MULTI-SCALE AND MULTI-PHYSICS MODELING OF THE STRENGTH OF GEOPOLYMER COMPOSITES

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EXECUTIVE SUMMARY

Geopolymers are a class of inorganic polymeric, X-ray amorphous materials consisting of alumina, silica, and alkali metal oxides [1]. Geopolymer composites exhibit appealing properties such as high thermal stability [2], small carbon dioxide footprint [3], and high strength, which makes them suitable for many applications including alternative cementitious materials [4], passive cooling systems [5], low-level nuclear waste encapsulation [6], and potential novel biomaterials. The research goal is to understand the impact of nanoporosity on stiffness and strength via molecular dynamics and finite element modeling. Nanoporosity is governed by monovalent cation and water content. In contrast, microporosity results from the mixing procedure and from poor bonding between the geopolymer matrix and the filler phase. To increase the performance of geopolymer composites several strategies were found: reduce the microporosity, select strong inclusions, increase the volume content of stiff inclusions, or select fillers with a high aspect ratio. These findings pave a new way toward novel, high-performance, and multi-functional composites.

RESEARCH CHALLENGE

Geopolymer composites are an emerging class of composites with great potential in civil engineering, mechanical engineering, aerospace, navy, automobile, and biomedical engineering. However, the widespread application and acceptance of geopolymer systems has been so far impeded by many roadblocks such as lack of long-term durability data [7], lack of in-service track record, and lack of standard geopolymer cements [8]. The computational approach selected based on molecular dynamics and finite elements offer a cost-effective and time-efficient means to accelerate discovery and innovation.

METHODS & CODES

At the nanoscale, atomic simulations were performed in LAMMPS, as shown in Fig. 2b. Various molecular structures were recreated using the Avogadro and Packmol software, for diverse alkali metal cations and Si:Al ratios. The amorphous structure was obtained through a melting and quenching sequence. Afterward, uniaxial tensile and compression tests along with shear tests were simulated to yield the strength behavior and failure micromechanisms. The software OVITO was utilized for visualization. At the mesoscale, the finite element package Abaqus was used (Fig. 2a). The microstructure was generated from OOF2D and MATLAB based on scanning electron microscopy observations of geopolymer composites. The constitutive behavior of the individual constituents was prescribed based on independent

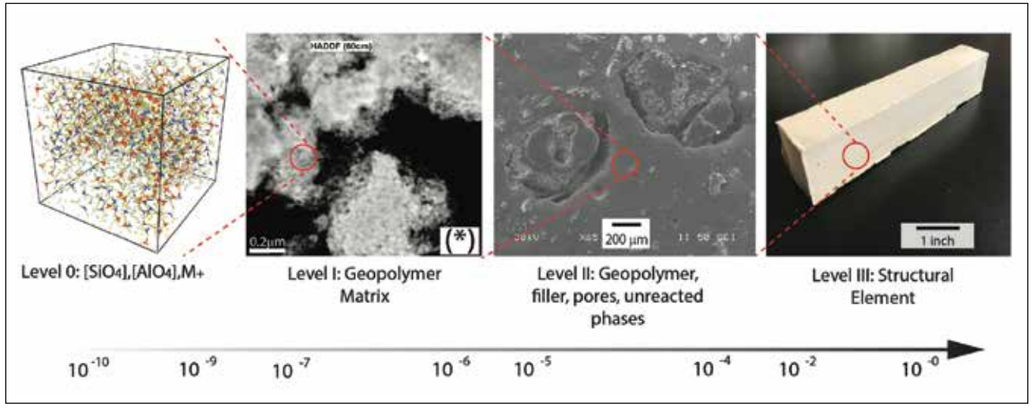

Figure 1: Multiscale nature of geopolymer composites. Our study spans levels 0 at the nanometer length-scale to level III at the macroscopic level.

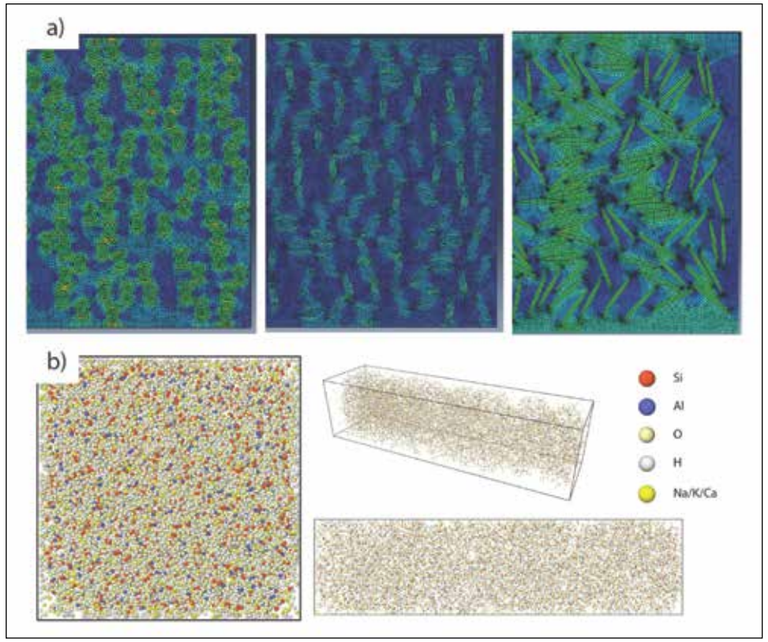

Figure 2: a) FEM model at mesoscale showing the stress distribution as a function of the filler aspect ratio. b) Molecular dynamics modelling of inorganic polysialate disiloxo.

experiments. Tensile tests with prescribed periodic boundary conditions were simulated to yield the effective response.

RESULTS & IMPACT

The strength and stiffness of amorphous geopolymers were correlated to its chemistry and density. The nanoporosity was found to be a function of the alkali and Si:Al ratio. At the mesoscale, the mechanical resistance of geopolymer composites to permanent deformation was elucidated as a function of the type, nature, size, and shape of the inclusions. Our theoretical and computational framework was validated on 31 different geopolymer-based systems, based on experiments carried out by various researchers over seven years. To our knowledge, it is the first time that a theoretical model has been proposed to upscale the constitutive behavior of geopolymers. In future efforts, we will model the evolution of the fracture toughness of pure geopolymer for various densities via molecular dynamics.

WHY BLUE WATERS

The Blue Waters platform was essential to carry out our molecular dynamics simulations as well as our finite element simulations. Standard desktop workstations do not have the required memory and computational power to resolve the complex systems involved. For molecular dynamics, it was crucial to be able to simulate large systems in a timely fashion. In the case of finite element simulations, the nonlinearity of the equations due to friction, contact, and plastic flow made it impossible to obtain results using a desktop workstation. In both cases, the Blue Waters supercomputer has enabled us to obtain novel results that bring new insights into the origins of strength and toughness in geopolymer composites.

PUBLICATIONS AND DATA SETS

Kataruka, A., S. Koric, W. Kriven, and A.-T., Akono, Strength Properties of Particulate Potassium-Based Geopolymer Composites. *ASCE Engineering Mechanics Institute Meeting*, San Diego, Calif., June 4–7, 2017.

Cui, Y., E. Guleryuz, and A.-T. Akono, Investigation of the Mechanical Properties of geopolymer binders using molecular dynamics simulations. *ASCE Engineering Mechanics Institute Meeting*, San Diego, Calif., June 4–7, 2017.

Kataruka, A., et al., Representative Elementary Volume Modeling of Geopolymer Composites. *14th U.S. National Congress on Computational Mechanics*, Montreal, QC, Canada, July 17–20, 2017.

Cui, Y., et al., Molecular dynamics study on the mechanical and fracture properties of geopolymer binders. *8th Advances in Cement-Based Materials American Ceramic Society*, Atlanta, Ga., June 26–28, 2017.

Kataruka, A., et al., A Parametric Study of Strength Properties of Particulate Potassium-Based Geopolymer Composites. *8th Advances in Cement-Based Materials American Ceramic Society*, Atlanta, Ga., June 26–28, 2017.