International Association of Chinese Infrastructure Professionals

Molecular dynamics study of interfacial mechanical behavior between asphalt binder and calcium silicate hydrate

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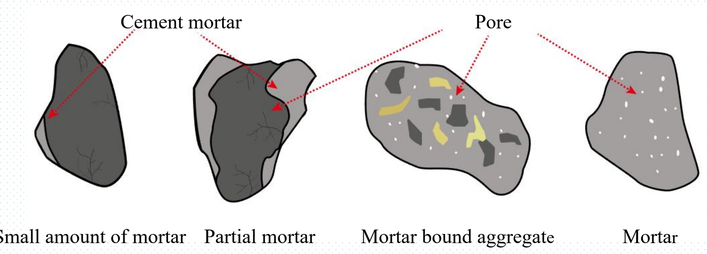
Introduction

- **The application of recycled concrete aggregates (RCA) in asphalt pavements is one of the ways to dissipate construction and demolition waste as well as replace natural aggregates for the purpose of conserve energy and reduce emissions.**
- **A considerable amount of mortar is adsorbed on the aggregate surface, and the mechanical behavior of asphalt/mortar interface is still unclear.**

RCA asphalt pavement.

Construction waste.



Mortar and pore characteristics of recycled aggregate from building solid wastes.

Objectives

- **To reveal the relationship between mechanical properties and microstructure of asphalt aggregate system.**
- **At the same time, the asphalt film thickness, strain rate, water content and other factors were studied.**

Materials and Methods

Simulation Model

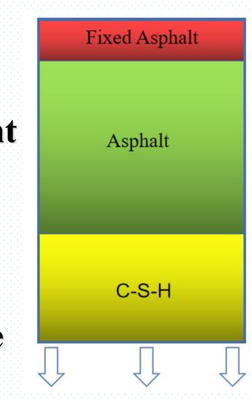
C-S-H

H_2O

Asphalt

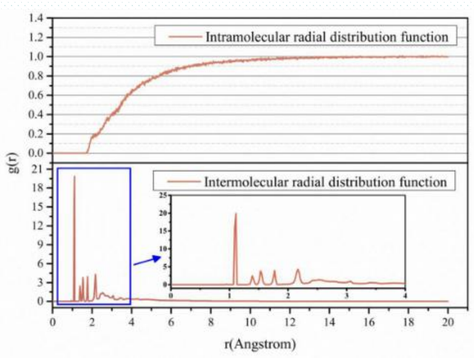
Simulation Details

- **The asphalt/C-S-H system model was relaxed with an NVT ensemble at 300 K for 500 ps to approximate constant temperature.**
- **It is necessary to apply the boundary condition in Z direction, fix the asphalt at the upper end, and move the calcium silicate hydrate at the lower end.**



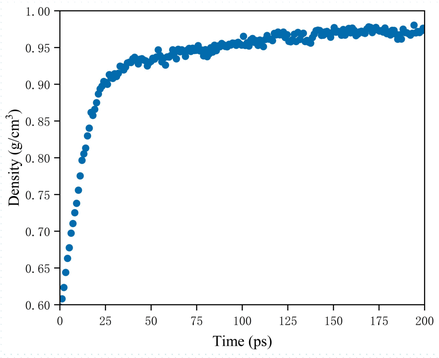
schematic of tensile simulation.

Model Validation



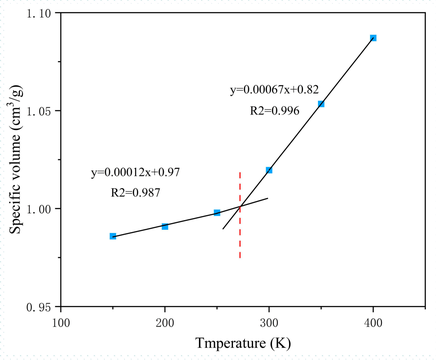
Radial distribution functions of neat asphalt.

- **The asphalt model is a short-range ordered,long-range disordered structure; the molecular interactions are mainly hydrogen bonds and van der Waals forces.**



Density evolution with equilibration of binder models.

- **Literature data for experimental asphalt is 1.03-1.04 g/cm³. The difference between the experimental and simulation results are approximately 0.06 g/cm3.**

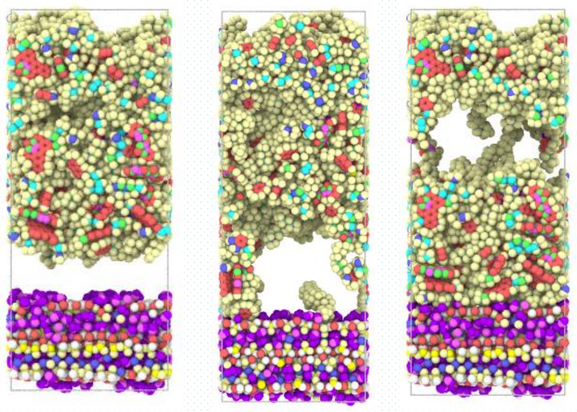


Specific volume versus temperature for asphalt

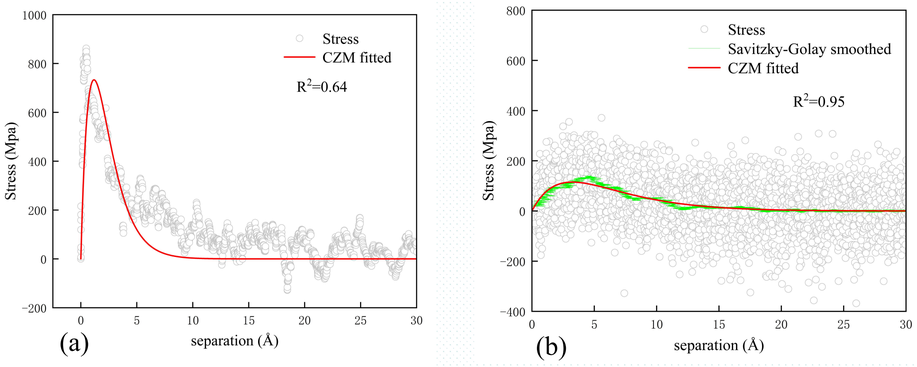
- **It can be observed that a steady increase of specific volume, which equals a steady decrease of density, was observed with increasing temperature.**

Results and Analysis

Failure Mode of Asphalt-CSH Interface



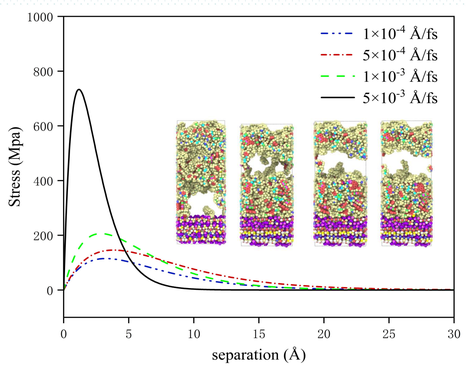
adhesive failure case and cohesive failure case.



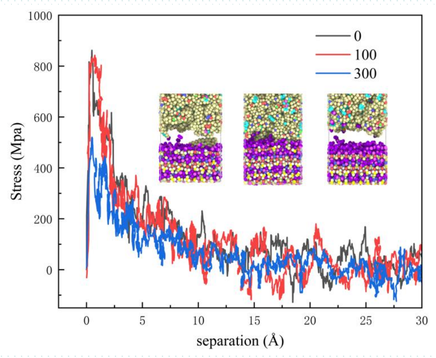
Stress-separation curve of pull-off MD simulation: (a) adhesive failure case; and (b) cohesive failure case.

- **When the loading rate decreases, the interface failure mode changes from adhesive failure to cohesive failure.**

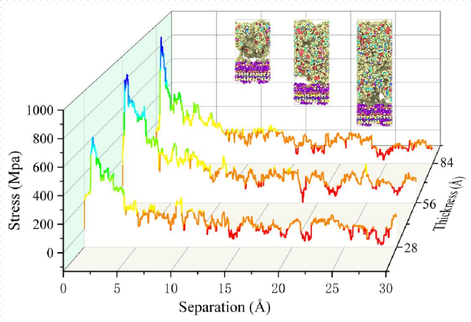
Effect of Strain rate, Moisture, Asphalt film thickness and Temperature



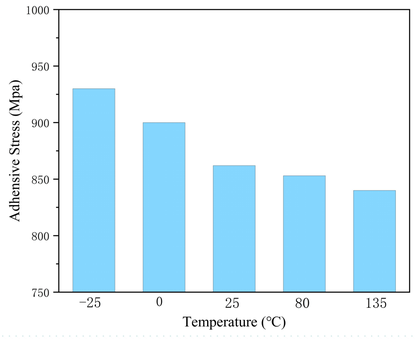
Effect of strain rates on stress-strains relationship.



Effect of moisture on stress-strains relationship.



Effect of asphalt film thicknesse on stress-strains relationship.



Effects of temperatures on predicted adhesive stress.

- **Cohesive failure is prone to occur at lower loading rates , whereas adhesive failure dominated at higher loading rates.**
- **The negative relation between interfacial bonding strength and moisture content demonstrates.**
- **this study did not find any significant changes in failure mode with different asphalt film thickness.**
- **A decreasing trend of interfacial tensile strength was observed with increasing temperature.**

Conclusions

- **The effects of loading rate, asphalt film thickness, temperature and water content on asphalt stability were studied. Cohesive failure tends to occur at lower loading rates, while adhesive failure dominates at higher loading rates. In addition, when the failure mode changes, there will be a significant difference in the failure strength. The value of adhesive failure is about 4 times of cohesive failure.**