

Examples (Former Interns)

HIP Presentation Slide Example



MD Toughness Predictions for Hybrids for Extreme Environments

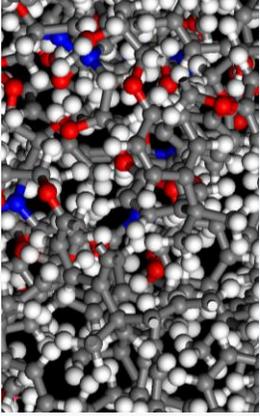
Logan Ward
Summer Intern, JEOM Program
Mentor: Dr. Mollenhauer
RXBC



LEAD | DISCOVER | DEVELOP | DELIVER

Project Overview

- **Goal:** Predict fracture toughness of a resin molecular dynamics.
 - Link constituent and component level behavior.
- **Advantages:** Determine material properties without physical experiments.
 - Multiscale virtual design

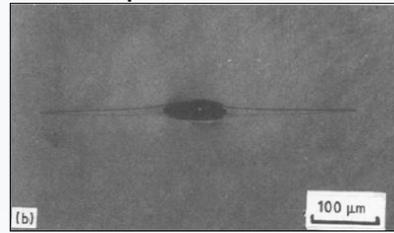


2



Fracture in Thermosets

- Macroscopic deformation occurs in epoxies
 - Thin films
 - Chain extension ahead of crack tip.
 - Extension leads to increased toughness



Kramer, Glad. *Journal of Materials Science*. 1991. 26.

- Altered by chain length and dilution
 - Less dilution → More extension
 - Higher M_w → More extension
 - More extension → Tougher

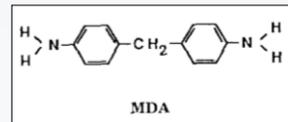
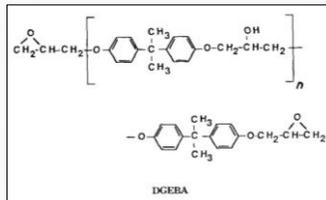


2



Initial System Selection

- The first resin system:
 - Epoxy: Diglycidyl ether of bisphenol A (DGEBA)
 - Curing Agent: Methylene dianiline (MDA)
- Various chain lengths
- Addition of non-reactive diluent
- Software works w/o modification



Both images: Kramer, Glad. *Journal of Materials Science*. 1991. 26.

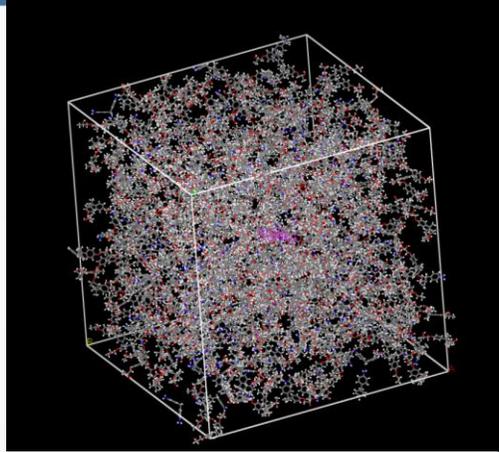
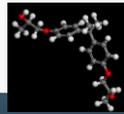
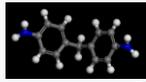
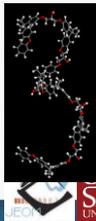


2



Model Creation

- Each molecule was made in Materials Studio
- A "cell" was generated by Discover.

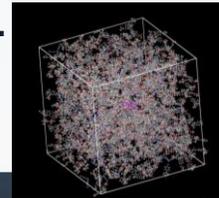


2



Simulation Scale

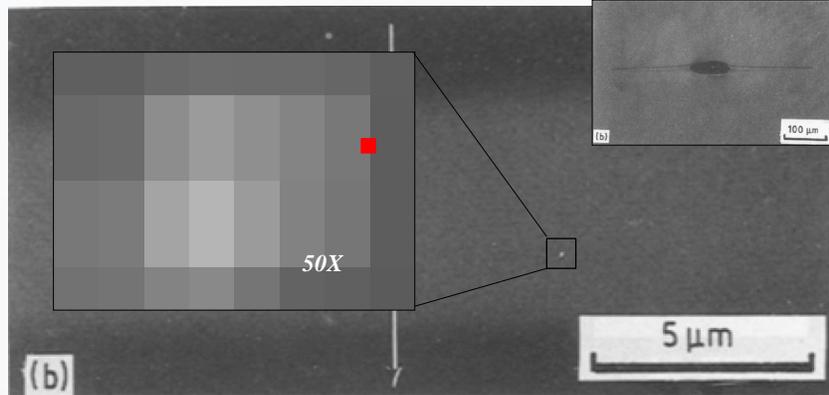
- Length scale: Around 70 Å.
- Time scales: Close to 1 ns, 1 fs resolution
 - Crack velocity: 0.34 Å/ps
(Fineberg in Dyn Fracture Mech, Shukla ed. p. 121)
- Number of atoms: ~30000 atoms cell
- Used periodic boundary conditions
 - Part of continuum of identical cells.



2



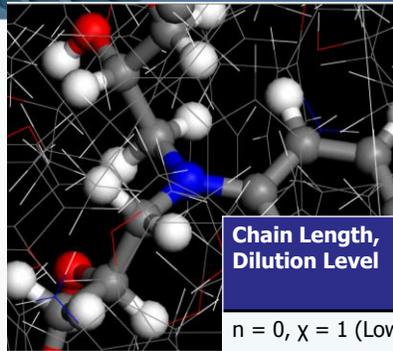
Simulation Compared to DZ



Kramer, Glad. *Journal of Materials Science*. 1991. 26.



Crosslinking



- Novel script by Accelrys
- Xlinks by search method
- Reaction extents > 88%
- Difference < 10 %

Strand: Length between two crosslinking sites

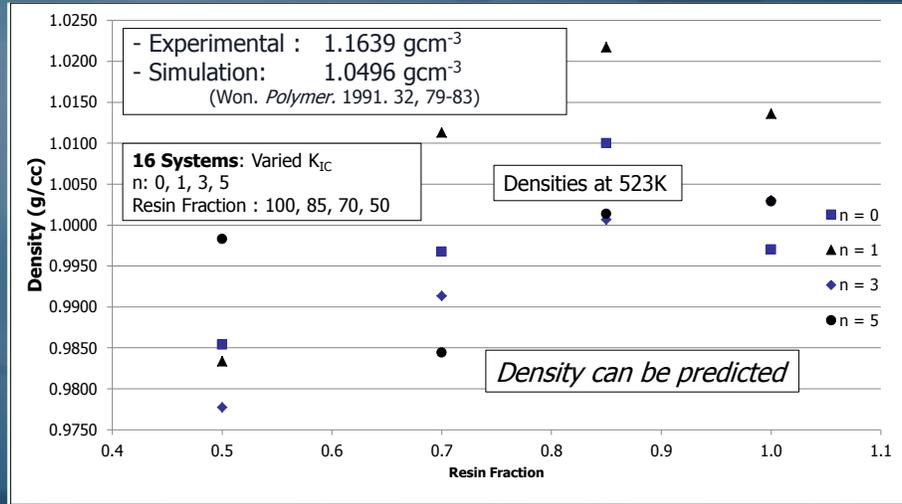
Chain Length, Dilution Level	Strand Density (10^{25} m^{-3})	
	Simulation	Experiment
$n = 0, \chi = 1$ (Low K_{IC})	123	135
$n = 5, \chi = 1$ (High K_{IC})	27.1	33.5
$n = 5, \chi = 0.7$	16.0	16.5
$n = 5, \chi = 0.5$ (Low K_{IC})	16.0	8.4

Values from: Kramer, Glad. *Journal of Materials Science*. 1991. 26.

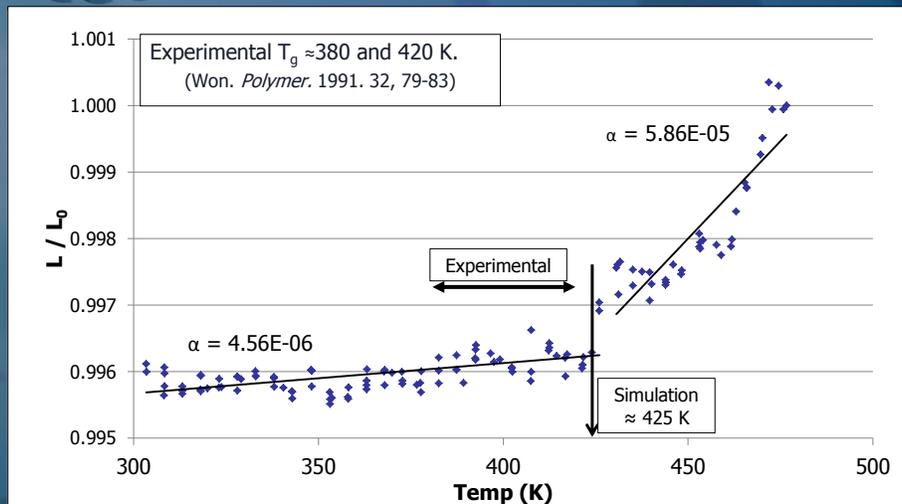




Density Prediction



Thermal Property Prediction



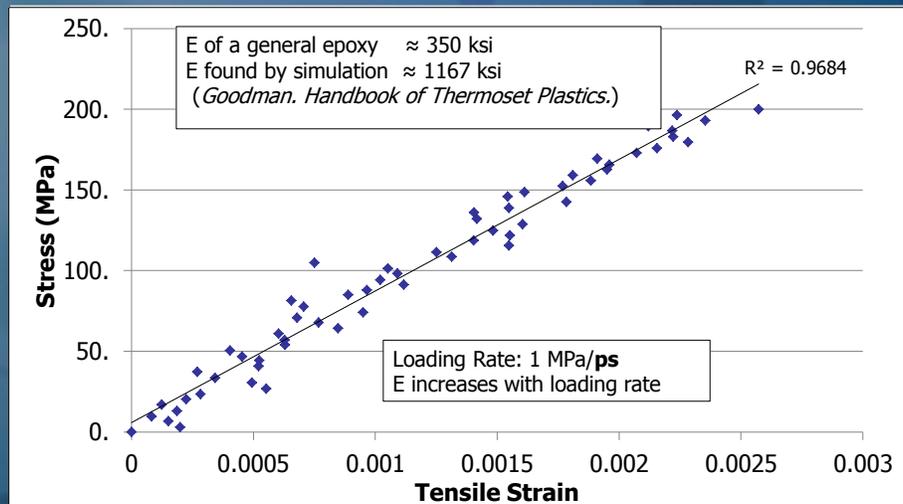


Mechanical Testing

- Uniaxial stresses, tensile and compressive
 - Testing between 20 MPa to 2.0 GPa
 - Constant stress rate (0.1-10 MPa/**ps**)
- Two conditions:
 - Bonds will not break (Few have completed)
 - Bonds can break (Not yet completed)
 - Under development

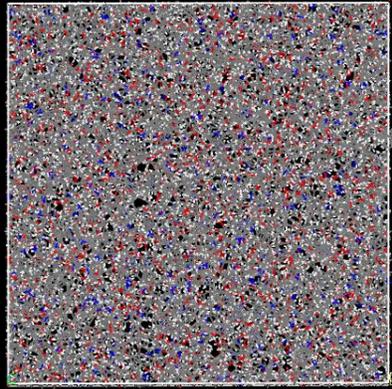


Mechanical Properties





Tensile Test



2



Chain Extension

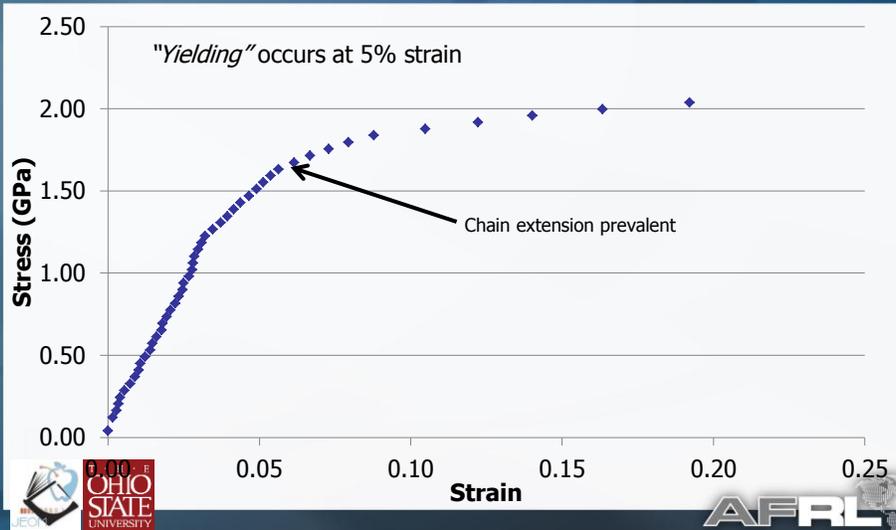
- Results show chain extension
 - End to end lengths increase
- Chain orientation effects extension
 - Greatest towards loading direction
- Event-triggered extension
 - Strain > 6%
- High free volume at high strains
 - Gaps/voids opening



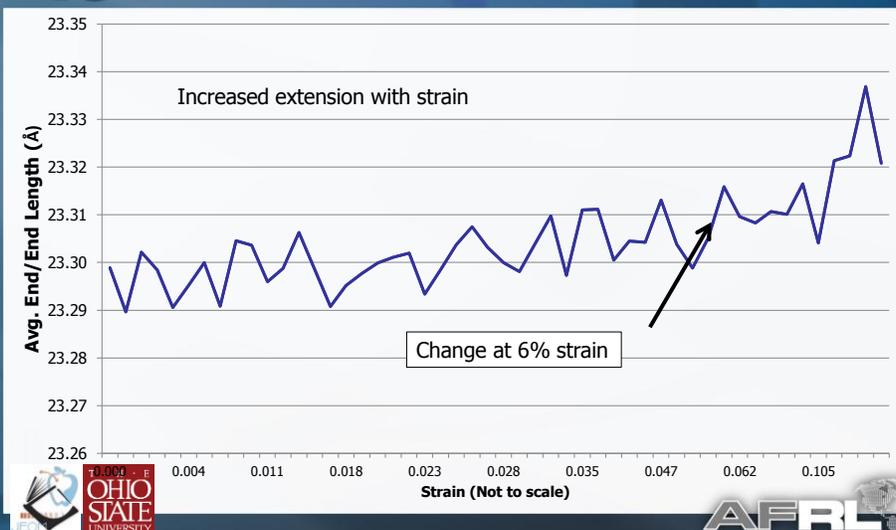
2



Behavior at High Stresses

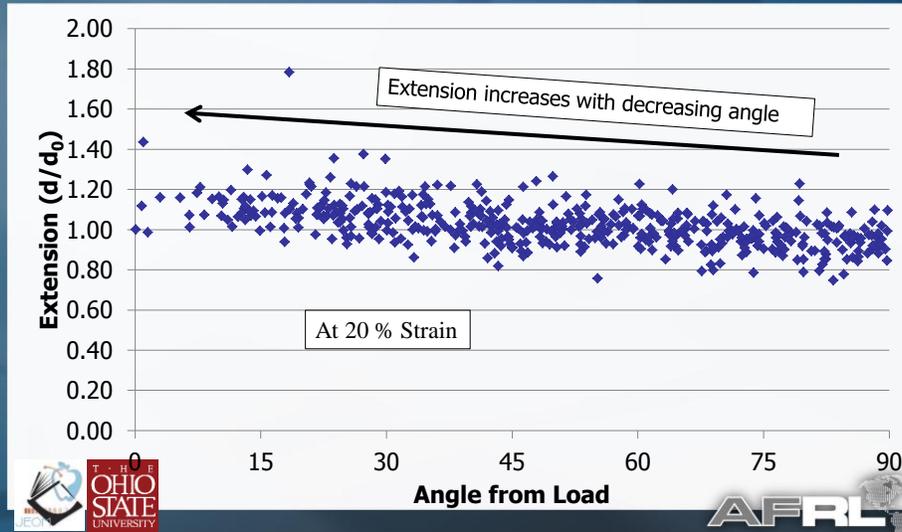


Chain Extension

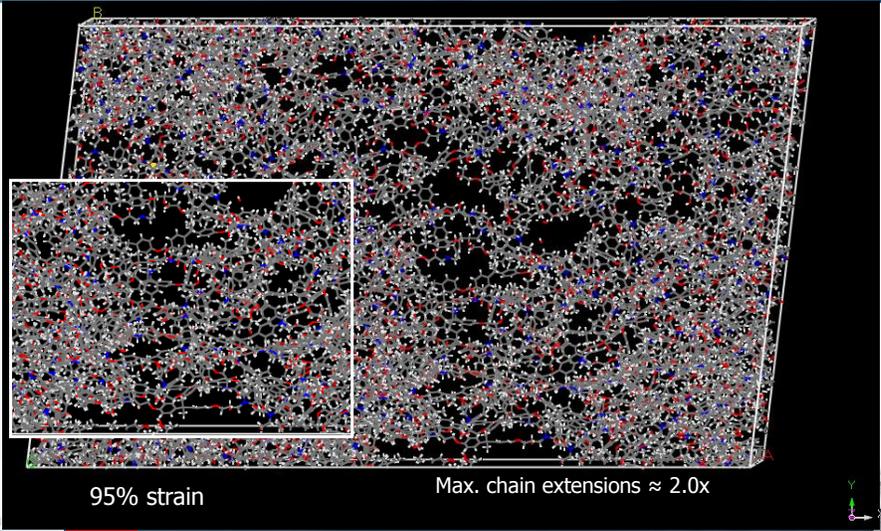




Chain Orientation



Behavior at High Strains





Possible Explanations

- Possible reasons for local behavior
 - Distribution of “free ends”
 - Greater mobility → more free volume?
 - Crosslinking topology
 - Rigid arrangement → less free volume?



2



Modeling Time

Step	Time
Cell Creation and Crosslinking	161 CPU hours
Relaxation	40 CPU hours
Cooling	740 CPU hours
Tensile	260 CPU hours
Total	7 CPU weeks

- Crosslinking took the most real time
- Waiting
- Parallelization
 - Short internship
 - 2048 cores
- 16, 30k systems
- 8, 5k systems



2



Conclusions

- Variety of highly Xlinked models
- Obtained realistic properties
- Tensile loading simulations are possible
 - Reasonable processing times
- Chain extension at high strains



2



Continuing/Future Work

- Different resin systems
 - Possible candidate: BMI resins
- Determining fracture toughness
 - Current strategy:
 - Tensile test w/ bond scission
 - Breaking energy stays in system
 - Monitor key parameters
 - Reproduce experimental behavior.
 - Effect of dilution, chain length



2



My Take-Backs

- Interest in computational science
 - Minor in Computer Science and Engineering
 - Computation science courses/degree
- Improved programming skills
 - More experience on a UNIX system
 - Introduction to FORTRAN and TCL
- More familiarity with materials science
 - Better introduction to fracture mechanics
 - Introduction to failure mechanisms in composites



2



Acknowledgements

- HPC Modern Office's JEOM Program
- Dr. James Moller
- Dr. Rajiv Berry
- AFRL DoD Supercomputer Resource Center



2



Questions?



LEAD | DISCOVER | DEVELOP | DELIVER

Computer Resources

- Two AFRL supercomputers:
Eagle and Falcon
- 2048 Processors each
- Local workstations:
Nova, Supernova, Comet





Costs of Scaling up

- Increasing number of atoms is expensive.
- 5000 → 30000 atoms: 25x more time

30000 atoms: ~250 hours **5000 atoms: <10 hours**

- | | |
|----------------------------------|----------------------------------|
| • Cell Creation and Crosslinking | • Cell Creation and Crosslinking |
| – 209 CPU hours | – 7.1 CPU hours |
| • Redensification | • Redensification |
| – 32 CPU hours | – 2.6 CPU hours |

Note: 250 hours does not count additional procedures

