Mississippi State University: Center for Advanced Vehicular Systems

Tribology and Friction of Soft Materials: Mississippi State Case Study

J.L. Bouvard
E.B. Marin, D. Oglesby, K. Solanki, B. Kirkland, M.F. Horstemeyer, P. Wang, and R.L. King

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Standard Form 298 (Rev. 8-98) Prescribed by ANSI Std Z39-18
Outline

1. Background of Mississippi State U.
2. MSU/CAVS Capabilities
3. Overall Strategy for Polymer Research
4. Multiscale Material Modeling
5. Case Study
6. Summary
Bagley College of Engineering
Degree Programs

Mechanical Engineering
Industrial Engineering

Software Engineering (Undergraduate only)

Aerospace Engineering

Biological Engineering

Biomedical Engineering (Graduate only)

Chemical Engineering

Civil Engineering

Computer Engineering

Applied Physics (Graduate only)

Electrical Engineering

Computer Science

Computational Engineering (Graduate only)
CAVS STRENGTH: People (about 250)
   Faculty: 47
   Staff: 58
   Graduate students: 85
   Undergraduate students: 79

CAVS GOAL: Become the nation’s premier interdisciplinary high-performance *vehicular* computing research facility.

NEXT STEPS: CAVS has a central focus on computational engineering to serve as our differentiator. We have now broadened the domain definition of the term “vehicular.” We are in the process of defining areas of research which are needed to complement the central focus.
CAVS/ MSU Capabilities

- **Materials Characterization Facilities**
  X-Ray CT Scan, High performance FEG-SEM, EVO–SEM, TALYSURF CLI 2000, Hysitron Nanoindenter, Axiovert Optical Microscope, Particle Size Analyzer, Spectroscopy, ...

- **High Temperature Characterization Facilities**
  TGA, DSC, DMA, Dilatometer, Microwave Sintering Furnace, Arburg Powder Injection Molding, Randcastle–Extruder, Powder Compaction Machine, ...

- **Mechanical Properties - Testing Facilities**
  Hopkinson Bar setup (compression, tension, and torsion), Instron (50 kN, and 100 kN load capacity), Biaxial Instron, MTS (5-25 kN load capacity), Hardness Tester, Structural Test Systems, ...

- **Computational capabilities**
  SunFire X2200 M2 (2048 Opteron proc.), IBM x335 Linux Supercluster (384 Pentium IV proc.), IBM x300 Linux Supercluster (1038 Pentium proc.), UltraSparc SUN

Websites:
http://www.cavs.msstate.edu/cavs4capabilities.php
http://www.dial.msstate.edu/cap/Analytical%20Services%20Laboratory%20Web%20Page%20August%202006.html
http://emcenter.msstate.edu
Goals
A. Develop material database capturing structure-property relationships for thermoplastics, elastomers, foams, and fabrics.
B. Develop internal state variable (ISV) material model. Model will be calibrated using database and verified/validated for a range of strain rates and temperatures.

Motivation
1. Increase the reliability and safety involving designing with polymeric materials for the automotive industry.
2. Better understanding of the mechanical response of polymers
3. Building a material database and developing material models for these materials

Materials
Plastics:
- Polycarbonate (PC)
- Acrylonitrile Butadiene Styrene (ABS)
- Polypropylene (PP)

Rubbers
- Natural rubber
- Santoprene (Vulcanized Elastomer)
- Styrene Butadiene Rubber (SBR)

Foams
- Polypropylene Foam
- Polyurethane Foam

Fabrics
- Kevlar
- Nylon
Polymer Overall Strategy (2)

**Experiments**
- Mechanical Tests
  - Low to High strain rates
  - Temperatures below/above Tg
  - Volumetric testing, relaxation, dissipation, strain paths, stress state
- Impact tests
- Fatigue tests
  - Mechanical / Fatigue tests
    - Test at different strain rates, temperature, Hz (stress/strain ratios, cyclic loading to failure)
    - Micro-structural studies
    - Failure mechanisms (crack initiation / growth)

**Materials**
- **PLASTICS**
  - Polycarbonate (PC)
  - Polypropylene (PP)
  - ABS
- **RUBBERS**
  - Natural Rubber
  - Santoprene
  - SBR
  - TPU
- **FOAMS**
  - PP foam
  - PU foam

**Modeling / Simulation**
- ISV material model (improved):
  - Identification / Calibration
  - FEA Implementation (ABAQUS)
  - Verification
- Fatigue model:
  - Identification / Calibration
  - FEA Implementation (ABAQUS)
  - Verification
- ISV material model:
  - Identification / Calibration
  - FEA Implementation (ABAQUS)
  - Verification
- Fatigue model:
  - Identification / Calibration
  - FEA Implementation (ABAQUS)
  - Verification

**Work supported by:**
- TARDEC (DoD)
- American Chemistry Council
- DOE

**People:**
- Faculty (8), Staff (3), PhD (3), UG (10)
Multiscale Polymer Modeling

Bridge 1 = Interfacial Energy, Elasticity (EAM, MEAM, MD, MS)

Bridge 2 = Mobility

Bridge 3 = Hardening Rules

Bridge 4 = Particle Interactions

Bridge 5 = Particle-Void Interactions

Bridge 6 = Elastic Moduli

Bridge 7 = High Rate Mechanisms

Bridge 8 = Density, T effects

Bridge 9 = Bonding, mobility

Bridge 10 = Nanoparticle, polymer interactions

Bridge 11 = FEA

Bridge 12 = FEA
Studying Polymers with Molecular Dynamics

Typical terms in Inter-atomic potential

\[ E_{bs}(r) = \sum_{\text{atoms}} \{ k \cdot (r-r_0)^2 \} \]

\[ E_{be}(r) = \sum_{\text{atoms}} \{ k \cdot (r-r_0)^2 \} \]

\[ E_{to}(\theta) = \sum_{\text{atoms}} \{ V_1 \cos \theta + V_2 \cos 2 \theta + V_3 \cos 3 \theta + V_6 \cos 6 \theta \} \]

\[ E_{vw}(\vec{r}) = \sum_{\text{nobonded}} \{ A(\vec{r})^{-12} - C(\vec{r})^{-6} \} \]

Nanoscopic specimen of idealized Linear amorphous polyethylene under uniaxial tension (T=100K, nc=200, n_monomers=1000)

Chains alignment (bond torsion)
Multiscale Polymer Modeling

- **Bridge 1**: Interfacial Energy, Elasticity (EAM, MEAM, MD, MS)
- **Bridge 2**: Mobility
- **Bridge 3**: Hardening Rules
- **Bridge 4**: Particle Interactions
- **Bridge 5**: Particle-Void Interactions
- **Bridge 6**: Elastic Moduli
- **Bridge 7**: High Rate Mechanisms
- **Bridge 8**: Density, T effects
- **Bridge 9**: Bonding, mobility
- **Bridge 10**: Nanoparticle, polymer interactions
- **Bridge 11**: FEA
- **Bridge 12**: FEA

- **Electronics Principles (DFT)**
- **Atomistics**
- **Coarse graining, MD and MC**
- **Nanoparticle Crack Interactions**
- **Fracture mechanics (ISV + FEA)**

Macroscopic ISV Continuum

- 100's Nm
- 10-100 µm
- 100-500 µm

Micromechanics (ISV and FEA)
Methodology Applied to Model Mechanical Response of Polymers

EXPERIMENTAL DATA

ISV MATERIAL MODEL

3-D Constitutive Equations + Numerical Integration Procedure

fitting algorithm developed for MATLAB

1-D Constitutive Equations

MODEL CALIBRATION TOOL

1-D Constitutive Equations

Impact Problem (ABAQUS Explicit)

FEA

Numerical Implementation in FEM Codes

Polycarbonate

PC Disk

Adaptive mesh domain

Axially symmetric model

Axisymmetric rigid elements RAX2

Axisymmetric deformable elements CAX4R

Size 0.1 mm and 1.45 mm

striker

Multiscale Experiments

16,000x

3.5mm Extension  11.5mm Extension  15.0mm Extension

Void Nucleation  Void Coalescence

16.3mm Extension  49.0mm Extension  Extension Until Failure

Nanoscale

Model
Cohesive Energy
Critical Stress

Analysis
Fracture
Interface Debonding

Experiment
TEM

Microscale

ISV Model
Void Growth
Void/Crack Nucleation

Experiment
SEM
Optical methods

FEM Analysis
Crystalline Plasticity

Mesoscale

ISV Model
Void Growth
Void/Crack Nucleation

Experiment
Fracture of Silicon
Growth of Holes

FEM Analysis
Idealized Geometry
Realistic RVE Geometry
Monotonic/Cyclic Loads
Crystal Plasticity

1. Exploratory exps
2. Model correlation exps
3. Model validation exps
1. Exploratory exps
2. Model correlation exps
3. Model validation exps
Compression Tests Results - Rubbers

Strain Rate Dependence (RT)

Santoprene

SBR

NR

Temperature Dependence (0.01 /s)

Santoprene

SBR

NR
**Goals**

A. Capture experimentally the mechanical properties of Thermoplastic Polyurethane (TPU)
B. Develop an internal state variable (ISV) material model for this material.
C. Develop a preliminary multiscale fatigue model to predict the failure of real structural component

**Approach**

♦ Carry out experiments using current testing methodologies:
  - Dynamic Mechanical Analyzer (DMA)
  - Thermogravimetric Analysis (TGA)
  - X-Ray Diffraction (XRD)
  - INSTRON (tensile and compressive testing)
♦ Develop ISV material model
  - Develop a model calibration procedure (MATLAB)
  - Model implementation in finite element code (ABAQUS).
♦ Develop a Multiscale Fatigue Model
♦ Perform finite element analysis to understand/improve the performance of a structural component design
Mechanical Behavior at the Coupon Level (monotonic loading)

- Strain rate dependence
- Temperature dependence
- Mullins’s effect (cyclic loading)
- Strain history effect
- Cyclic strain history effect
- Strain rate history effect
Stress - Life With Frequency Effects

Mechanisms leading to failure?
Fatigue Behavior: Internal Heat Build-up Leads to Failure

Failure = specimen deformed 5% from steady state length
ISV Material Model Prediction

- Branch A: Elastic rubbery spring
- Branch B: Hyperelastic rubbery spring
- Nonlinear viscous dashpot
- Frictional element

**Maximum strain level**
- Illustration of stress-strain curves for different strain levels.

**Mullins’ effect**
- Comparison of test data (black squares, red triangles) with model predictions (blue circles, blue triangles).

**Relaxation tests**
- Graphs showing stress relaxation with time for different strain levels.

**Strain rate dependence**
- Stress-strain curves for various strain rates (0.1/s, 0.05/s, 0.01/s) compared to model predictions.
ISV Material Model prediction (isothermal problems)
Thermal Fatigue Simulation at Medium Frequency for Various Stress Levels
Component Life Prediction

Wheel dynamometer testing

Simulations accurately predict internal temperature increase and cycles to failure

Thermocouples embedded for internal measurements
Summary

1. Multidisciplinary Center

2. Lab equipment / Computational capability

3. Multiscale experiments

4. Multiscale modeling frameworks with ISV approach.

5. Application to Polyurethane insert component