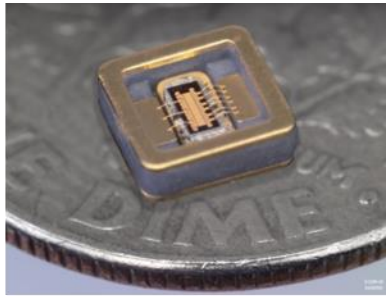
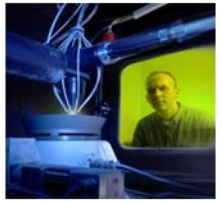
MECHANICAL

- Containers
- Mechanisms
- Machining
- Solid Modeling
- Prototyping
- Special Materials and Processes
- Welding Technologies

ENGINEERED MATERIALS

- Ceramics
- Polymer Develop. and Production
- Materials Engineering
- Organic / Inorganic / Metallurgy
- Gas Transfer Systems




Simulation Technology

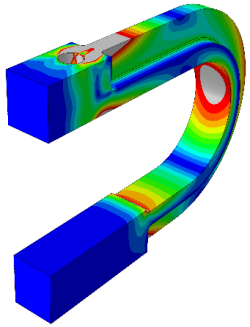
Value in Using Simulation Tools for Small Lot Production Environments

- **Reduce or eliminate actual prototype builds.**
- **Reduce time to evaluate processes, designs, and/or fixturing.**
- **Allows for a more robust process, product or fixture.**
- **Uncover production problems before they occur.**
- **Allows for environmentally friendly 'virtual' evaluations.**
- **Aid if production failures do occur.**

Simulations can make you agile and flexible to change for rapid response to needs and requirements.

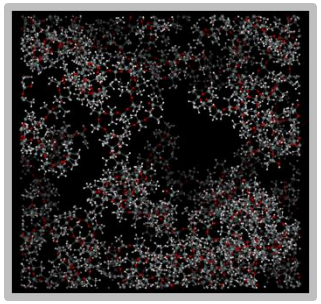
Simulation Technology History

- **Have used Finite Element Analysis (FEA) to troubleshoot mechanical issues since 1979**
  - 1979 – 1985: NASTRAN
  - 1985 – 2015: Abaqus



- **Simulation group, AESA, has grown from a few individuals to ~23 FTEs and conducts 150-200 projects per year**

- **First molecular dynamics simulation in 2014**



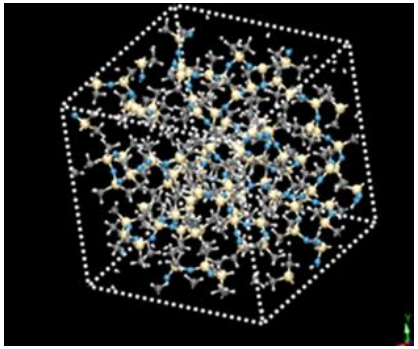
- **First *ab initio* simulation in 2015**

Molecular Dynamics Fundamentals

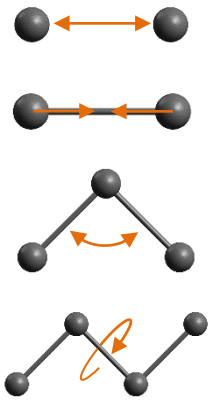
$$\frac{d^2 r_i}{dt^2} = \frac{F_i}{m_i} \qquad F_i = -\nabla_{r_i} V(r_1, \ldots, r_N)$$

Numerically solve them from *t* to *t+Δt*, *t+ 2Δt* to obtain a trajectory (output data).
Temperature and Pressure are calculated and controlled by thermostat and barostat.

$$K = \frac{3}{2} N \kappa_B T \qquad PV = N \kappa_B T + \frac{1}{D} \left\langle \sum_{i=1}^{N} r_i \cdot F_i \right\rangle$$

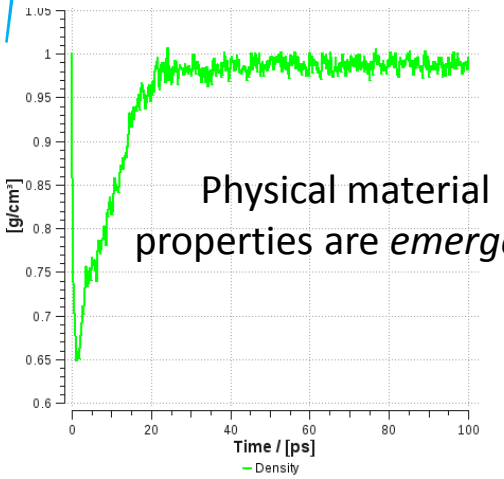


Initial positions and velocities



Interatomic potentials

Symplectic Time Integration

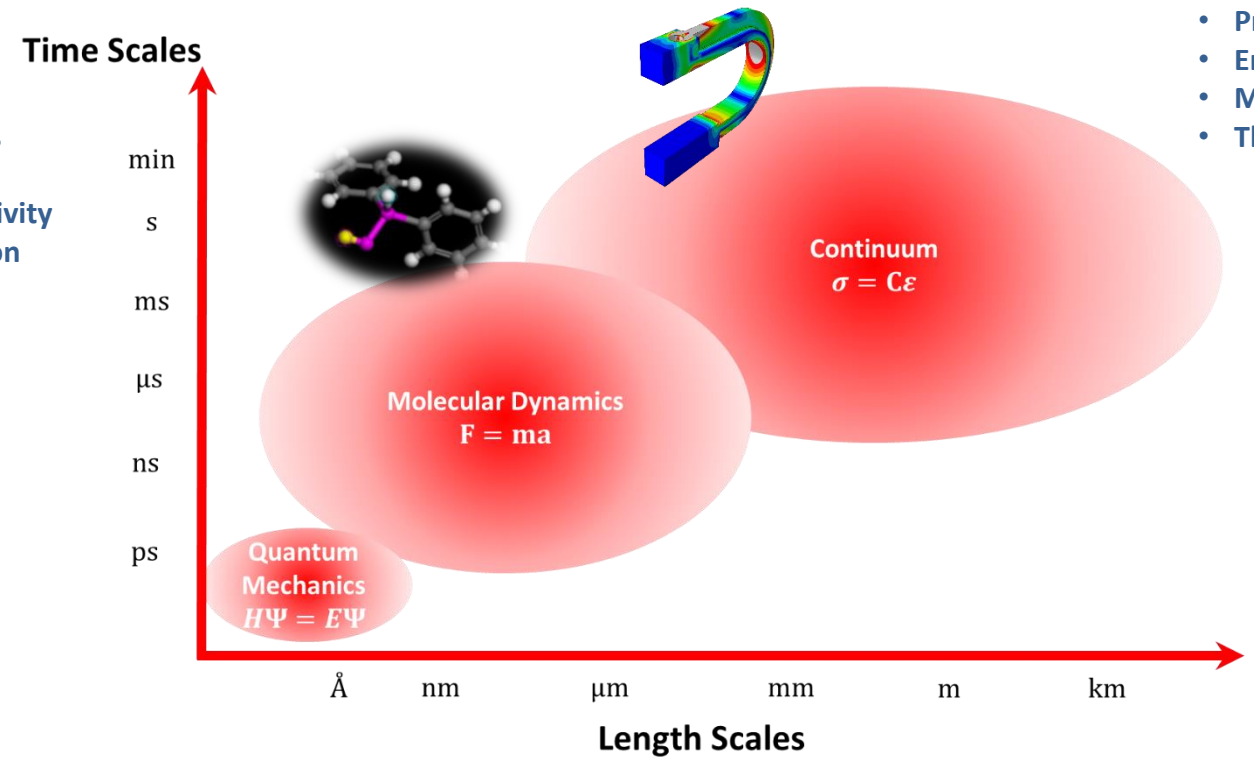


Physical material properties are *emergent*

Model & Simulation Applicability

Molecular and Quantum Modeling

- Density
- Young Modulus
- Shear Modulus
- Shear Yield Stress
- Heat Capacity
- Thermal Conductivity
- Thermal Expansion
- Mass Diffusion
- Transition Temps
- Cohesive Energy
- Surface Tension
- Molar Volume
- Solubility
- Gas Permeability



Continuum Modeling

- Product Performance
- Energy Absorption
- Mechanical response
- Thermal conductivity

Activation Energy: Why we took the plunge

- **In 2013 an employee with 30+ years of experience of processing the base material for cellular silicones retired.**
- **Loss of "tribal knowledge" led process to the brink of being out-of-control. Questions arose:**
  - What will happen if we replace the mixing blade?
  - What affect does filler particle size/distribution have?
  - Do the variations in room temperature cause the variance?
  - If a butterfly flaps its wings…?
- **NSC was preparing 3 years of experiments to regain knowledge and confidence in process.**

NSC needed an answer, fast!

Glassware: Getting the Right Tool for the Job

- **Polymer production requested help from AESA to model the process's chemistry.**
  - AESA has depth in continuum solutions (EM/Thermal/Mech/Fluid),but none in discrete chemistry.
- **The task was wide-open, all solution methods were on the table. Should we:**
  - Write our own computational chemistry software to model this specific issue?
  - Outsource to academia?
  - Use open-source / free software exclusively?
  - Use commercial software?

To guide us, we used lessons learned through AESA's extensive history with finite element analysis

Building a Finite Element Code

Geometry	Discretization	Solve	Analyze

• ACIS
• Parasolid
• Open CASCADE
• CGM
• SOLIDS++
	• Topology
	• Shape
	• Unstructured
	• Adaptive
	• Higher Order
		• Linear Solvers
		  • Trilinos
		  • PETSc
		  • Hypre
		  • Paralution
			• Excel
			• Matlab
			• Python
			• Blot
			• Paraview
			• VisIt

Of course you can also write any of these yourself!

Code Development and Rapid Response

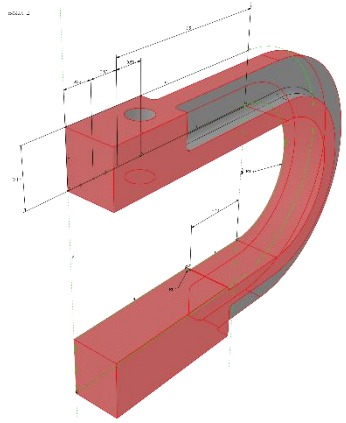
- **This model does not suit well to a rapid-response production environment**

- **Would require either a few omniscient analysts, or an entire infrastructure built around developing codes (like that found at Sandia National Labs)**

- **Equal, if not more, time spent debugging issues with code than debugging production issues**

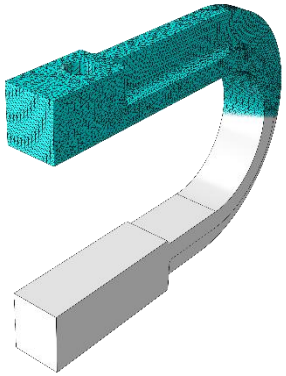
- **AESA instead uses a commercial FEA software with the following general characteristics:**

High quality and easy to use interfaces to:

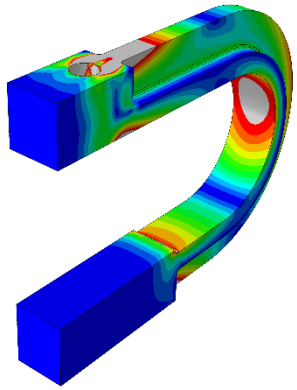


Rapidly construct accurate geometry

We rely on vendor's quality assurance
We trust them!



Rapidly build an accurate physics model



Rapidly analyze comprehensive results

Total time to build, run and analyze simulation: **4 hours**

Applying to Computational Chemistry

Software Functionality Criteria

Low

- Ease of installation
- Simulate multiple materials?
- User privilege level required
- White docs (industry case studies)

Desired

- Correlation tool
- Easy to simulate
- Easy to post-process
- Low Cost (<$50k)
- LAMMPS engine
- GPU capabilities
- Quality of Tech Support
- OS flexibility / interoperability
- Ability to customize

Needed

- Graphics
- Easy to build amorphous cells
- Scripting interface
- Ability to run jobs simultaneously
- **Good** tutorials & documentation

Critical

- Atomistic capabilities
- Mesoscale capabilities
- Crosslinking capabilities
- Works with our HPC platforms / queuing

Software Selection

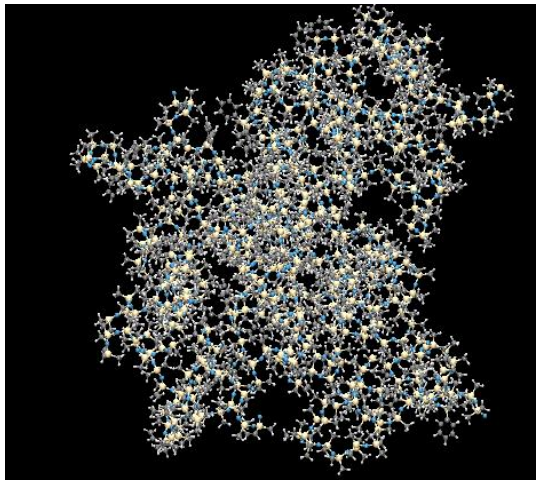
- **After an initial review of nearly 30 software tools, 3 were selected for evaluation**
  - Scienomics: MAPS
  - Materials Design: MedeA
  - Accelrys: Materials Studio

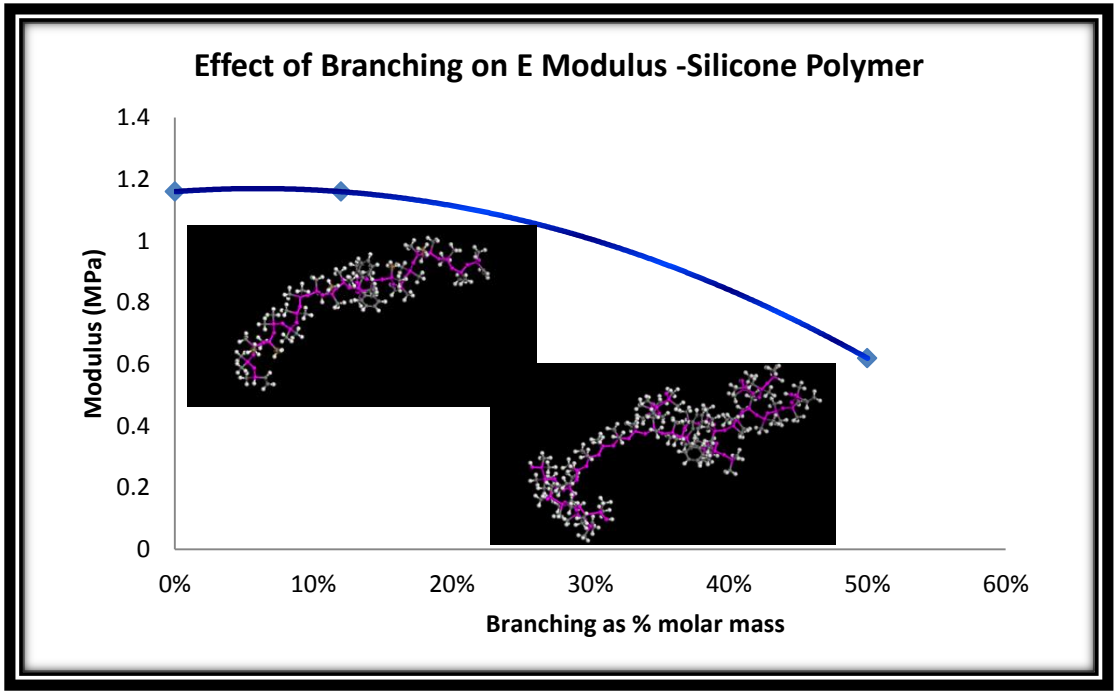
    Now Dassault Systemes BIOVIA

Use LAMMPS

- **Now armed with a tool, we tackled the problem at hand!**

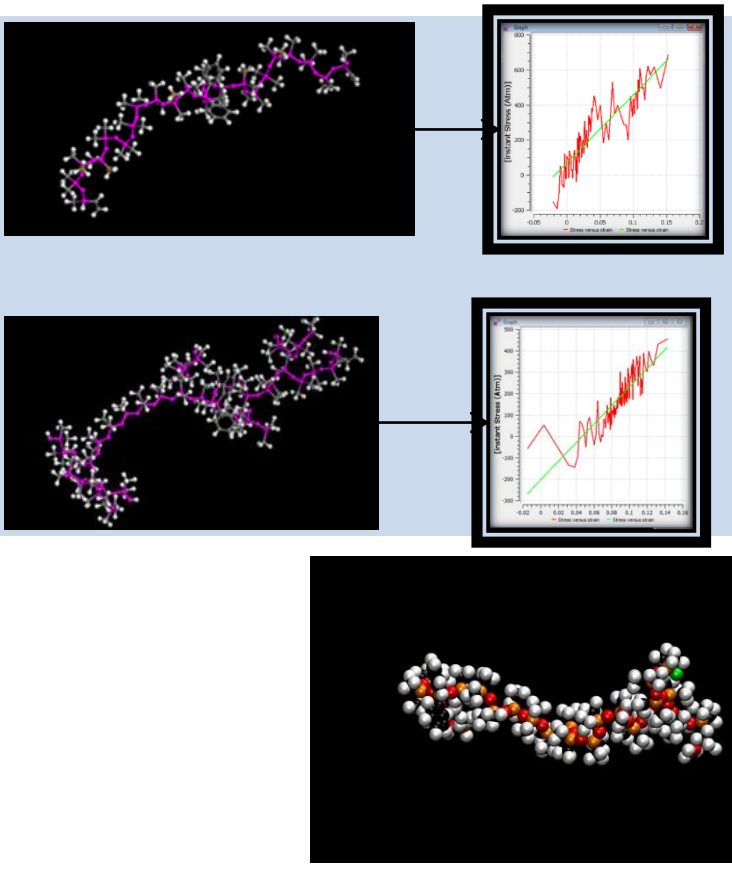
Investigating Silicone Polymer Production





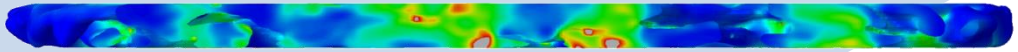
Allowable branching limits were determined using MD
This matched predictions derived from experiment.

Investigating Silicone Polymer Production



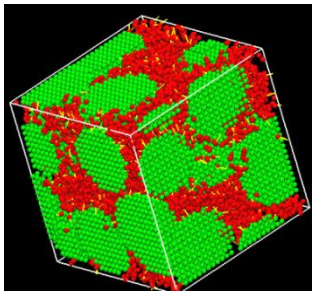
FEA to Compute Mechanical Response

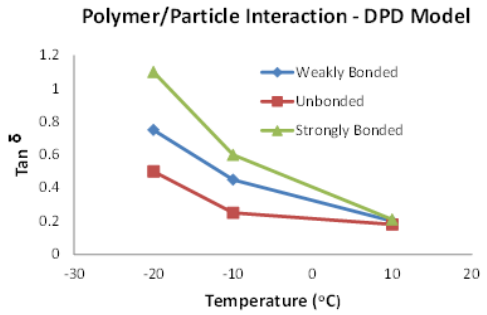
Computed Tomography



Contours of Strain-Energy Density (J/m^3)

Reinforced Silicone Polymer





Viscoelastic Stress/Strain

$$\sigma = \sigma_0 \sin(t\omega + \delta)$$
$$\varepsilon = \varepsilon_0 \sin(t\omega)$$

Loss Modulus

$$E'' = \frac{\sigma_0}{\varepsilon_0}\sin(\delta)$$

Storage Modulus

$$\mathrm{E}' = \frac{\sigma_0}{\varepsilon_0}\cos(\delta)$$

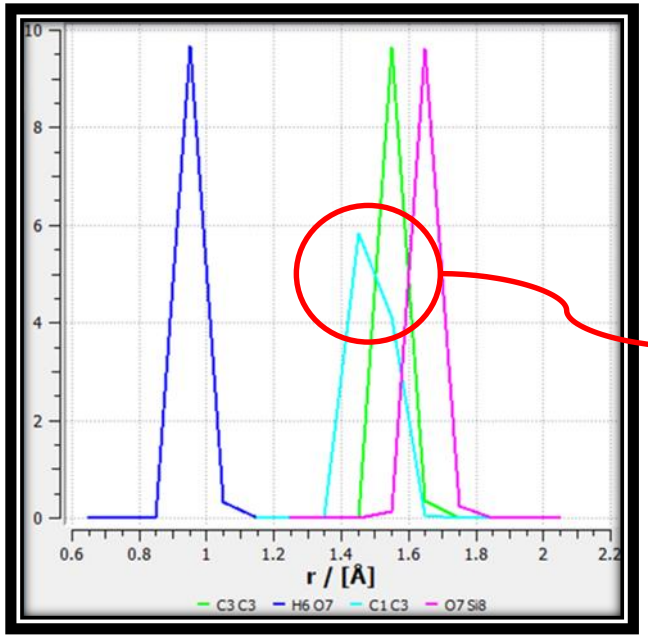
$$\tan(\delta) = \frac{E''}{E'}$$

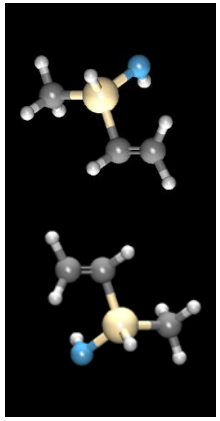
Experiment shows tan delta increased with time, as predicted by simulations

Simulations were used to set parameters for experimental methods investigating particle/polymer interactions and aging

Crosslinking in Silicone Polymer

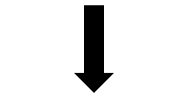
Bond Distribution Analysis:
-Crosslink formation as function of process conditions
-Probability of secondary reactions (via Gibbs Energy)

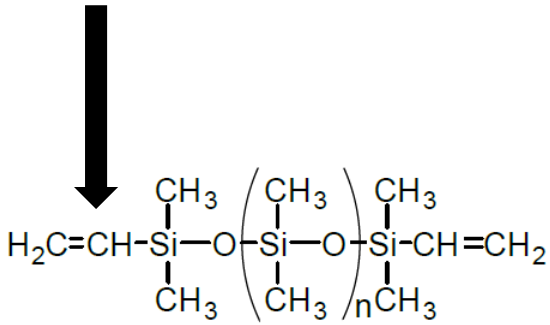




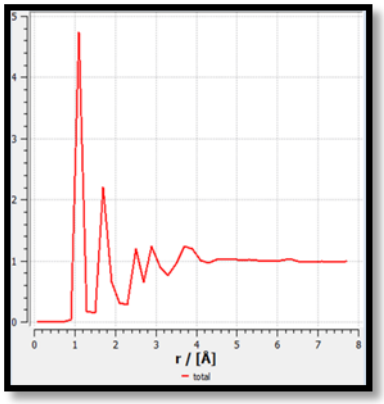
Effect of End Group
Vinyl = Crosslinks <200°C
Silanol = No reaction below 200°C

Silanol vs Vinyl functional group

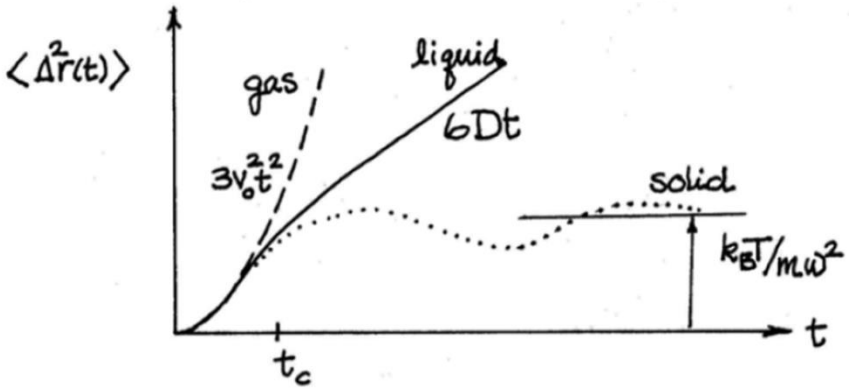




Change in Structure of Silicone Polymer

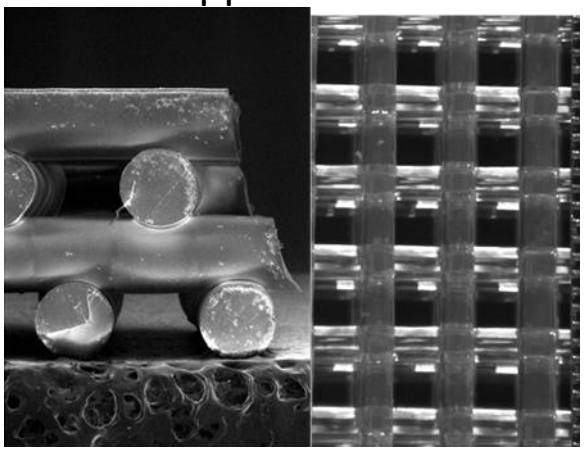


Molecular Dynamics can provide information regarding dynamic change of structure, yielding phase transformation.



Courtesy of Sid Yip. Used with permission
Professor Emeritus M.I.T

Important for Direct-Ink-Write applications



Results

- **Cost savings of $210k per year (Materials and Labor)**
- **Provided confidence that production could downscale this process**
  - Provided support for acquisition of $380k of capital equipment
- **By providing parameters for experiments, simulations reduced the search space, thus reducing the number of experiments by 70%**

Summary

- **Molecular dynamics has proven to be a useful tool for NSC and its usage is being expanded**
  - If we have time we will look at a few expansions
- **NSC's usage of LAMMPS is dependent on**
  - External tools that accelerate and/or enable construction of simulations
  - Trusting that features in these tools and in LAMMPS have been thoroughly validated / verified
- **With the right tools and people, molecular dynamics can provide value to rapid-response production environments**

Acknowledgements

- **Jim Mahoney –** Honeywell FM&T, Engineering Fellow
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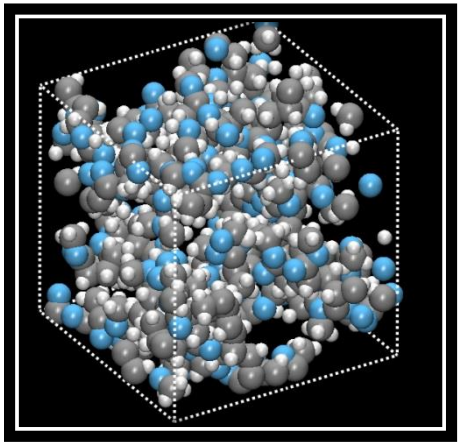
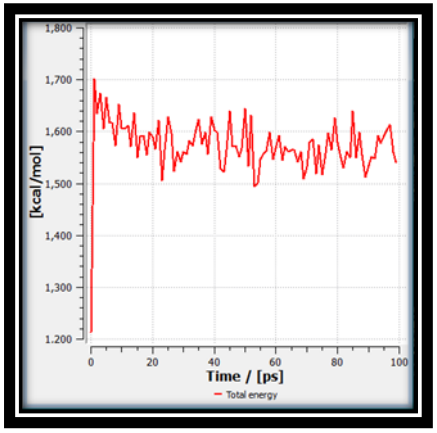
- **Lalitha Subramanian PhD –** Scienomics
- **Andreas Bick PhD –** Scienomics
- **Dr. Paul Rulis –** University of Missouri-Kansas City
- **Dr. Ridwan Sakidja –** Missouri State University
- **Rachel Cramm Horn –** UMKC Student Intern

And of course, LAMMPS and everyone who has contributed, whether as a developer, sponsor, or deliverer of chocolate chip cookies!

Polymer Solubility and Compatibility

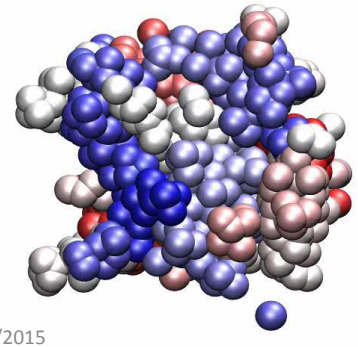


Polymethylacrylate (PMA)



$$\delta = \left(\frac{|\langle E_i \rangle|}{\langle V \rangle} \times 6947.28 \right)^{1/2}$$

Polymer solubility can be calculated for any given chemical formulation



Solubility $(J/cm^3)^{1/2}$
Molecular Dynamics = 18.5
Experimental Value = 19.9

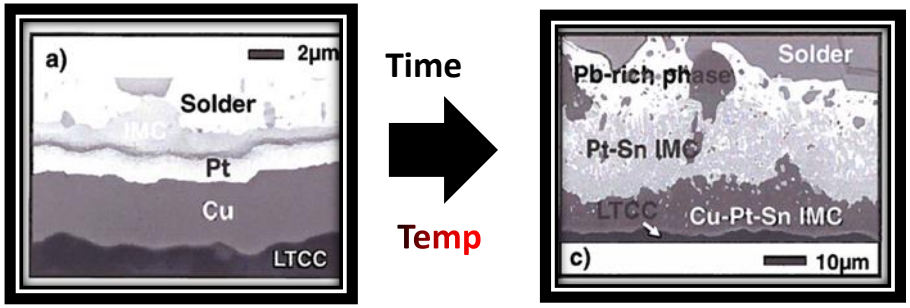
Total time to build, run and analyze simulation: **4 hours**

Thin Film Diffusion

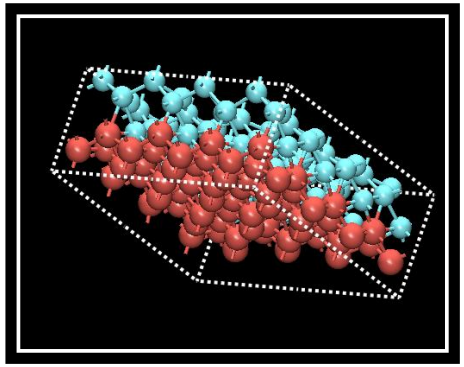
Solder Material – Thermal Aging

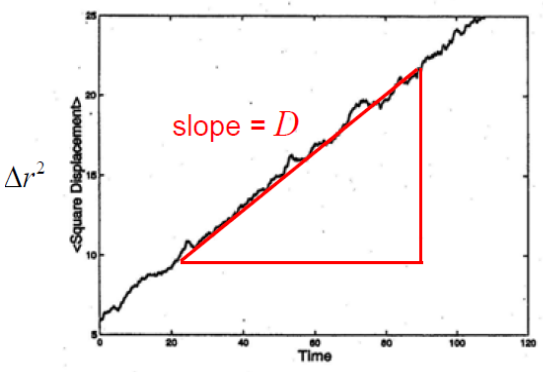
Goal: Improve understanding of metal diffusion observations in thin film aging experiments

Approach: Model diffusion via molecular dynamics



$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

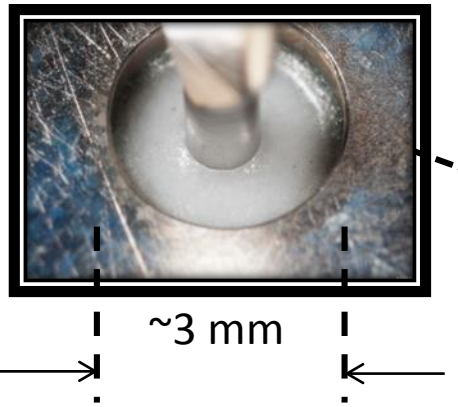




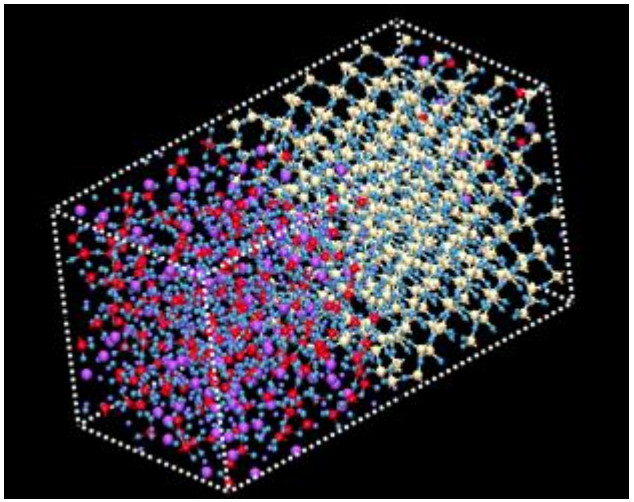
$$D = p\frac{\Delta x^2}{\Delta t}$$

$$\langle \Delta r^2(t) \rangle = \frac{1}{N}\sum_i \left(\vec{r}_i(t) - \vec{r}_i(0)\right)^2$$

Characterizing Material Interfaces



Glass Ceramic – Metal Interface



Minimizing the total energy gaps
minimizes residual stress
Control via annealing process