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RPPR Final Report
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STEM Degrees: 2 **STEM Participants:** 3

Major Goals: The major goals of this project are to:
1) advance the capabilities of gradient-damage models to provide robust simulations of fragmentation, with a particular emphasis on representing localized failure surfaces;
2) develop new methodologies to address the stochastic nature of fracture and fragmentation for quasi-uniform loading conditions;
3) construct a relatively simple, quasi two-dimensional fragmentation experiment, allowing for state-of-the-art measurements of stress fields over a range of strain rates, that can be widely employed for model validation.

Accomplishments: We made significant progress in this project advancing goals 1) through 3).

On goal 1, we have established the ability of cohesive-based gradient-damage models to represent pervasive failure phenomena under quasi-uniform states of stress. These problems are challenging to deal with for continuum-mechanics theories because in reality the bifurcations are driven by defects at length scales that are simply below the level of resolution in the models. This is where goal 2 was essential, because what is needed is to introduce variations in material or fracture properties at the macro-scale. Methods for doing this in a manner that is robust and allows for spatial convergence in quantities of interest are not trivial, however.

We developed new approaches in this work that connect variations in material properties to the resulting fracture patterns. The new approach relies on polynomial chaos expansion and a global sensitivity analysis to measure which factors in the variation of the output (i.e. damage fields) are connected to the variation of each input (Young's modulus, fracture toughness) or any combination thereof. For cohesive-based gradient damage models, the studies we performed in this project demonstrated how both variations in critical fracture energies and thresholds for fracture influence fracture patterns.

We have also studied the sensitivity to the underlying regularized fracture model. In particular, we have compared energetic-based gradient damage models to more recent ones that employ a strength envelope in stress space to govern nucleation in the bulk. These studies have shown that the different models do yield qualitatively and quantitatively different results, despite behaving similarly under biaxial states of stress. We expect these results to be important when models are used to explain fracture patterns in fragmentation problems, for example.

Finally, for goal 3), we have developed a relatively simple fracture experiment. It is not quite two-dimensional, but it is close. The experiment consists of bonding a thin layer of a ceramic to an aluminum substrate, and subjecting the system to a rapid temperature change. For specimens in which the aluminum substrate is a cylinder, we have shown that pervasive fracture occurs in the ceramic film on the surface during the thermal shock. We have also shown that qualitative aspects of the experiment can be reproduced by the strength-based gradient damage model.

Training Opportunities: This project provided training for PhD students Tianchen (Gary) Hu and Bo Zeng, as well as Masters student Casper Versteeg.

PhD student Tianchen (Gary) Hu received training in the use of K-L expansion methods to construct fields with spatial variation. He also received training in numerical methods for fracture and constrained minimization problems.

PhD student Bo Zeng also received training in the use of K-L expansion methods to construct fields with spatial variation. She also received training in the use of a strength-based model for crack nucleation and crack growth. Finally, she received training in the design and analysis of thermo-mechanical experiments.

MS student Casper Versteeg received training in dynamic fracture mechanics, as well as code development in C++.

Results Dissemination: Our efforts on this project have been disseminated in a number of important ways.

Casper Versteeg's masters thesis on dynamic fracture is hosted by Duke University libraries.

Bo Zeng's masters thesis on this topic is hosted by Duke University libraries.

Tianchen Hu's doctoral dissertation, involving parts of this project, is hosted by Duke University libraries.

Our primary mechanism for dissemination has been through the journal publication describing it:

T. Hu, J. Guilleminot, and J. Dolbow (2020). "A phase-field model of fracture with frictionless contact and random fracture properties: Application to thin-film fracture and soil dessication," Computer Methods in Applied Mechanics and Engineering, volume 368, number 113106.

PhD Student Gary Hu presented the results from this project at the 15th US National Congress on Computational Mechanics, in Austin, Texas in July of 2019.

PI Dolbow gave an invited seminar at the University of Texas Austin that primarily focused on the aforementioned paper. This was delivered on February 18, 2020.

PI Dolbow gave a presentation based on the work done in this project at the virtual World Congress on Computational Mechanics, held in January of 2021.

PhD student Bo Zeng presented the results from this project at the 15th World Congress on Computational Mechanics, in Yokohama Japan (virtual) in July of 2022.

PhD student Bo Zeng presented the results from this project at the 17th US National Congress on Computational Mechanics, in Albuquerque, NM in July of 2023.

At least one more manuscript describing the results from the most recent strength-based studies and the thermo-mechanical experiment is expected to result from this project.

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Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
National Academy Member: N

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Authors: Tianchen Hu, Johann Guilleminot, John E. Dolbow
Keywords: phase-field models; soil dessication; traction-free surfaces; frictionless contact; random field; uncertainty quantification

Abstract: We present a new derivation for a phase-field model of cohesive fracture that allows for fully-damaged surfaces to properly transmit tractions under frictionless contact conditions. The model is derived from an energy minimization standpoint, and the governing equations are presented in a general Allen–Cahn form, unifying both brittle and cohesive fracture models. A novel elastic energy split is proposed to enforce frictionless contact conditions along the regularized crack set. A fixed-point iterative algorithm is used to solve the system of equations, and an active-set strategy is incorporated to enforce the crack set irreversibility. The model is then applied to study the mechanical-fracture coupling in the fracture of thin films and soil desiccation problems in which intricate crack networks form. We present results for one-dimensional, two-dimensional, and fully three-dimensional configurations, and examine the relationship between the generalized driving energies for fracture an

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An Integrated Experimental and Computational Investigation of Fragmentation in Transparent Polymers: Final Report

John E. Dolbow

August 20, 2023

Abstract

Many fracture problems of interest are characterized by the response of systems that are rapidly over-stressed, in which the state of stress is in excess of the strength of the material. This is obviously an unstable configuration, and the system tends to respond by failing once the strength has been exceeded for a sufficiently long period. Moreover, failure tends to be pervasive, characterized by the formation of many cracks that interact with one another in non-trivial ways. These problems are difficult to model with state-of-the-art continuum mechanics theories because in reality the fracture process is triggered by defects at scales that are simply not resolved. This project advanced a class of gradient-damage models to describe this class of problems, along with methods to introduce stochastic variations in material properties. These models were then deployed to investigate the sensitivity of fracture patterns in thin films subjected to biaxial states of stress to underlying variations in material and fracture properties. Our studies reveal a sensitivity to variations in the critical fracture energy, but also the strength model for the material. Finally, a relatively simple thermo-mechanical experiment was developed to investigate the ability of these models to explain fragmentation in an actual system.

1 Introduction

The response of structures and materials to rapid loading conditions has been a topic of interest to the engineering and materials science communities for decades. The primary application of interest has been the response of structures to a range of extreme loading conditions, from rapid impact to explosive blasts. These problems tend to be characterized by pervasive failure, in which initially intact structures break apart and interact in non-trivial ways as part of a fragmentation process. Fragmentation involves a wide range of phenomenon, from the initiation of small flaws from defects, to rapid crack growth and coalescence, to the formation of smaller structures that interact through contact. Quantities of interest include basic fields at the macroscopic level, such as how the distribution of fragments is impacted by the strain rate, the maximum velocities fragments can attain, and etc. These problems are challenging and expensive to study experimentally, and so quite a bit of work has focused on the development of simulation-based science. While numerical analysts have had success "tuning" existing models and methods to particular systems, truly predictive capabilities have remained elusive.

PI Dolbow's lab has become a leader in the development of gradient-based damage models to simulate this class of phenomena. Nevertheless, much work remains to make these approaches truly predictive and useful for practical simulations of pervasive failure. A significant challenge with quasi-brittle materials concerns the relatively small size of the fracture process zone. Even with modern computational resources, resolving such length scales presents significant challenges in three dimensions. In addition, fragmentation problems are not deterministic. The response of the system can be thought to be composed of two pieces: a mean response that is fairly deterministic, and a stochastic perturbation whose magnitude depends on a whole host of factors. The latter includes, for example, the distribution of defects at small length scales and uncertainty surrounding residual stress fields. While the latter is often overlooked in simulations, it can play a significant role in impacting the fragmentation response.

2 Objectives of the Proposed Research

The objectives of this research project, broken down by project years, are as follows:

- To develop new methodologies to address the stochastic nature of fracture and fragmentation for quasi-uniform loading conditions. (year 1)
- To advance the capabilities of gradient-damage models to provide robust simulations of fragmentation, with a particular emphasis on representing localized failure surfaces. (year 2)
- To construct a relatively simple, quasi two-dimensional fragmentation experiment, allowing for state-of-the-art measurements of stress fields over a range of strain rates, that can be widely employed for model validation. (year 3)

3 Findings

Our primary tool for developing new models and methods in this project concerned a thin film bonded to an elastic substrate and subjected to biaxial tension, as shown in Figure 1. This did represent a departure from our original plan to study thin spinning disks of material. This departure was made because the biaxial stretched layer has been widely studied by other researchers, and it contains many of the same features. In particular, it gives rise to pervasive failure under the action of a spatially uniform state of stress.

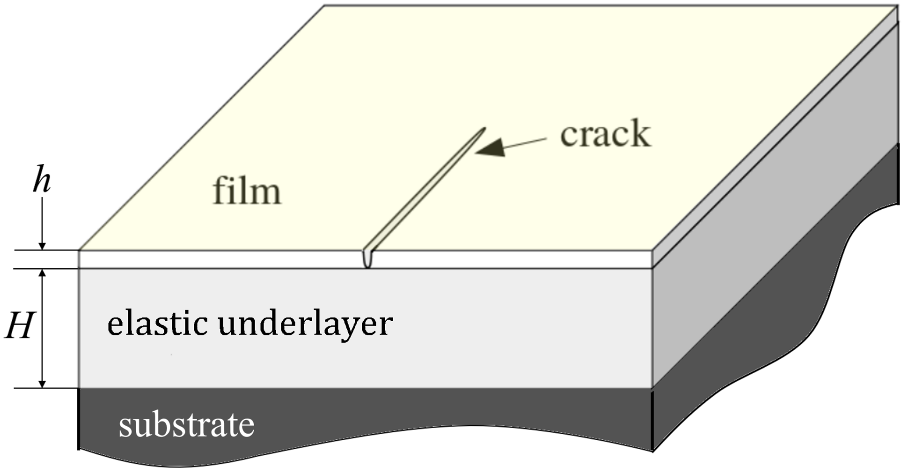
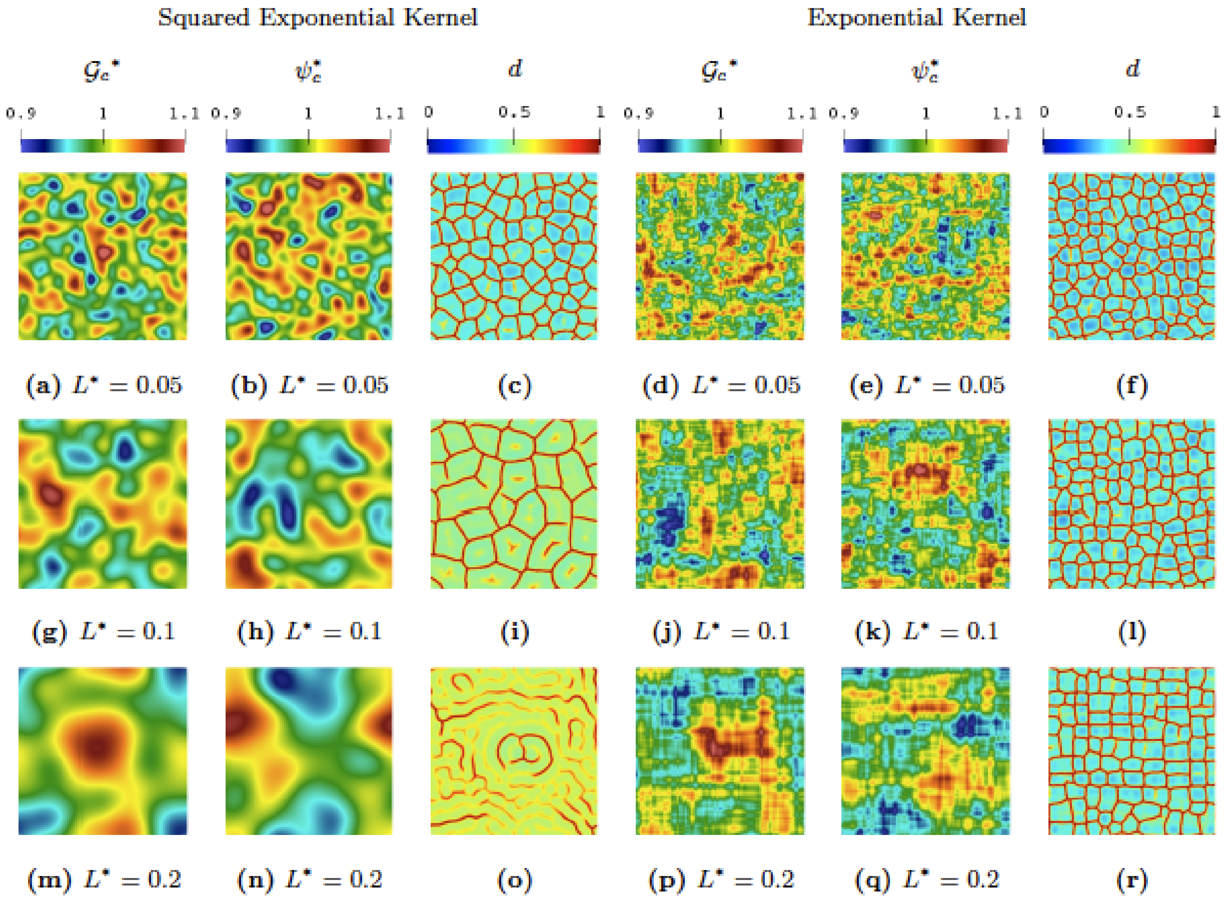


Figure 1: Two-dimensional model for thin-film cracking. A mismatch in material properties between the film and the elastic underlayer gives rise to a biaxial state of stress in the film.

We developed methods to introduce spatially-correlated fields for the critical fracture energy G_c and the energetic trheshold for damage, ψ_c. The resulting fracture patterns predicted by the model, using various kernels for the K-L expansion (squared exponential vs. exponential) are shown in Figure 2. Our studies indicate that the fragment distribution is mostly sensitive to variations in the critical fracture energy. Moreover, the fracture pattern itself appears to show much more sensitivity to the squared exponential kernel than the exponential kernel.



(a) $L^* = 0.05$ **(b)** $L^* = 0.05$ **(c)** **(d)** $L^* = 0.05$ **(e)** $L^* = 0.05$ **(f)**

(g) $L^* = 0.1$ **(h)** $L^* = 0.1$ **(i)** **(j)** $L^* = 0.1$ **(k)** $L^* = 0.1$ **(l)**

(m) $L^* = 0.2$ **(n)** $L^* = 0.2$ **(o)** **(p)** $L^* = 0.2$ **(q)** $L^* = 0.2$ **(r)**

Figure 2: Damage fields resulting from six pairs of realizations with different correlation models and normalized correlation lengths.

These kinds of models were employed to determine the optimal set of hyperparameters to match an actual experiment of pervasive failure in a thin film. The procedure for identifying these hyperparameters is summarized in Figure 3, and the results comparing the simulated fracture pattern to the experiment are shown in Figure 4.

For the second objective, our work focused on applying analogous methods to an emerging phase-field model for fracture that incorporates a strength envelope for fracture. This work was a collaboration with Professor Oscar Lopez-Pamies group at the University of Illinois, who has developed the new model. Their model is attractive as, in addition to being more physical, results in fracture patterns that are much more localized spatially. Figure 5 compares the resulting fragment counts using the cohesive based gradient damage model to the nucleation model employing a strength envelope. Interestingly, despite both models being tuned to behave similarly under bi-axial tension, there are qualitative and quantitative differences in the results. These findings may indicate that other quadrants of the stress space play an important role that is under-appreciated.

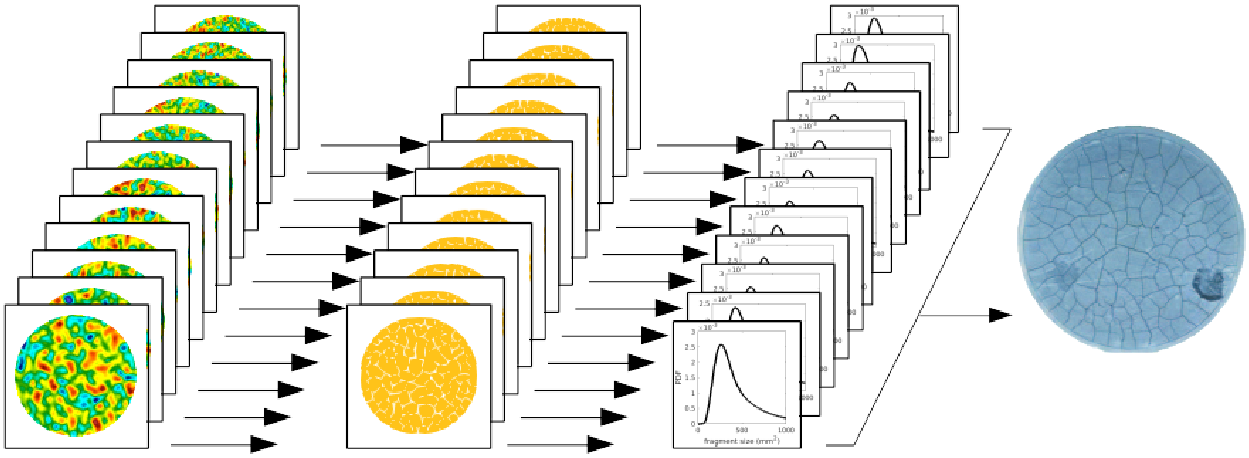
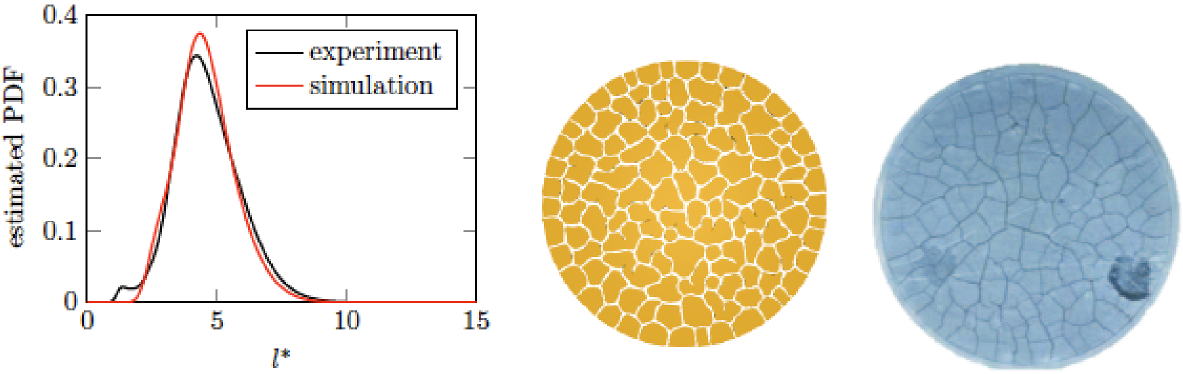


Figure 3: Procedure for finding the optimal hyperparameter to match the experiment.



(a) **(b)** **(c)**

Figure 4: a) Estimated PDFs of the dimensionless fragment size extracted from the experimental result and the calibrated stochastic model. b) Fracture morphology obtained using the calibrated fracture properties. c) Photograph of cracks from a thin film experiment.

For the third objective, in the last year of the project, we developed a relatively simple thermo-mechanical experiment of thin film fracture. In particular, the setup consists of mounting a thin film of ceramic to an Aluminum base, as shown in Figure 6. The thin film is made of a ceramic material called BegoStone which is commercially available. It was selected here instead of a transparent polymer because it has a very high contrast in coefficient of thermal expansion compared to the Aluminum. As shown in the Figure, the layer was polished down to a uniform thickness of approximately 0.6 mm. Then the sample is thermally shocked to a temperature of 250 Celsius, and the fracture pattern on the surface is captured.

A comparison of the fracture pattern that appears in the experiment compared to the model-based simulation calculations (using the new nucleation model) is shown in Figure 7. We find that the results of the experiment are reproducible, and that the model appears to provide a reasonable match with both qualitative and quantitative aspects of the fracture pattern on the surface of the layer.

counted by flooding algorithm, 'crack' by $d \geq 0.95$

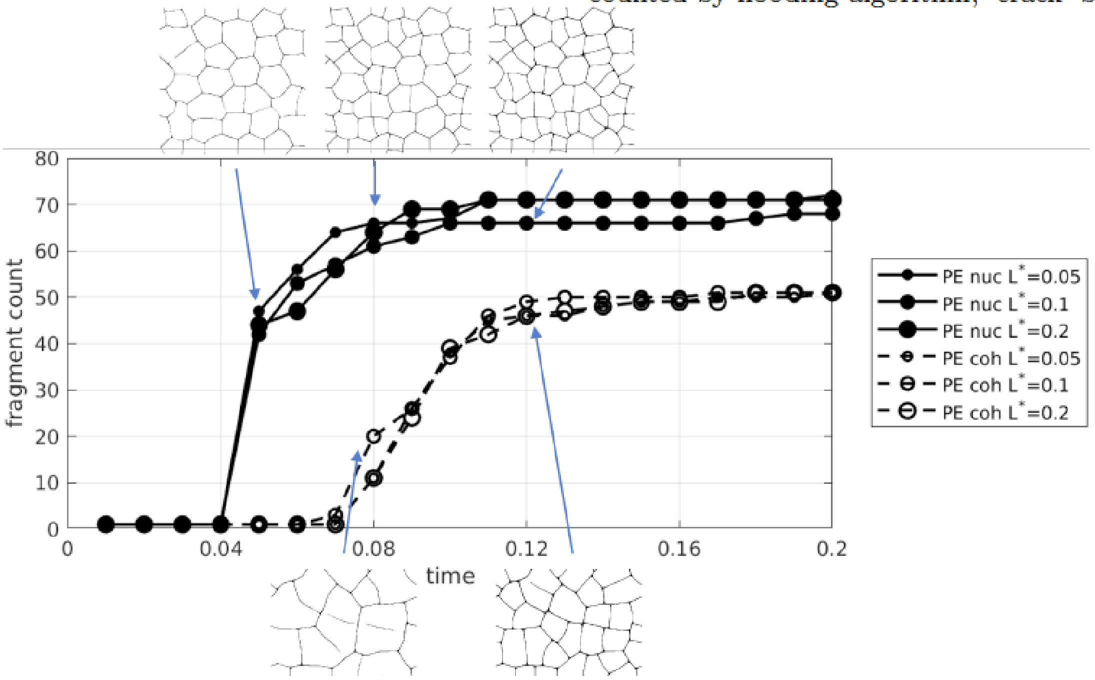
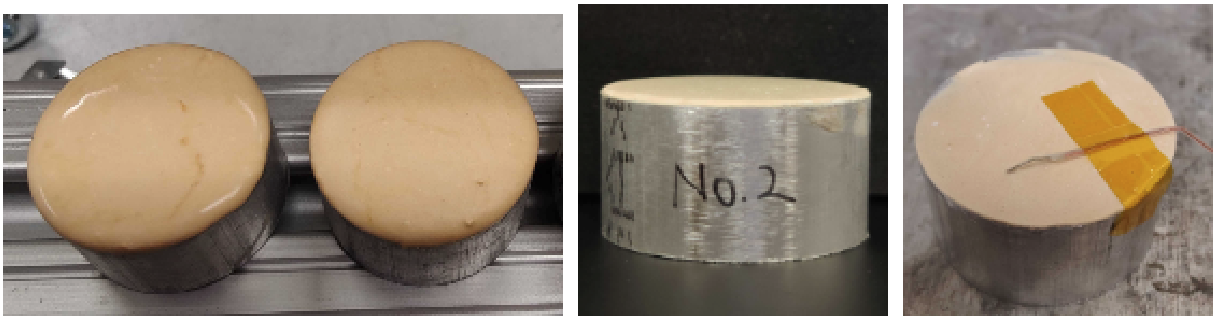


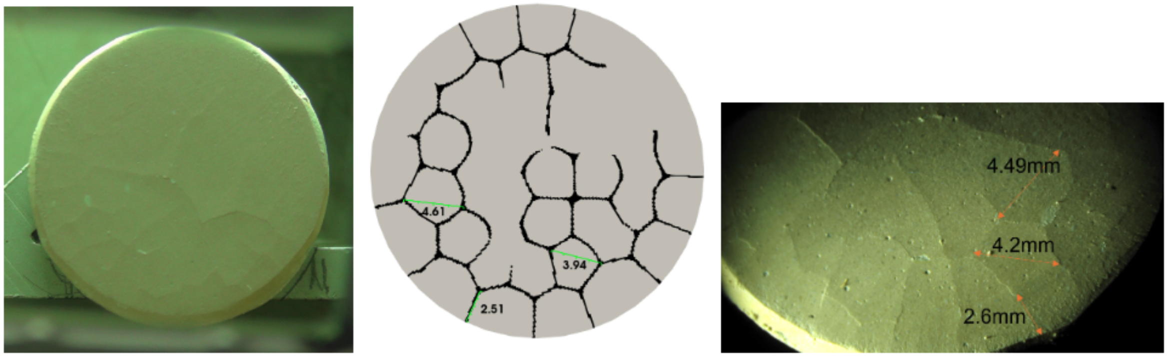
Figure 5: Comparison of fragment counts with time for the cohesive model vs. a nucleation model employing a strength envelope.



(a) raw samples (b) polished (c) reference

(d) setup inside the chamber (e) setup outside the chamber

Figure 6: Experimental setup for thermo-mechanical fracture. a) Layers are of a ceramic slurry are first deposited on top of aluminum cylinders. b) The layers are subsequently polished down to yield a thin film on top of the thick substrate. c) A reference sample is used to monitor the surface temperature during the experiment. d) The inside of the thermal chamber, and 2) the use of a camera outside the thermal chamber.



(a) Begostone fracture result (b) simulation result (c) measure of fragment size

Figure 7: a) resulting fracture pattern on the surface of the BegoStone layer in the thermo-mechanical experiment. b) A simulation result using the nucleation model. c) A detailed view of the experimental surface, with measurements of the fragment sizes.