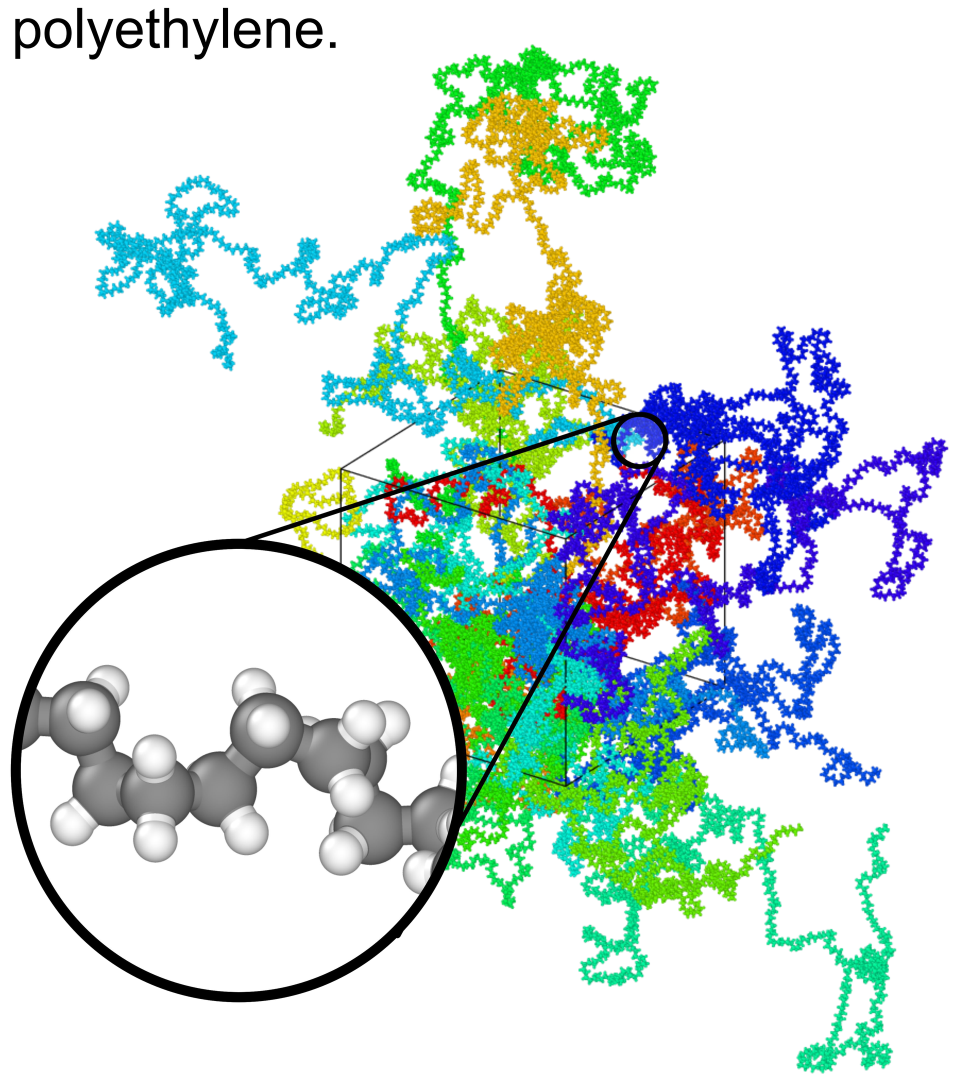
Molecular Modeling of Amorphous Polyethylene

University of Delaware | Center for Composite Materials

Timothy Longoria (BChE)[2], Sanjib C. Chowdhury, Ph.D.[1] and Prof. John W. Gillespie Jr.[1]
University of Delaware | Center for Composite Materials[1] | Department of Chemical & Biomolecular Engineering[2]

Introduction

- Polyethylene is a polymer material often found in commercial goods with a wide range of applications due to its variable properties. PE fibers are also found in protection systems such as vests, helmets and armor backing plates.
- Polyethylene systems have been studied previously with molecular simulations using non-reactive force field.
- Further investigation with reactive AIREBO force field will reveal more insight into the deformation and stress-strain response of amorphous polyethylene.



Amorphous polyethylene model of 17 chains with a degree of polymerization of 500.

Objectives

- Predict thermo-mechanical properties of amorphous polyethylene as a function of molecular weight
- Understand the deformation and damage mechanisms

Methodology

Create model with the desired number of chains and molecular weight using MAPS

↓

GAFF

- High pressure and temperature relaxation
- Annealing: high temperature heating and cooling to determine glass transition temperature Tg

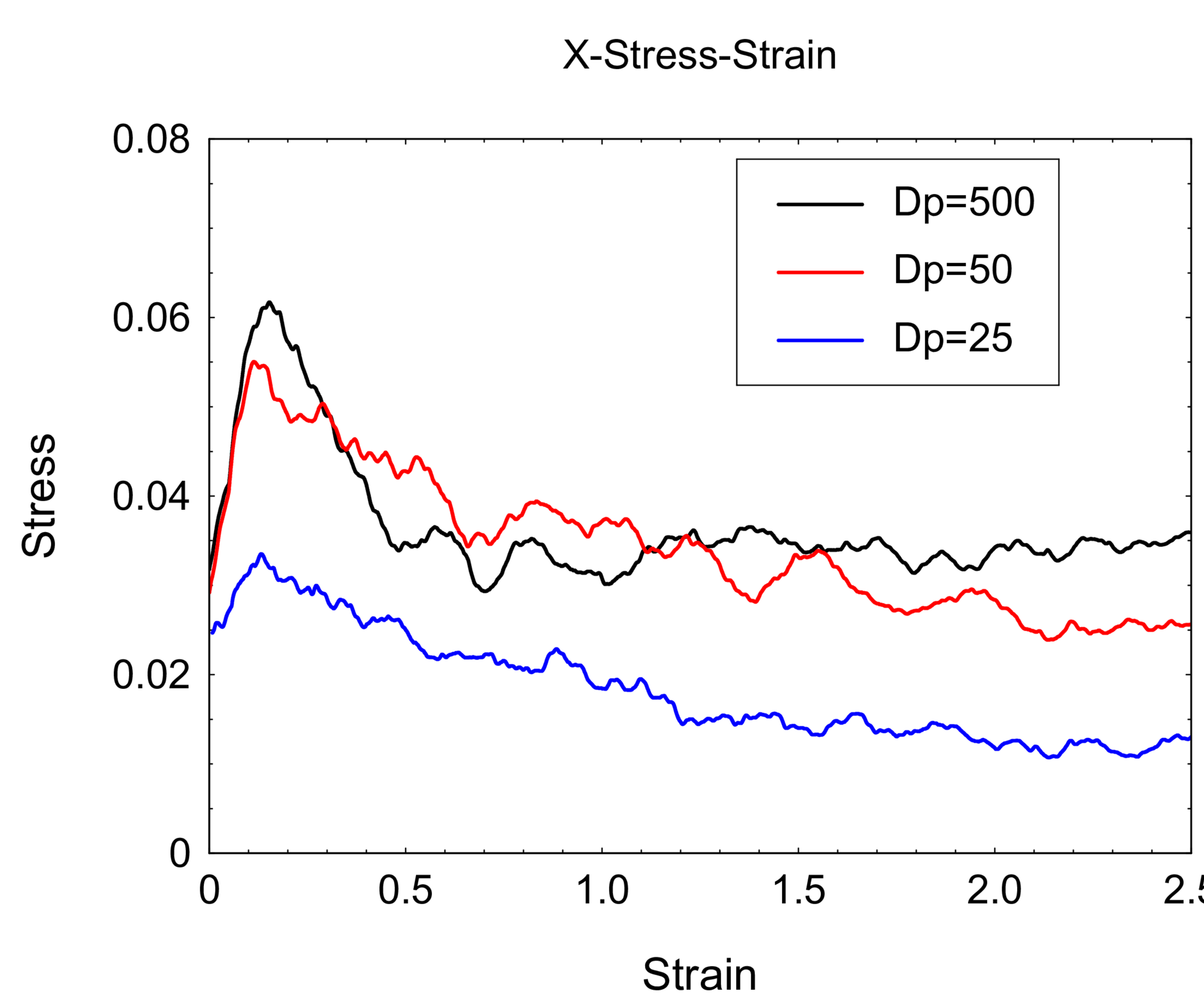
↓

AIREBO-M

- Relaxation at 300K
- Mechanical tensile loading

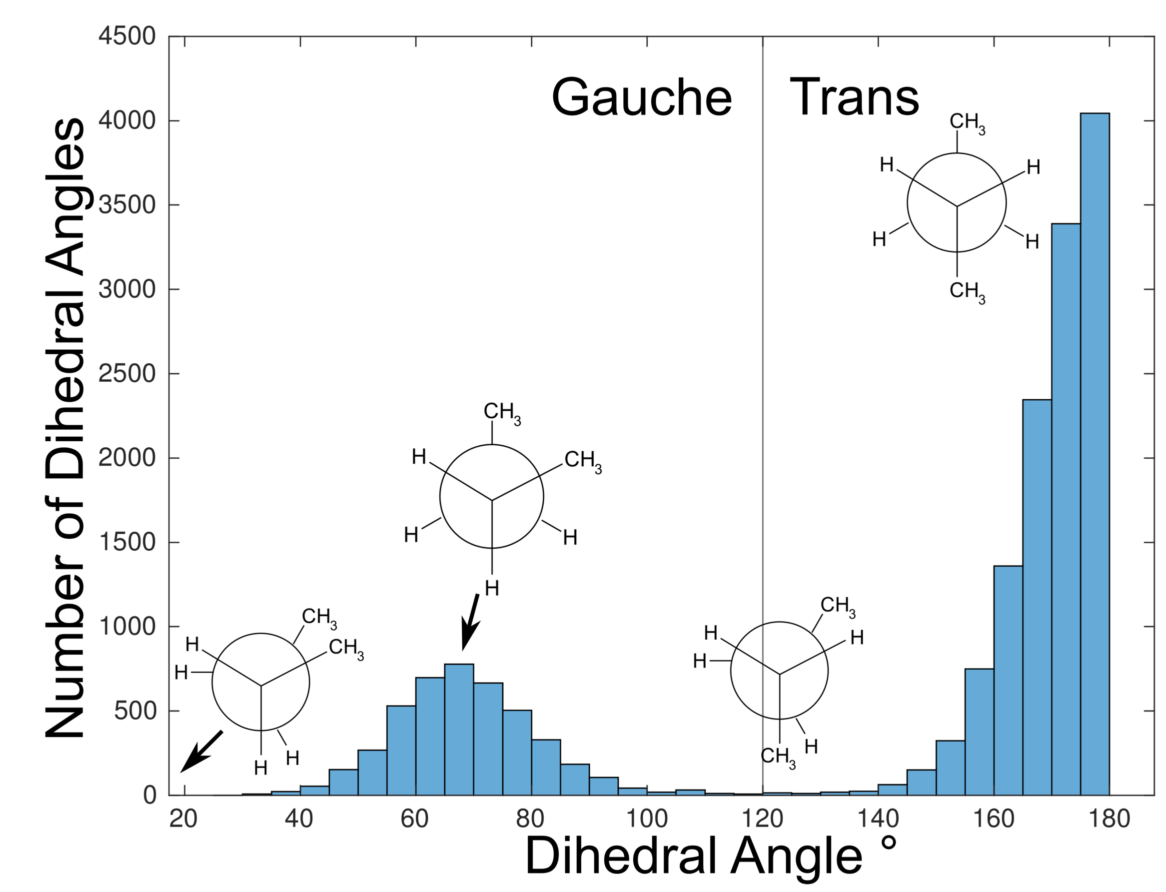
Results and Discussion

- Stress strain response



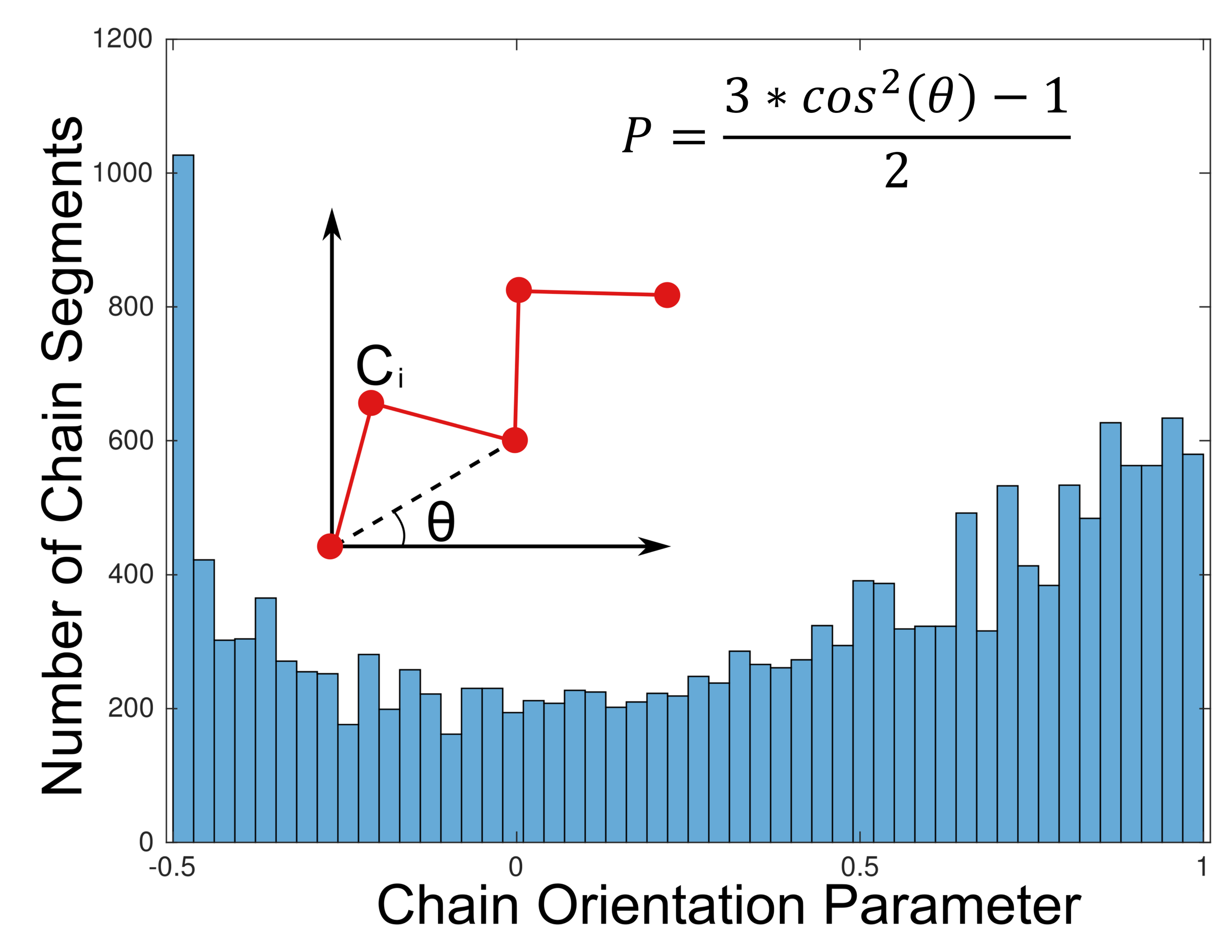
Results and Discussion

- Dihedral Angle



The distribution shows gauche configuration centered around 65° and trans 180°

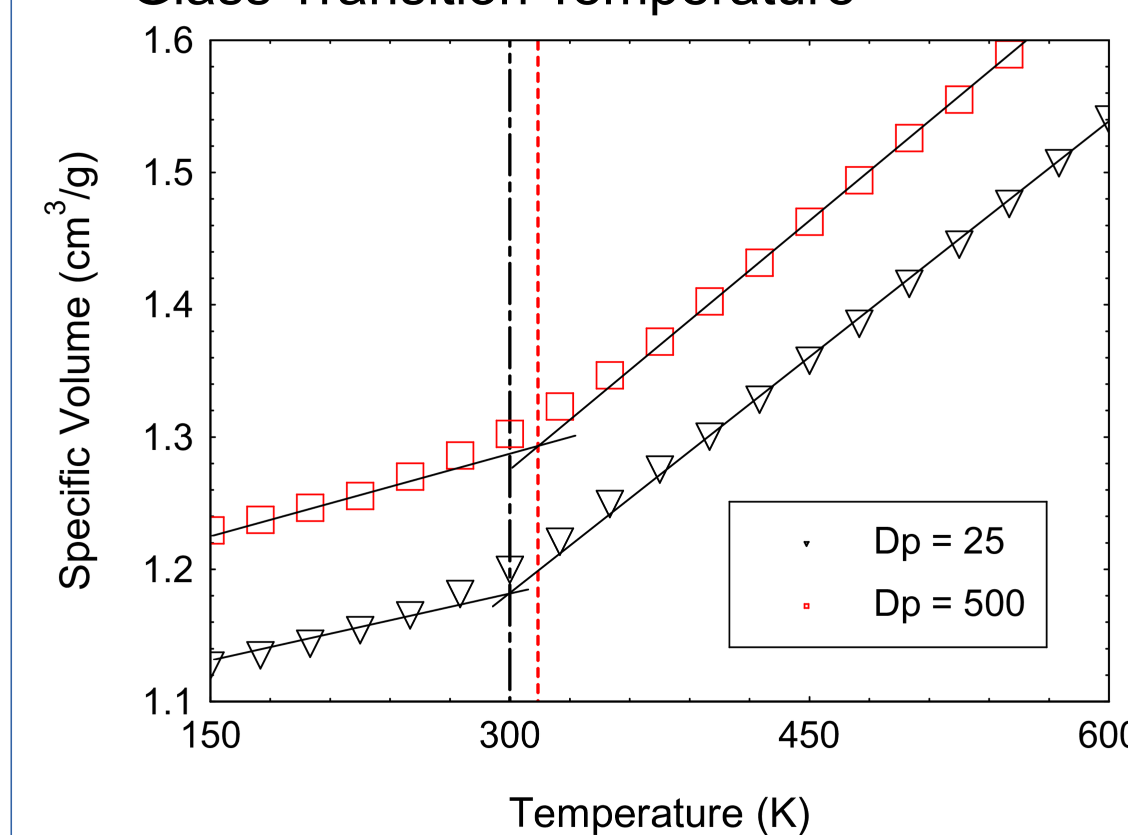
- Chain Orientation



A value of -0.5 represents a perpendicular segment, 0 random, and 1 a segment parallel to the x-axis. An increase in values near 1 are seen as tensile loading aligns the chains along the loading axis.

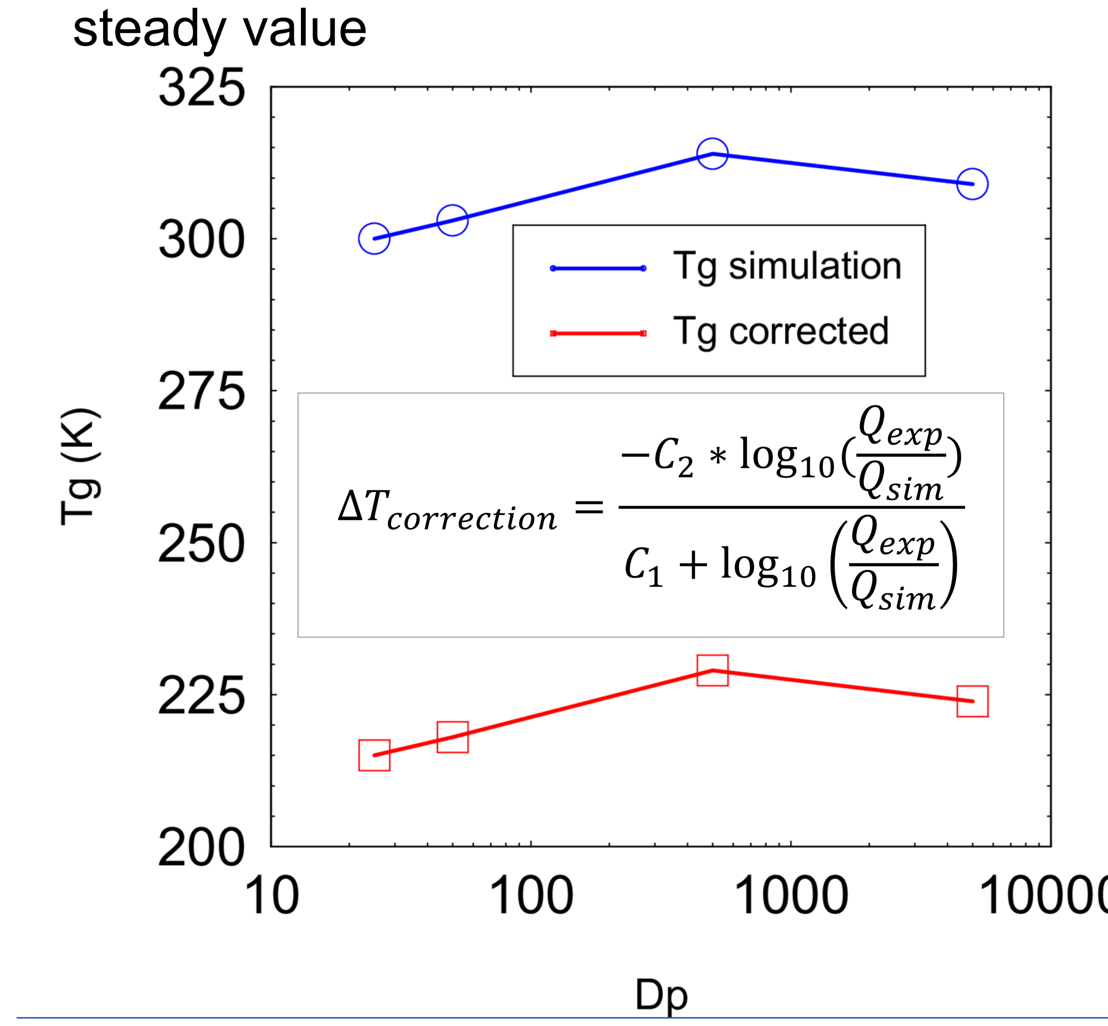
Results and Discussion

- Glass Transition Temperature



Summary and Conclusions

- Molecular modeling of amorphous polyethylene reveals details of deformation and damage mechanisms. Damage is controlled by chain slippage instead of chain scission for the MWs considered here
- Higher molecular weight systems show greater yield strength due to entanglement of the chains
- Increasing degrees of polymerization show glass transition temperatures approaching a steady value



Acknowledgments

This work is supported by the Army Research Laboratory under Cooperative Agreement Number W911NF-21-2-0208.