PROPOSITION DE SUJET DE THESE

Intitulé : An adaptive continuous/discrete coupling strategy for microstructure-dependent fracture simulations

Référence : **MAS-DMAS-2025-15**
(à rappeler dans toute correspondance)

Début de la thèse : October 2025	**Date limite de candidature :** April 2025

Mots clés

Porosity, Cracks, static and dynamic damage, FEM-DEM coupling, Lagrange multipliers, edge-to-edge coupling

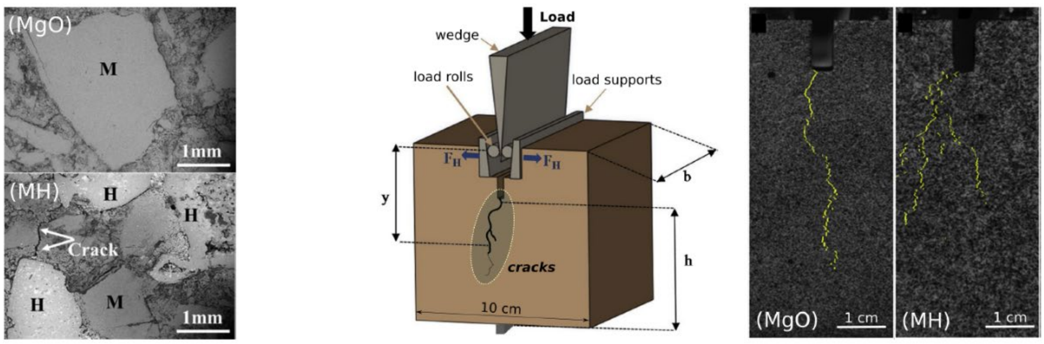
Profil et compétences recherchées

We are looking for candidates with a Master's degree or an engineering diploma in physics, solid mechanics or materials engineering, with a very good knowledge and skills in computational science, numerical tools and numerical simulation. Experience in nonlinear modeling and/or fracture mechanics would be appreciated.

Présentation du projet doctoral, contexte et objectif

Brittle materials like ceramics have a wide range of industrial applications thanks to their good mechanical and thermal strengths, as well as their chemical stability and resistance to corrosion. They can be used for example as coatings to protect and enhance the performance of other materials. A technique used to produce "thick" coatings (up to 100 µm) is plasma spraying, producing so-called plasma sprayed ceramic coatings (PSCC) and are generally used in high-tech applications where their use can significantly increase performance. This is the case for aerospace applications or for highly sensitive defense systems that need to be protected against external threats.

Despite their large applications, the characterization of their fracture properties is always a challenging task: most of the classical tests make it difficult to track the fracture path and propagation speed, even at low test speed. This applies to tests such as tensile, Brazilian or even Compact-Tension tests, to cite only quasi-static tests: the strain energy stored in the specimen is suddenly released when cracks initiate, and quickly leads to complete ruin of the specimen. One of the most efficient test is the so-called Wedge Splitting Test (Figure 1b), which allows identifying the specific fracture energy of brittle materials, such as ceramics, in which the fracture toughness is highly influenced by the presence of micro-cracks within the microstructure. In addition, these micro-cracks promote energy consumption and make the material tougher. The Figure 1 shows for example a refractory material where the microstructure plays a major role on the crack path.



(a) MgO and MH materials [6], (b) Illustration of the Wedge Splitting Test, (c) Cracks path,

Fig. 1: Wedge Splitting Test, pure-Magnesia and Magnesia-Hercynite specimens and the observations of the crack paths [1].

From the numerical point of view, the most complex task is to accurately model the specimen local behavior. A previous PhD thesis work [2] focused on the possibilities offered by the Discrete Element Method (DEM) to model heterogeneous materials such as PSCC at the microstructure scale. A strategy for creating 2D and 3D numerical domains representing the microstructure was proposed [3]. Some simulations for different loading cases in quasi-statics and fast dynamics were carried out on the models to study the effect of the microstructure on the propagation of compression waves, to obtain macroscopic behavior laws and to study the induced damage. Nevertheless, one of the major limitations of such numerical representations at the microscale is the computational cost when the simulation needs to be compared to real experimentations. A full mutiscale modeling is indeed required to simulate a mechanical test at the engineering scale (≈ cm) and to take into account the details of a sub-millimetric microstructure. This can be achieved by using the quite accurate but costly DEM to track failure propagation, together with the quite cost-efficient Finite Element Method (FEM) where a high level of accuracy is not required. Such a modelling strategy has been developed during the PhD thesis of Yahya [4]: the simulation starts with a domain fully described with FE and, when a user defined criterion is reached, the dedicated FE region is replaced with an on-the-fly generated discrete domain. The mechanical fields are then transferred from the FE region to the DE one, and the computation goes on until fracture.

The aim of the proposed research work is to increase the cost-effectiveness and robustness of the preliminary approach proposed by Yahya et al. [4] to simulate more complex cases where standard continuous methods still show limitations. In these specific limiting cases the description of the microstructure is indeed required to simulate multiple cracks initiation, branching and interactions, and dynamic fragmentation.

Three numerical softwares or librairies will be used and coupled together :

• EUROPLEXUS is a Finite Element based computer program for the analysis of fluid-structure systems subjected to fast transient dynamic loading, jointly developed by the French CEA Saclay and by the JRC of the European Commission ;

• GranOO is an open source workbench dedicated to discrete element based simulations. It is developed by researchers from the IRCER, I2M and LAMIH laboratories, and implements several types of bonds and discrete element shapes ;

• CWIPI is a coupling library, developed by ONERA, which ensures the exchange of interpolated fields across a non-conforming geometric interface.

This computing part of the PhD proposal will then be validated with respect to three experimental test cases, selected to gradually move towards validation of the protocol for fast-dynamic loadings : a Wedge Splitting Test, commonly used to characterize the tensile strength and fracture toughness of quasi-brittle materials, a Split Hopkinson Tensile Bar test, commonly used to characterize the dynamic failure behavior of brittle and ductile materials and a laser shock test leading to a very high strain rates and a spalling damage.

References

[1] I. Khlifi, O. Pop, J.-C. Dupré, P. Doumalin, and M. Huger. Investigation of microstructure-property relationships of magnesia-hercynite refractory composites by a refined digital image correlation technique. Journal of the European Ceramic Society, 39(13):3893–3902, 2019.

[2] V. Longchamp. Modélisation du comportement de c´céramiques projetées plasma sous choc par simulation discrète `a l´´échelle de la microstructure. Theses, HESAM Université, Mar. 2024.

[3] V. Longchamp, J. Girardot, D. André, F. Malaise, A. Quet, P. Carles, and I. Iordanoff. Discrete 3d modeling of porous-cracked ceramic at the microstructure scale. Journal of the European Ceramic Society, 44(4):2522–2536, Apr. 2024.

[4] F. Yahya, C. Hubert, N. Leconte, and L. Dubar. A fem/dem adaptive remeshing strategy for brittle elastic failure initiation and propagation. International Journal for Numerical Methods in Engineering, 125(15), May 2024.

Collaborations envisagées

The PhD student will be a full member inside the consortium bringing together four public laboratories (I2M, IRCER, LAMIH, CERAMATHS) and ONERA. Periodic scientific discussions and exchanges, short-period journeys and multiple seminars will be the basis of the collaborations in this project. Supervisors of this project are also members of two scientific communities in the field of the subject : (i) the European COST (COoperation in Science and Technology) Open Network on DEM Simulations [https://www.cost.eu/actions/CA22132/] and (ii) the french national joint laboratory FR CHOCODYN [https://chocodyn.cnrs.fr/].

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