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Collaborative Research: An Integrated Microstructure-Based Approach to Property Prediction for Cement-Based Materials

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Principal Investigator: Landis, Eric N.

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Submitted By:

Landis, Eric - Principal Investigator

Title:

Collaborative Research: An Integrated Microstructure-Based Approach to Property Prediction for Cement-Based Materials

Project Participants

Senior Personnel

Name: Landis, Eric

Worked for more than 160 Hours: Yes

Contribution to Project:

Post-doc

Graduate Student

Name: Ellis, Nathan

Worked for more than 160 Hours: Yes

Contribution to Project:

This person is supported by the project as a regular graduate research assistant. His research conducted as a part of this project will lead to an MS degree in civil engineering.

Name: Phillips, Megan

Worked for more than 160 Hours: Yes

Contribution to Project:

Graduate Research Assistant, primarily responsible for microtomography experiments and data analysis. Works directly with PI and other research assistants.

Name: de Wolski, Sean

Worked for more than 160 Hours: Yes

Contribution to Project:

Originally came on project as an Undergraduate Research Assistant, however, transitioned to Graduate Research Assistant during this reporting period. Primary responsibility is in-situ load frame, including electronics, control, and data acquisition. Participated in experimental work at Advanced Photon Source.

Undergraduate Student

Name: Livingston, Clarissa

Worked for more than 160 Hours: Yes

Contribution to Project:

This student is conducting research as a part of this project as an undergraduate research assistant. Part of her work is independent, and part is in support of the graduate research assistant.

Name: Fogg, Lacey

Worked for more than 160 Hours: No

Contribution to Project:

This student is providing support to both the graduate research assistant and the other undergraduate research assistant.

Name: Lingley, Sarah

Worked for more than 160 Hours: Yes

Contribution to Project:

Undergrad Research Assistant. Assisted with preparation of specimens and data analysis.

Name: Dumas, Katie

Worked for more than 160 Hours: No

Contribution to Project:

Undergraduate research assistant

Name: Martin, Katrina

Worked for more than 160 Hours: No

Contribution to Project:

Undergraduate research assistant

Technician, Programmer

Other Participant

Research Experience for Undergraduates

Organizational Partners

Argonne National Laboratory

Project staff conducted experiments at the Advanced Photon Source (APS) at ANL. Facilities and assistance were provided by the DND-Collaborative Access Team, APS Sector 5.

Other Collaborators or Contacts

Denis T. Keane, Director of the DND CAT at the Advanced Photon Source, Argonne National Laboratory. Dr. Keane collaborated on the x-ray microtomography experiments, providing necessary support at the x-ray beamline. Dr. Keane and PI Landis also collaborated on a tutorial publication related to this and other joint projects.

Activities and Findings

Research and Education Activities: (See PDF version submitted by PI at the end of the report)

Research activities over the latter half of the project have involved comparisons of physical and numerical specimens of micro-concrete tested in the split-cylinder configuration. As noted in the interim progress reports, the micro-concrete was formed of spherical glass aggregates embedded in a fine-grained mortar matrix. The positioning of the glass aggregates was determined through micro-tomographic analyses of the physical specimens. This information was used to discretize the numerical specimens so that, at least in terms of aggregate positioning, a one-to-one correspondence was established between the physical and numerical specimens. For the fracture analyses, strength and stiffness of the mortar matrix were calibrated using the test results of physical specimens without glass aggregates. No additional calibration efforts were made, so that the analyses of the specimens with glass aggregates can be regarded as semi-predictive. Fracture patterns and load-displacement curves up to peak load were compared and good agreement was found (see Figs. F-1 to F-3 attached to this report), thus validating some aspects of the model. In Fig. F-3, the results for the U- and E-series correspond to untreated and acid-etched glass aggregates, respectively. Acid-etching was done to improve the bond properties between the glass and mortar matrix.

More recently, the model has been used to explore potential variations in peak strength due to: 1) random variations in the positions of the glass aggregates; and 2) changes in aggregate content. Models were constructed for 100 nominally identical specimens (differing only in random placement of the acid-etched glass aggregates) for aggregate weight fractions of 10, 20, and 30%. Histograms of peak strength, normalized by the experimental mean peak strength for an aggregate content of 10 wt%, are shown in Fig. F-4. The normalized peak strength for the case of 10 wt% of aggregates is quite close to the experimental mean value. With increasing aggregate content, mean peak strength provided by the model decreases. The rate of strength decrease with increasing aggregate content agrees well with the numerical experiments of Lilliu (2007).

In project year 3, we tested physical specimens with 0, 10, and 50 wt% of untreated and acid-etched glass aggregates. Peak loads were accurately recorded, but displacement measurements were complicated by a faulty sensor. Models were constructed for 10 nominally identical specimens containing 50 wt% of acid-etched aggregates. (The smaller number of models is due to their higher computational expense, since finer meshes are needed to resolve the more closely packed aggregates and their interfaces with the matrix.) Figure F-5 shows the dependence of peak strength on aggregate content, according to the physical and numerical test results; the error bars indicate one standard deviation about the mean strength values. The composite strength values have been normalized by the matrix strength, so that the two different test groups (of project years 3 and 4) can be compared. From these results, several points can be made:

1. The physical and numerical test results agree well for all tested/simulated amounts of glass aggregates. Only the strength and stiffness of the matrix were calibrated, whereas the other quantities were assumed from the literature, so that these numerical results can be viewed as predictions.

2. The variation of strength for the numerical models is significantly smaller than that observed in the physical test results. This is reasonable considering the potential sources of variability in the physical test specimens, such as positioning of the glass aggregates, unevenness along the loading surfaces, differences in specimen size and geometry, and the presence of some large air voids. Potential sources of variability in the models are limited to the random positioning of the glass aggregates and some minor degree of mesh bias.

A 3-D sub-voxel resolution vector displacement field algorithm was finally implemented and validated in the final project year. The program determines the movement of any voxel in two successive images of the same specimen, and it is accurate to within 0.1 voxels 92% of the time. Because we were not able to implement this program until the final project year, the findings from this work are not yet significant. Currently we are using the code to measure 3-D strain fields in the specimens tested, and comparing the measurements to results predicted by strain invariant based failure theories.

Collaborative Activities

The findings described within this report depended on routine contact and data exchange by the PIs at the collaborating institutions. Throughout the project duration, the PIs conferred by phone and met at jointly attended conferences. This past project year included a visit by Landis to UC Davis to meet with Bolander?s group and review the most recently obtained data. One outcome of that meeting has been a proposal for one of the UC Davis PhD students to continue the work at UMaine upon graduation.

Findings:

Major Findings

This collaborative research involved the coordinated use of micro-tomographic imaging/analysis and three-dimensional lattice modeling to improve current understandings of brittle-matrix composite materials, such as concrete, under mechanical loadings. Emphasis was placed on tracing the development of pre-critical cracking within the material meso-structure. This was accomplished by establishing a one-to-one correspondence between the meso-scale features in the physical and numerical specimens, which were subjected to similar boundary conditions.

The outcomes of the work conducted under this award are a major step in our movement towards physical (microstructure-based) computational modeling of concrete materials. High-resolution 3-D imaging of heterogeneous materials provides spatial mappings of the material phases and developing features (e.g., microcracks), from which realistic 3-D models can be created and validated. As seen from the project results, including Figs. F-1 to F-5 attached to this report, these models can accurately simulate not only bulk load-deformation properties, but also crack patterns and failure modes. As such, numerous numerical experiments can be run on different random structures to study material structure-property relationships and the sources of response variability.

More specific outcomes/findings of this collaborative project are:

1. These methods of analysis are complimentary. The tomographic images provide much higher spatial resolution of material structure and damage within the specimens, relative what has been achieved with the lattice model. One the other hand, the tomographic measurements of crack development were taken at discrete load stages (and the number of stages per specimen was small, due to limited access to the APS facilities). The numerical model provided an event-by-event (quasi-continuous) description of the fracture processes. These two disparities (i.e., the differences in abilities to resolve the spatial and event-sequencing aspects of material fracture) point to opportunities for improvement of both methods.

2. The tomographic images provide benchmarks for validating the lattice models. In some instances, the patterns of cracking through the composite material agree quite well, as seen in Fig. F-2. The experimental and simulated load-displacement curves for each type of glass aggregate surface are shown in Fig. F-3. As matrix stiffness and strength were calibrated with an independent data set, these simulation results are predictions, at least to some degree. This high degree of correspondence between experimental results and 3-D modeling of fracture at the material meso-scale is a significant accomplishment in concrete materials study, especially considering the small scale at which the tests were conducted.

3. The bulk of previous fracture modeling of concrete materials at the mesoscale has been for tension-dominant loadings. Tensile fracture induced by orthogonal compression, as occurs during the split cylinder testing considered here, has received much less attention even though it is an important practical concern (e.g. diagonal compression-shear failure of concrete beams). Such multi-axial stress conditions place additional demands on the fracture model, particularly for lattice models, which are inherently disadvantaged by their use of one-dimensional elements. To address this issue, the PI?s developed an element fracture criterion based on tensorial measures of stress calculated at the element nodes. When loaded in compression, the lattice model of the split cylinder specimen develops lateral tension over it midsection (in close agreement with theory and without mesh bias).

a) For the case of the fine-grained matrix, without glass aggregates and assumed to be homogeneous, peak load matches the theoretical strength and exhibits practically no scatter. For 25 numerical specimens, differing only in random discretization of the matrix, the coefficient of variation of split cylinder strength is only 0.0030. This ability of the fracture model, implemented within an irregular lattice model of a continuum, to remove mesh bias from the solution is a noteworthy outcome of this research.

b) For the case of the micro-concrete, composed of spherical glass aggregates within the fine-grained matrix, fracture begins with debonding along the lateral surfaces of the glass aggregates most centrally located within the load path (Fig. F-1). Increasing interface strength increases the loads at which this debonding initiates and matures. For the interface-to-matrix strength ratios (of 0.25 and 0.5) and low aggregate contents considered at that stage of the project, however, interface strength did not have an appreciable effect on composite strength. Failure initiates just before or at peak load, and consists of interfacial cracks extending into the matrix and coalescing to form a failure surface through most of the specimen depth. Although this characterization of failure is not new, the event-by-event tracing and quantification of the failure process are significant advances. Representation of broken elements by their Voronoi facets is unique to the PI?s work and provides a more easily interpretable depiction of fracture surfaces, in comparison to what is done with other lattice models.

4. Direct comparisons of numerical specimens with the project year 4 data set, shown in Figs. F-2 and F-3, served to partially validate the modeling approach. As a next step, the PIs constructed 100 nominally identical specimens, differing only in random positioning of the glass aggregates, for each of several weight fractions of aggregates. As shown in Fig. F-5, the simulated mean values of split cylinder strength agree well with the experimental means for the range of weight fractions considered. Both result types exhibit variations in strength about the mean values. The numerical specimens exhibit much less scatter. This is reasonable considering the only potential source of variability in the numerical specimens comes from the random positioning of aggregates, whereas the potential sources of variability in the physical specimens are more numerous. These preliminary results are noteworthy as they point to the model?s potential for exploring the effects of material/structural variability on structural performance.

5. Several 3D image processing algorithms were developed to facilitate analysis of the very large data sets. Of note was a method to segment the glass bead aggregates based on texture rather than the more common intensity approach. Intensity-based segmentation was not possible because the x-ray absorption of the beads was in a narrow band that was straddled by the more widely banded absorption of the cement hydrates. This segmentation was a critical step in matching spatial distributions of aggregates between real and simulated specimens.

Training and Development:

At UMaine, two graduate research assistants (one MS and one PhD) are committed to the project. In addition, numerous undergraduate assistants worked assigned this project at various times. As a result of their work on this project, the
students have become skilled or are in the process of gaining skills in a number of areas, including closed-loop mechanical testing, x-ray imaging (both synchrotron-based and conventional sources), tomographic reconstruction, digital image processing (2D and 3D). In addition, the students are getting experience in overall research management, laboratory skills, statistics and data analysis.

At UC Davis, two graduate students (one Ph.D. student and one M.S. degree student) have significantly contributed to the project activities. The M.S. student has completed her degree requirements and is now working for an engineering firm in Austin, Texas. The Ph.D. student has completed his course work, passed the qualifying exam, and is now concentrating on the project activities for his dissertation research. Two undergraduate students contributed significantly to the project goals. One worked on the improving the efficiency of the pre-processor used for the project analyses; the other undergraduate student improved graphical post-processing capabilities for the same analysis package. Both undergraduate students attended regular meetings with the PI?s research group (including graduate students and visiting scholars), where they were exposed to other aspects of the project activities and goals, including the experimental work of the PI at

UMaine. The first student will stay on the project for the next project period, whereas the other undergraduate student will be graduating. Along with development and use of the analysis tools, the students are contributing to the user manuals that will eventually accompany the analysis tools by the end of the project.

Outreach Activities:

Journal Publications

Landis, Eric N. and Bolander, John E., "Explicit representation of physical processes in concrete fracture", Journal of Physics D, p. , vol. , (2009). Accepted,

Landis, E. N., Keane, D. T., "Tutorial Review: X-ray microtomography", Materials Characterization, p. 1305, vol. 61, (2010). Published, 10.1016/j.matchar.2010.09.012

Books or Other One-time Publications

Asahina, D.; Landis, E. N.; Grassl, P.;
Bolander, J. E.
, "Role of Phase Interfaces During Pre-
Critical Cracking of Particulate Materials", (2009). Conference Proceedings, Accepted
Editor(s): Onate, E, and Owen, D.R.J.
Bibliography: International Conference on Partcile-
Based Methods (Particles 2009)

E. N. Landis and J. E. Bolander, "ntegration of 3D Imaging and Discrete
Element Modeling for Concrete Fracture
Problems", (2010). Proceedings, Published
Editor(s): K. A. Alshibli and A. H. Reed
Collection: Advances in Computed Tomography for
Geomaterials
Bibliography: ISTE, London, 2010, pp. 117-123.

E. N. Landis, M. C. Bridges, and J. E.
Bolander, "3D Tomographic Imaging Applied to Split
Cylinder Fracture", (2010). Conference Proceedings, Published
Editor(s): B.H. Oh, O.C. Choi, and L. Chung
Collection: Recent Advances in Fracture Mechanics of Concrete, Proceedings of FraMCoS 7
Bibliography: pp. 100-104

J. E. Bolander and E. N. Landis, "Modeling of Phase Interfaces During
Precritical Crack Growth in Concrete", (2010). Conference Proceedings, Published
Editor(s): B.H. Oh, O.C. Choi, and L. Chung
Collection: Recent Advances in Fracture Mechanics of
Concrete, Proceedings of FraMCoS 7
Bibliography: pp. 536-539

Web/Internet Site

Other Specific Products

Contributions

Contributions within Discipline:

As reported in the major findings, we believe we have integrated spatial data from experiments into models to a degree not yet achieved. This integration makes the long term goal of physical models to capture micromechanical mechanisms much closer, and as such will vastly improve our predictive simulation capabilities for concrete and other particulate composite structures.

Contributions to Other Disciplines:

The collaboration between Landis and Dr. Denis Keane (noted in the collaborations section) produced a paper 'Tutorial Review: X-ray microtomography', that introduces techniques developed in this work to the wider materials science community.

Contributions to Human Resource Development:

Contributions to Resources for Research and Education:

Contributions Beyond Science and Engineering:

Conference Proceedings

Categories for which nothing is reported:

Activities and Findings: Any Outreach Activities

Any Web/Internet Site

Any Product

Contributions: To Any Human Resource Development

Contributions: To Any Resources for Research and Education

Contributions: To Any Beyond Science and Engineering

Any Conference

Project Activities/Findings

The research has proceeded on parallel tracks at UMaine and UC Davis as outlined in the project proposal. As detailed below, several issues have arisen that has prevented us from keeping with our original schedule, however, the delays are not substantial, and will not affect our ability to carry out the proposed research tasks.

Activities at UMaine

Work to date has focused on two fronts at UMaine. The first is the development of a subpixel resolution 3D vector deformation field program. Under a previous project we developed a 3D displacement field routine not unlike commercially available 2D digital image correlation programs. Our current version is a fast algorithm that calculates 3D displacement fields to the nearest whole voxel. However, the research done under this project requires us to have better resolution to link with computational models.

The second front where we have made progress is on small scale split cylinder tests. The research issue we are addressing is the refinement of a simple mechanical test that can be done in-situ during tomographic scanning. The restrictions of tomographic imaging make in situ scanning difficult. To date we have refined a combined screw/piezoelectric actuated small scale load frame, which will be used for tomographic scanning at the APS this coming year.

As part of the preliminary work, we have cast an array of specimens using both normal and artificial aggregate. The artificial aggregates are spherical ceramic beads that will be useful for simulation purposes. Notched beam specimens have been cast and tested under closed loop control to obtain stable post-peak crack propagation. Specimens of both regular and artificial aggregates were tested and the differences noted (as expected, spherical aggregates lead to specimens with less interlock, and therefore more brittle behavior) for future reconciliation with numerical simulations. In addition, during notched bending tests acoustic emission activity was recorded as an alternate continuous measure of energy dissipation. Although not originally part of the proposed research program, the work will provide an way to validate the continuous energy dissipation predicted by numerical simulation.

As noted above, two unexpected issues arose that have delayed the UMaine activities to a limited extent. First, a graduate research assistant who had been identified as an excellent fit for the project failed to get a U.S. visa, and was therefore unable to enroll in our graduate program. An alternative U.S. student was quickly identified and started on the project in March of this year. This delay put the project approximately six months behind schedule. The second issue is that the x-ray source in-house microtomography system that we planned to use for this project failed early this year. The group responsible for maintenance and operation of this instrument is currently weighing alternatives for bringing the unit back online. In the mean time, a new instrument with much higher spatial resolution was recently acquired by the PI, and is being tested for suitability for this project. Should the instrument prove suitable, there should be little or no delay with respect to in-house imaging necessary to complete this project.

Activities at UC Davis

The research activities at UC Davis have focussed on the development and extension of lattice models to simulate the micromechanics of fracture of cement-based composites, with particular attention to simulating interfaces present at the micro- and meso-scales. Early work anticipates the eventual close-linkage of the simulation activities with the experimental work described above.

Some current work involves the 3D simulation of fracture along aggregate-matrix interfaces in conventional cement-based composites, where the interface tends to be weaker than the inclusion and matrix phases of the composite. Spherical inclusions are studied first, since much of the experimental testing will employ spherical ceramic beads as aggregates within microconcrete specimens. The computation approach differs from most other lattice models in that it allows for precise control over interface orientation and thickness. Preliminary simulations have shown that, under far-field tension, fracture initiates where the interface is perpendicular to the direction of principle tension, followed by increasingly mixed mode behavior as interface fracture progresses. Animation sequences have been produced showing, side-by-side, gradual breaking of the inclusion-matrix interface and the corresponding fracture events plotted in the Mohr-Coulomb stress space.

Later in the project, the computational approach will be used to study interface fracture for other inclusion geometries. For this purpose, inclusion discretization procedures have been generalized to accommodate the meshing of arbitrary (convex) polyhedral shapes. The procedure relies only on the definitions of vertex coordinates and the vertex connectivities of the individual facets of the polyhedron. After placing nodal sets to introduce the vertices, the polyhedron edges, facets, and internal volume are systematically defined (in that order) by placing nodes via random sequential addition, subject to minimum distance constraints.

The visualization of fracture in three-dimensions is important for interpreting the computational results and their correspondence to the images obtained experimentally by the PI at UMaine. Some of the PI's previous post-processing algorithms have been restructured and extended to improve visualization capabilities and facilitate third-party use.

Inverse analysis provides a systematic means for linking the experimental and model components of the project to extract knowledge about interface properties (and other aspects of fracture at the micro- and meso-scales). Several techniques for inverse analysis are being studied, including gradient-based routines (e.g. the Levenburg-Marquardt scheme used by the PI in previous work) and more recently developed approaches that do not rely on gradient information.

Project Training/Development

At UMaine, one graduate assistant and two undergraduate assistants have been assigned to this project. As a result of their work on this project, the students have become skilled or are in the process of gaining skills in a number of areas, including closed-loop mechanical testing, quantitative acoustic emission acquisition and analysis, 3D image processing, and x-ray tomographic imaging and analysis.

At UC Davis, three graduate students and one undergraduate student have participated in the code development and modeling aspects of this project. This student team is also producing manuals to facilitate the use of the programs by future students and other researchers. Through group discussions and independent study, the students are learning basic information about the imaging techniques used in the experimental component of this research project.

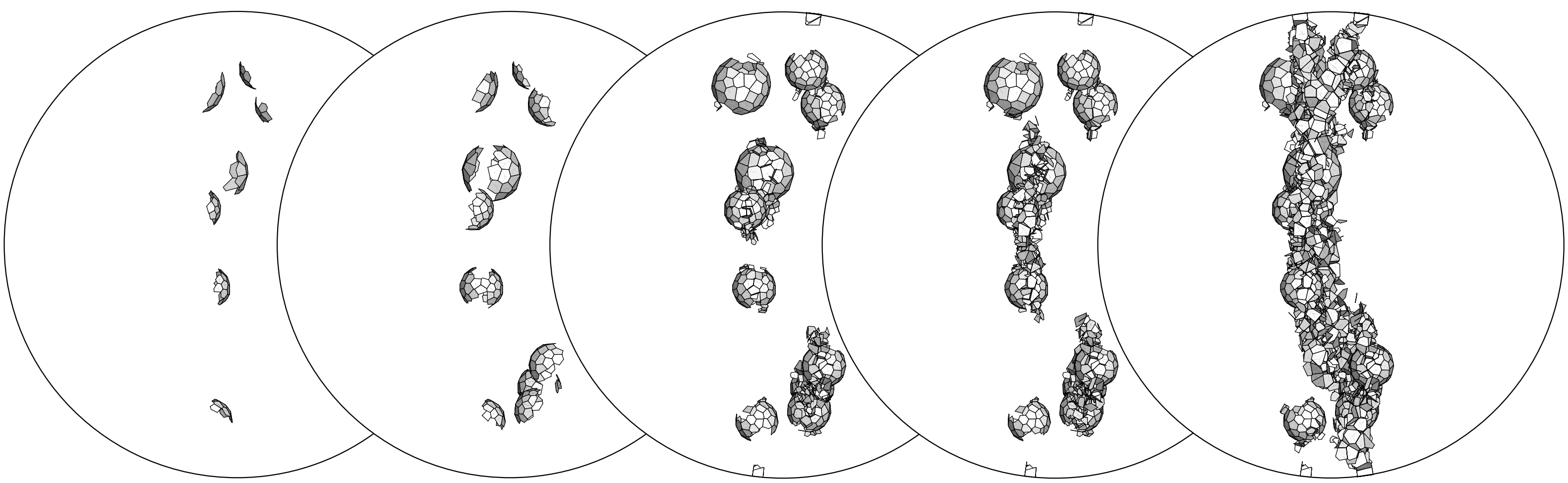

Figure F-1: Frontal view of several stages of the 3-D fracture process

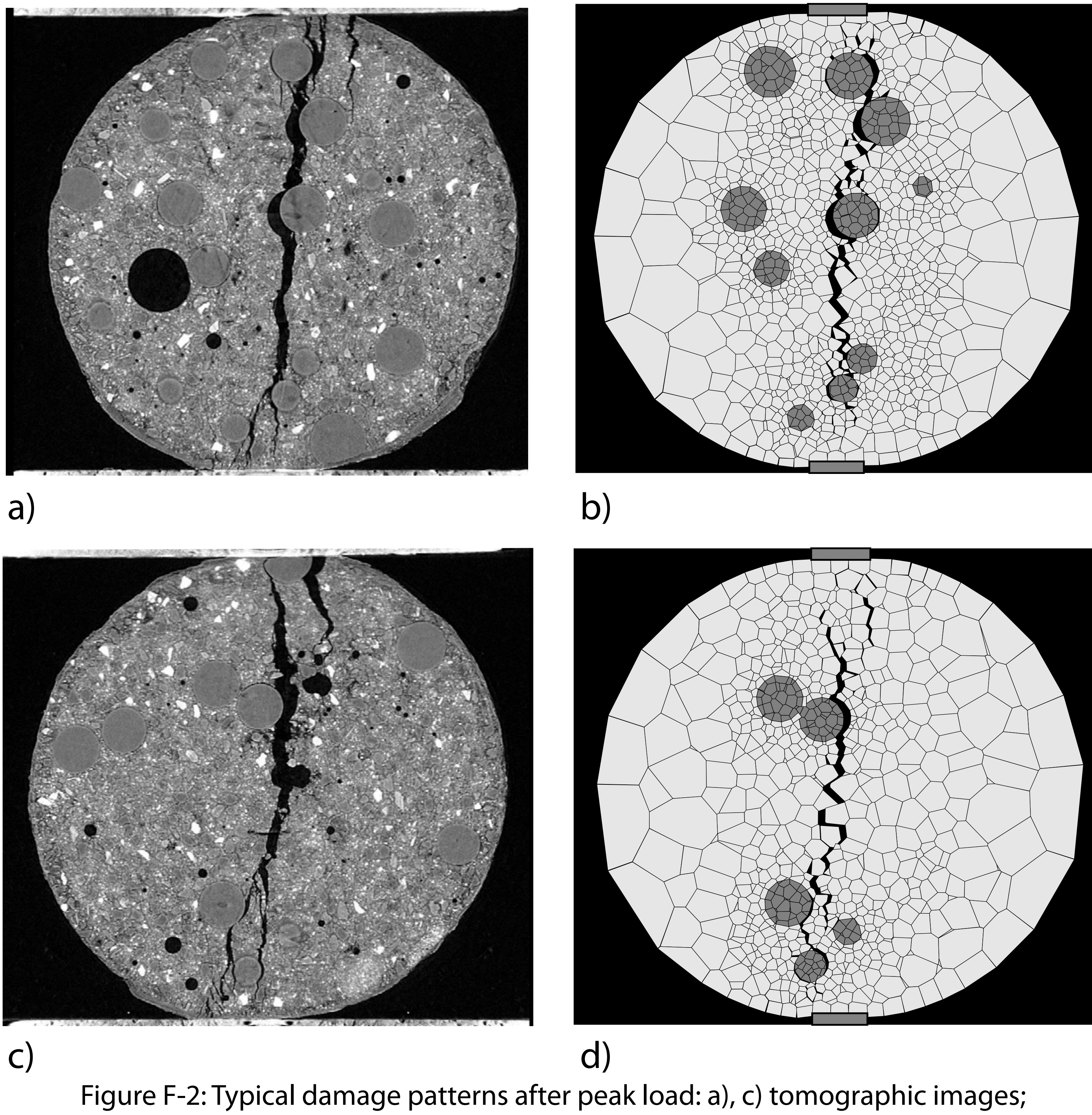

Figure F-2: Typical damage patterns after peak load: a), c) tomographic images; and b), d) lattice model results. Cross-sections of the three-dimensional images and model results are being compared.

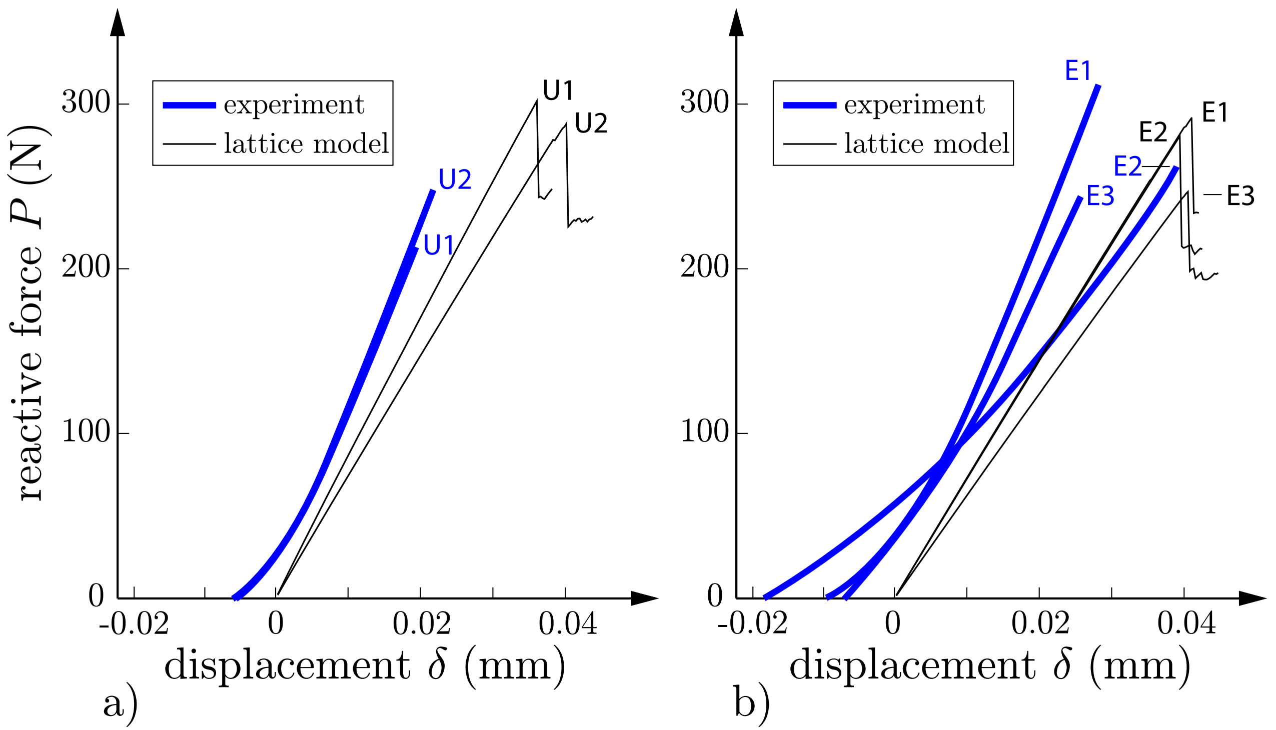

Figure F-3: Load-displacement response of split-cylinder specimens:
a) unetched glass aggregates; and b) etched glass aggregates

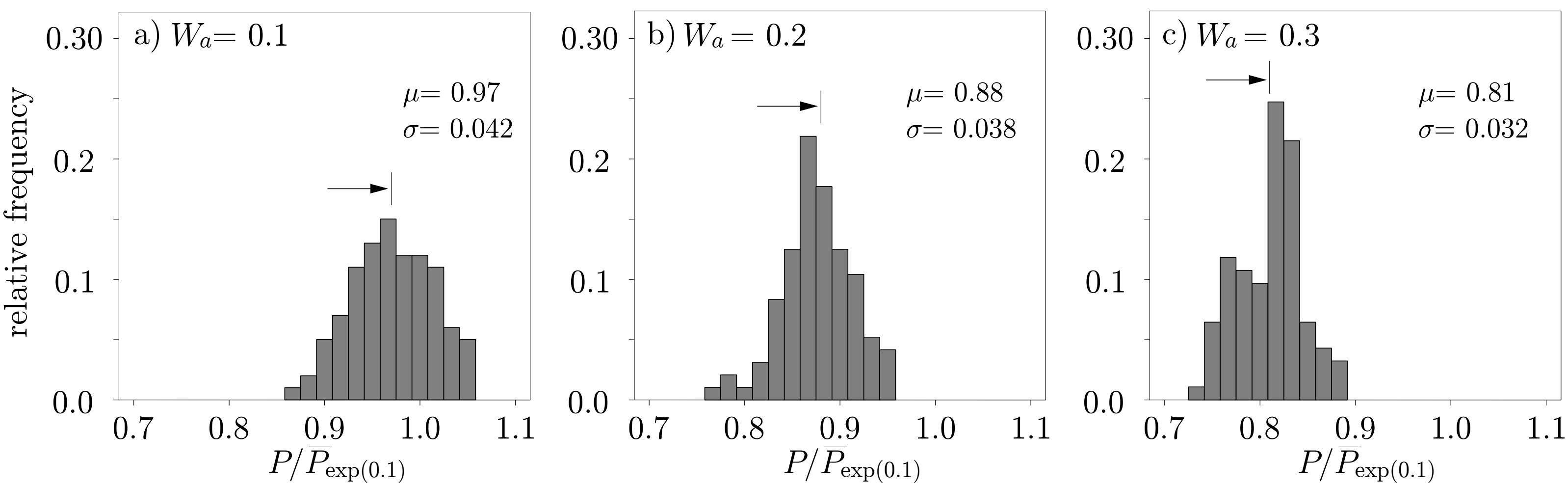

Figure F-4: Frequency distributions of split-cylinder strength based on 100 nominally identical models differing only in random placement of aggregates (W_a= weight fraction of aggregates; μ = mean value; σ = standard deviation)

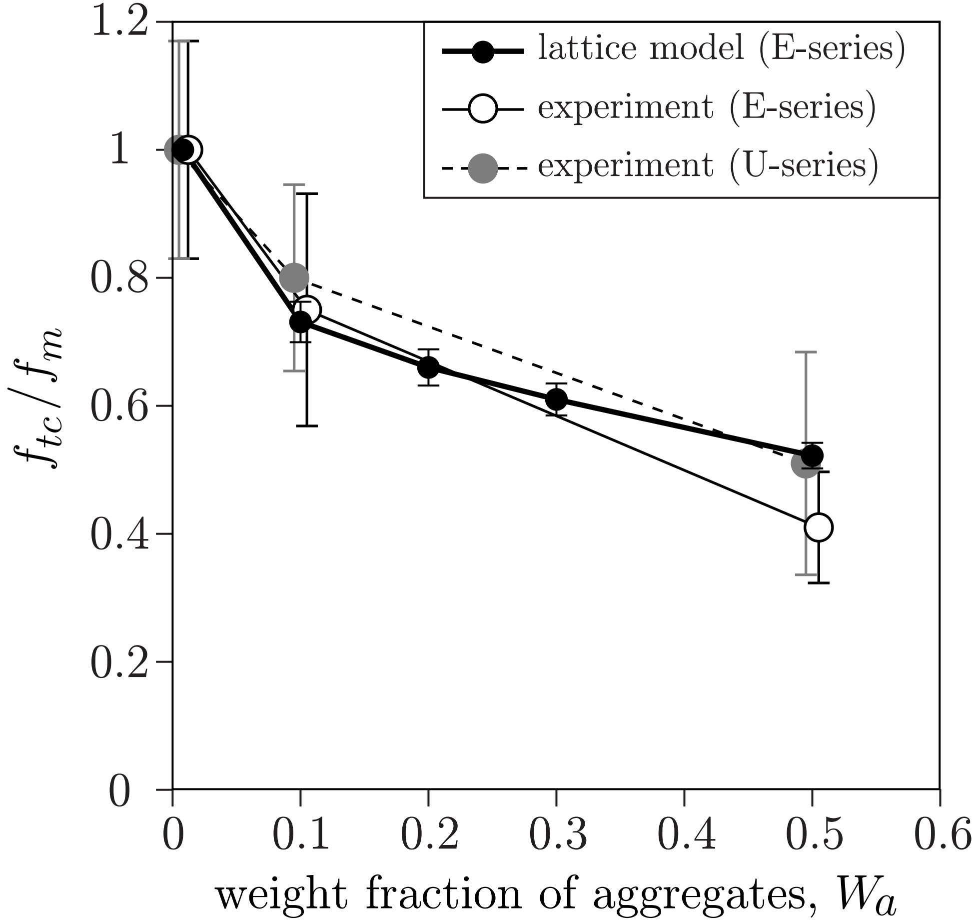

Figure F-5: Normalized split-cylinder strength for different weight fractions of aggregates