

# Stochastic Coarse Graining from Atomic to Continuum Scale Models of Fracture in Amorphous Silica Glass

*MSc/PhD Project Proposal for Mathematics for Real-World Systems CDT*

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**Background.** Despite the potential for significant technological and economic impact, remarkably little is known about the fundamental fracture mechanisms that cause many materials to break. Accurate simulations of these kinds of processes at the atomic scale have recently been made practical using multiscale approaches.<sup>1</sup> The effect of individual defects on crack paths can now be studied to high precision.<sup>2</sup> What is missing for an effective mean-field theory is a model reduction procedure that can capture information lost during coarse graining, allowing defect nucleation and growth in random microstructures to be modelled. The overarching aim of this project is to develop such a procedure.

**Overall Scope.** Continuum elasticity remains accurate surprisingly close to defects, with non-linearity and discreteness localised to a nanoscale region<sup>3</sup>, suggesting that it is possible to remove some of the empiricism in current continuum models by incorporating atomistic information that need not be computed on-the-fly. However, to move beyond perfect crystals, microstructural variation must be effectively included, making this a complex problem to attack. In this project this will be addressed by averaging over representative configurations at the microscale, then identifying and extracting the key information to a higher scale. Keeping track of information lost during coarse graining will enable uncertainty quantification.

**MSc and PhD Projects.** The MSc project will consider a simple material for which microstructural variation is an issue: amorphous silica glass. The student will use an existing code developed by project supervisors to generate crack path trajectories in glass structures. They would then develop a deterministic continuum crack growth criterion (e.g. Griffith) fitting the data. Finally, they would formulate a PhD project that incorporates:

- A strategy to include microstructural uncertainty into the above procedure
- Propagation of model, microstructural and epistemic uncertainty
- Implementation within an end-user finite element code.
- Application to industrially relevant problems

**Applications.** The long-term goal of the project is to develop models which improve our understanding of failure processes and suggest strategies to control them. The current generation of continuum models rely heavily on empirical crack growth criteria and constitutive equations, and the lack of true predictive power in this area is a cause of great concern to industry. Options for industrial co-funding and/or partners include:

- Supervisor's industrial links: AWE, NPL, TWI, Rolls Royce, US Air Force lab
- JLR/Tata steel and Thalys - CDT partners

<sup>1</sup> J.R. Kermode et al, Nature **455**, 1224 (2008).

<sup>2</sup> J.R. Kermode et al., Nat. Commun. **4**, 2441 (2013).

<sup>3</sup> V. Ehrlacher, C. Ortner, and A.V. Shapeev, arXiv [math.NA] 1 (2013).