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

Advanced Materials: Models and Methods Forum
March 18, 2010
**Report Documentation Page**

Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.

<table>
<thead>
<tr>
<th>1. REPORT DATE</th>
<th>2. REPORT TYPE</th>
<th>3. DATES COVERED</th>
</tr>
</thead>
<tbody>
<tr>
<td>18 MAR 2010</td>
<td>N/A</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4. TITLE AND SUBTITLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tribology and Friction of Soft Materials: Mississippi State Case Study</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>5a. CONTRACT NUMBER</th>
</tr>
</thead>
<tbody>
<tr>
<td>W56 HIZV-08-C-0236</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>6. AUTHOR(S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>J.L. Bouvard; E.B. Marin; D. Oglesby; K. Solanki; B. Kirkland; M.F. Horstemeyer; P. Wang; R.L. King</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mississippi State University: Center for Advanced Vehicular Systems</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>8. PERFORMING ORGANIZATION REPORT NUMBER</th>
</tr>
</thead>
<tbody>
<tr>
<td>20625</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)</th>
</tr>
</thead>
<tbody>
<tr>
<td>US Army RDECOM-TARDEC 6501 E 11 Mile Rd Warren, MI 48397-5000, USA</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>10. SPONSOR/MONITOR’S ACRONYM(S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TACOM/TARDEC</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>11. SPONSOR/MONITOR’S REPORT NUMBER(S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20605</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>12. DISTRIBUTION/AVAILABILITY STATEMENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approved for public release, distribution unlimited</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>13. SUPPLEMENTARY NOTES</th>
</tr>
</thead>
<tbody>
<tr>
<td>The original document contains color images.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>14. ABSTRACT</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>15. SUBJECT TERMS</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>16. SECURITY CLASSIFICATION OF:</th>
<th>17. LIMITATION OF ABSTRACT</th>
<th>18. NUMBER OF PAGES</th>
</tr>
</thead>
<tbody>
<tr>
<td>a. REPORT unclassified</td>
<td>SAR</td>
<td>24</td>
</tr>
<tr>
<td>b. ABSTRACT unclassified</td>
<td></td>
<td></td>
</tr>
<tr>
<td>c. THIS PAGE unclassified</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>19a. NAME OF RESPONSIBLE PERSON</th>
</tr>
</thead>
</table>

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
(Academic only)

Aerospace Engineering

Biological Engineering

Mechanical Engineering

Chemical Engineering

Civil Engineering

Biomedical Engineering
(Graduate only)

Applied Physics
(Graduate only)

Electrical Engineering

Computer Science

Computational Engineering
(Graduate only)
CAVS Today

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
Polymer Overall Strategy (1)

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

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.

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

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

Macroscale ISV Continuum

Micromechanics (ISV and FEA)

Coarse graining, MD and MC

Coarse graining

A

B

100's Nm

10-100 µm

Nanoparticle/ crack
Interactions
Fracture mechanics (ISV + FEA)

Electronics Principles (DFT)

Atomistics (EAM, MEAM, MD, MS)

Fracture mechanics (ISV + FEA)

100-500µm

1-1000 µm

100's Nm
Typical terms in Inter-atomic potential

\[ E_{bs}(r) = \sum_{\text{atoms}} \{ k_1 (r - r_0)^2 \} \]  

\[ E_{be}(r) = \sum_{\text{atoms}} \{ k_2 (r - r_0)^2 \} \]

\[ E_{to}(\theta) = \sum_{\text{atoms}} \{ V_1 \cos \theta + V_2 \cos 2\theta + V_3 \cos 3\theta + V_4 \cos 4\theta \} \]

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

Studying Polymers with Molecular Dynamics

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

Van der Waals interaction

Chains alignment (bond torsion)
Multiscale Polymer Modeling

- Bridge 1 = Interfacial Energy, Elasticity
- 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

---

Macroscopic ISV Continuum

- Coarse graining, MD and MC
- Atomistics (EAM, MEAM, MD, MS)
- Electronics Principles (DFT)

- Fracture mechanics (ISV + FEA)
- Micromechanics (ISV and FEA)

- 100-500 µm
- 10-100 µm

---

Nanoparticle/crack interactions

100's Nm
Methodology Applied to Model Mechanical Response of Polymers

EXPERIMENTAL DATA

ISV MATERIAL MODEL

MODEL CALIBRATION TOOL

1-D Constitutive Equations

3-D Constitutive Equations + Numerical Integration Procedure

fitting algorithm developed for MATLAB

Impact Problem (ABAQUS Explicit)

Axisymmetric rigid elements RAX2
Axisymmetric deformable elements CAX4R
Size 0.1 mm and 1.45 mm

FEA

Numerical Implementation in FEM Codes
Multiscale Experiments

Nanoscale
- Model
  - Cohesive Energy
  - Critical Stress
- Analysis
  - Fracture
  - Interface Debonding
- Experiment
  - TEM

Microscale
- ISV Model
  - Void Nucleation
- FEM Analysis
  - Idealized Geometry
  - Realistic Geometry
- Experiment
  - SEM
  - Optical methods

Mesoscale
- ISV Model
  - Void Growth
  - Void/Crack Nucleation
- Fem Analysis
  - Idealized Geometry
  - Realistic RVE Geometry
  - Monotonic/Cyclic Loads
  - Crystal Plasticity
- Experiment
  - Fracture of Silicon
  - Growth of Holes

1. Exploratory exps
2. Model correlation exps
3. Model validation exps
Multiscale Experiments

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

Strain Rate Dependence (RT)

Temperature Dependence (0.01 /s)
MSU/ CAVS Case Study

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?

Nominal Stress vs. Cycles for different frequency effects:
- Low Frequency
- Medium Frequency
- High Frequency

Test stopped, temperature reached equilibrium.
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
- Nonlinear viscous dashpot
- Frictional element

Branch B
- Hyperelastic rubbery spring

Maximum strain level
- Test Strain max = 50%
- Model Strain max = 50%
- Model Strain max = 100%

Mullins’ effect
- Test N=1
- Model N=1
- Model N=2
- Test N=2
- Test N=4

Relaxation tests

Strain rate dependence

Test 0.1/s
- Test 0.05/s
- Test 0.01/s
- Model 0.1/s
- Model 0.05/s
- Model 0.01/s
ISV Material Model prediction (isothermal problems)
Thermal Fatigue Simulation at Medium Frequency for Various Stress Levels

Temperature vs. Cycles graph showing experimental and simulated data for different stress levels (5MPa, 6MPa, 8MPa, 10MPa).
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