A Micro-scale Approach to Evaluate the Asphalt Low Temperature Properties

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1. Introduction

2. Evaluation of Fatigue properties of asphalt binder, mastic and mixture

3. Application of Phase-Field Method and MD Simulations in Asphalt Binder Fracture

4. Conclusions and Challenges
Research Objectives

- The fatigue cracking and fracture are the two most common distresses on state highway.
- What are the root causes and how to evaluate them?
Introduction

- **Numerical Modeling**
  - Finite Element Method; Phase-Field Method; Molecular Dynamics Simulation

- **Experiments**
  - Direct Tension Test; X-ray Tomography; Atomic Force Microscopy

- **Digital Mix Design**
  - Digital Specimen and Digital Test
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Experiment: fatigue test

Direct Tension Tester (DTT) is altered to build up a new fatigue test procedure.
Evaluation of Fatigue properties of asphalt binder, mastic and mixture

- New fatigue test procedure can be written.
- Cyclic tensile loading can be applied.
- Test temperature can be controlled.
Evaluation of Fatigue properties of asphalt binder, mastic and mixture

Materials

- Asphalt Binder
  - PG 70-22 Binder

- Asphalt Mastic
  - PG 70-22 Binder + Quartz Filler

- Asphalt Mixture
  - PG 70-22 Binder + Aggregates with controlled size (0.5~4.76mm)
Evaluation of Fatigue properties of asphalt binder, mastic and mixture

➢ X-ray Tomography

X-ray system (Wang, 2003)

Sky Scan 1174 Compact X-ray system
Evaluation of Fatigue properties of asphalt binder, mastic and mixture

Fatigue Test Comparison

<table>
<thead>
<tr>
<th>Specimens</th>
<th>Average final strain</th>
<th>Average number of cycles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Binder</td>
<td>0.0059</td>
<td>105</td>
</tr>
<tr>
<td>Mixture no filler</td>
<td>0.0124</td>
<td>1676</td>
</tr>
<tr>
<td>Mixture with 30% filler</td>
<td>0.0459</td>
<td>12226</td>
</tr>
<tr>
<td>Mastic with 20% filler</td>
<td>0.0587</td>
<td>16395</td>
</tr>
<tr>
<td>Mastic with 30% filler</td>
<td>0.0684</td>
<td>19208</td>
</tr>
<tr>
<td>Mastic with 40% filler</td>
<td>0.0652</td>
<td>17457</td>
</tr>
</tbody>
</table>
Evaluation of Fatigue properties of asphalt binder, mastic and mixture

Numerical Modeling

Single Aggregate  Multiple Aggregates
Digital specimen and digital test

- Center node of the loading surface
- Number of loadings and final strain

<table>
<thead>
<tr>
<th></th>
<th>Lab results</th>
<th>Simulation results</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Number of</td>
<td>Strain</td>
</tr>
<tr>
<td></td>
<td>loading</td>
<td></td>
</tr>
<tr>
<td></td>
<td>cycles</td>
<td></td>
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Phase Field and Interface

Material between intact ($\phi=1$) and fully broken ($\phi=0$) states, is considered as $0<\phi<1$. Two kinds of interface can be used.

Figure 1 (a) Sharp interface (b) Diffuse interface*

*http://nele.studentenweb.org/research/?subject=PFM
Fundamental Concepts in PFM

- A model for a phase field can be constructed by physical arguments if one has an explicit expression for the free energy of the system.
- The driving force of the system is either Chemical potential or the gradient of Chemical potential.

I. Free energy \((f(\phi))\)
   - A thermodynamic potential that measures the "useful" or process-initiating work of a system.
   - It is calculated by MD simulation.

II. Chemical potential \((G \text{ or } \mu)\)
   - A measure of the potential that a substance has to produce in order to alter a system.
   - It is calculated as the variational derivative of free energy with respect to order parameter.
Phase kinetics

- Spinodal decomposition*
  Two components can separate into distinct regions (or phases) with distinctly different chemical compositions and physical properties.
- A simple example
  The figure shows that a cup of red ink is well mixed with water. After a certain time, ink and water will get separated due to different gravitational potential energy.

  Asphalt fracture develops since fracture phase and intact phase has different chemical potential and they get phase separated.

*Figure is from http://pruffle.mit.edu/3.00/Lecture_32_web/node3.html
Application of Phase-Field Method in Asphalt Binder Fracture

- Phase field equations
  - Total free energy is expressed as
    \[ F = \int_{\Omega} (f_{gr} + f_{local} + f_{el}) d\Omega \]
  - The gradient energy density \( f_{gr} = \frac{1}{2} \lambda |\nabla \phi|^2 \).
  - The local free energy density \( f_{local} = \frac{\lambda}{4\epsilon^2} (1 - \phi)^2 (1 + \phi)^2 \) is a commonly used double well potential.
  - The elastic energy density \( f_{el} = \frac{E(\phi)}{2(1+\nu)} \left( \frac{\nu}{1-2\nu} (\varepsilon_{ii})^2 + \varepsilon_{ik} \varepsilon_{ik} \right) \)
    Where \( E(\phi) = E + (E - E_0) h(\phi) \) is the elastic modulus
    and \( h(\phi) = -\frac{1}{4} \phi^3 + \frac{3}{4} \phi + \frac{1}{2} \) interpolates the void phase (\( \phi = -1 \)) and the intact phase (\( \phi = 1 \));
    Possion’s ratio \( \nu = 0.3 \) is phase-independent.

- Allen-Cahn equation (Non-conserved case)
  \[ \frac{\partial \phi}{\partial t} = -M \frac{\delta F}{\delta \phi} \]
Application of Phase-Field Method in Asphalt Binder Fracture

- A simple case with self-adaptive meshing
MD simulations

Molecular structure of crack tip in the molecular dynamics (MD) model: (a) & (b) initial view molecular structure from different views (c) molecular structure after tension failure.

Atoms are missing at the dislocations.
Multi-scale Approach

Multi-scale Approach based on MD and PFM
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Conclusions and Challenges

Conclusions

- Filler improves binder fatigue resistance. 30% optimum filler content.
- Digital Specimen and Digital Test improve understanding.
- Phase-field Method could capture and simulate the asphalt fracture.
- A multi-scale approach could tie macro properties such as the stress concentration with molecular structure.

Future Plan

- Further verification and validation
Thank you!