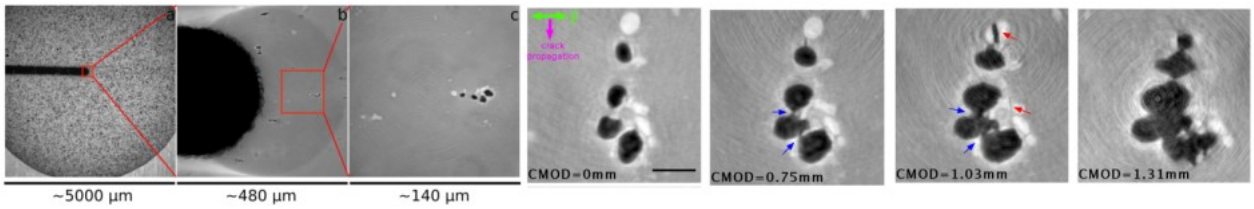
AI-based damage nucleation models assessed on big 4D data and micromechanical finite element simulations

PhD thesis at Mines Paris

Industrial and scientific context

Strong, formable, damage-tolerant and recyclable materials are crucially needed to reduce CO2 emissions in the transport industry, particularly concerning vehicles with combustion engines but also electric cars. Damage nucleation has gained particular interest in industry as recycling of alloys often leads to higher impurity content and associated amount of brittle intermetallic particles in the alloys. In forming and associated ductile fracture, the damage nucleation on micrometre-sized brittle particles remains poorly understood and hard to predict. Computerized predictions, as well as simulation data, obtained on realistic virtual microstructures, are needed in materials-by-design frameworks that seek to control and enhance the mechanical response of microstructures. Damage evolution is driven by the local stress state, which is itself a complex result of the load distribution within the microstructure of the material. Experimental (4D, i.e. space and time) data, image analysis, meshing tools and full-field computational methods (e.g. finite element) have been developed in an effort to obtain a unified and reliable damage model at the macroscopic scale that works under a wide variety of loading conditions. Nevertheless, the role of stress or strain as well as of particle nature, size and shape remains unclear and hard to predict, yet crucial for formability and fracture. The underlying physics responsible for damage nucleation and evolution is still nowadays an open question. The complexity of such mechanisms suggest that the problems should be tacked at lower scales, i.e. at micrometre scale, which put such study far away from industrial applications. On the other hand, results from literature show that the use of macroscopic phenomenological models do not allow to obtain a generic and unified damage nucleation model, which lead to ad-hoc ingredients that allow to fit some experimental observations. The nucleation of damage and its evolution is currently driven by phenomenological macroscopic laws that are far too simple and cannot accurately reproduce the complexity observed in real systems.

Machine learning techniques could offer alternative strategies to such phenomenological damage laws. Large experimental 4D datasets, of prime importance in this context, are available and can be used in order to develop machine learning pipelines. To train these models and perform inverse identification, experimental observations could be adequately supplemented by simulation data. Yet, this approach suffers from two main drawbacks. First, state-of-the-art micromechanical computations are most often based on meshing of the structures whereas deep-learning pipelines are often based on images. Second, the computational time involved in carrying out 4D simulations on representative volume can be extreme. To address these problems, we propose to use specific graph-based machine-learning methods to leverage existing experimental and computational methods at the microscopic scale, at which the microstructure of the material can be resolved. In particular, Graph Convolutional Networks (GCNs) are deep-learning pipelines that are useful to deal with data generated on fairly-general discrete domains where interdependency between objects is explicitly represented and have lately been adapted to treat mesh-based physical simulation or to deal with crack coalescence and phenomena occurring at the crack tips. The methods yield much more rigorous identification procedures by taking into account mesh-dependency explicitly in PDE solvers, and therefore can be validated unambiguously.



Aluminium sample with a notch, in visible light microscopy image and high/ very high resolution Laminography (left) and development of several voids (black) nucleated at secondary phase particles (white) during loading (right). The scale bar corresponds to 10 µm.

Scientific objectives

The PhD study will focus on developing new machine-learning methods to capture and understand damage nucleation in engineering materials, making use of a combination of 4D experimental data representing damage evolution and micromechanical simulations. Our starting point are a set of in-situ 3D imaging experiments with deep-sub micrometer resolution. Existing data will be supplied by the “Centre des Matériaux” (CDM) to the project. Recent progress in synchrotron laminography has allowed to investigate damage mechanisms in such 4D experiments in flat sheet samples under mechanical load (see figure). Spatial resolution far below the micrometer scale were obtained in nano-laminography. A first objective therefore concerns the automated tracking of the particles and extraction of damage nucleation kinetics, using advanced segmentation tools. The second objective concerns the identification of damage laws by machine learning methods, as a way to avoid the tedious trial-and-error calibration of mechanical models. Since damage strongly depends on the local stress state of the material, an accurate numerical model should be able to capture stress heterogeneities. The PhD study will employ intensively numerical models available at “Centre de Mise en Forme des Matériaux” in order to create a “numerical twin” of the real material and as well as a surrogate material for the calibration of the different damage and constitutive laws. The micrometre-sized real geometrical features that are observed in the material must be present in the numerical twin. The coupling between the proposed numerical twin and the aforementioned machine learning techniques allows to test and calibrate advanced nucleation models. Ultimately more accurate models allow to enhance our understanding of the underlying physics responsible for damage nucleation and evolution. These simulation using the initial microstructure of real particles will serve as numerical twin to which will be applied mechanical loading and different damage nucleation laws with different parameters. The meshes will serve as graphs for training of AI networks. The trained network will then help to identify the best damage nucleation laws and associated parameters by comparison with the damage scenarios obtained from big data and 3D imaging. The third objective concerns the development of new deep-learning frameworks tailored to physical problems. Mesh structures for graph-convolutional networks will be implemented as a natural representation of finite element simulations,. The material evolution will be studied via spatio-temporal graph-convolutional networks in an effort to take into account in-situ experimental data.

Environment of the PhD thesis

The thesis will be directed by François Willot (Center for Mathematical Morphology -CMM) and Thilo Morgeneyer (Centre des matériaux -MAT) and will be jointly supervised as well by Santiago Velasco-Forero (CMM) and Daniel Pino Munoz (Centre de mise en forme). It will be based in the CMM lab of Fontainebleau as well as in the MAT lab of Evry, both part of Mines Paris.

The doctoral school for this PhD thesis is ED 621 “Ingénierie des Systèmes, Matériaux, Mécanique, Énergétique” with doctoral specialty “Mathematical Morphology” (axe thématique “Mathématiques et systèmes”).

PhD candidates with excellent background in either machine-learning techniques or mechanics and in numerical methods are sought for. The thesis will be partly funded by the PSL “AI4Science” grant (European Marie Skłodowska-Curie Marie Curie program). Therefore only students (of any nationality) **who studied 3 years in the last 4 years outside France are elligible.** Please contact us for questions.

Contact: F. Willot (francois.willot@mines-paristech.fr) T. Morgeneyer (thilo.morgeneyer@mines-paristech.fr) S. Velasco Forero (santiago.velasco@mines-paristech.fr) D. Pino Munoz (daniel.pino_munoz@mines-paristech.fr)

Please include, with your application: a CV, letter of motivation, master/engineering schools grades, articles or project reports you have written.