MICROSCALE DISCRETE ELEMENT SIMULATION OF SHOCK WAVE PROPAGATION IN PLASMA SPRAYED CERAMICS

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Abstract
The macroscopic behavior of plasma sprayed zirconia coatings is greatly affected by their microstructure, and phenomena that occur at this scale, such as micro-craking and cracks closure. The present study investigates the effect of micro-porosities and micro-craking on compressive waves mitigation, material compaction, and macroscopic fracture. A procedure to generate 3D digital twins that faithfully represents the microstructure is developped using the discrete element method (DEM) and analysis of scanning electron microscope (SEM) images. Static and dynamic compressive loadings are applied to 3D and 2D twins to identify their macroscopic behavior. Local damage mechanisms and their influence on the waves mitigation and the macroscopic damage are observed and discussed related to the current knowledge in the literature.

1. Introduction
Ceramic coatings produced by plasma spray are characterized by a complex microstructure composed of numerous cracks and pores, which directly affect the macroscopic properties of the material. The objective of this study is to investigate their influence on the mitigation of laser-induced shock waves [1], by the mean of a microscale numerical model. High-precision 3D visualizations of the microstructure are acquired with a FIB-SEM [2]. Digital twins of the observed microstructure are generated using image processing and analysis techniques derived from the work in [2-3], and the discrete element method (DEM). This method is selected because of its ability to describe heterogeneous media [4], to represent discontinuous phenomena such as multi-cracking [5], and to perform dynamic simulations [6]. To address the multiscale nature of the problem, two case studies are proposed: i) a 3D model on which compression is applied to study its macroscopic mechanical response and ii) a simplified 2D model capable of modeling millimeter thick coatings to simulate the propagation of laser-induced shock waves. These simulations are able to deal with complex crack initiation and propagation thanks to the DEM framework.

2. Results
In this DEM based modeling, a continuous medium can be modeled by a set of discrete elements (DE) connected by mechanical bonds. Then, pores bigger than the selected DE size are represented by deleting DE, whereas cracks, which are smaller than the DE size, are represented by deleting bonds (*cf.* Fig.1). With this approach, digital twins of 25×25×25 µm³ statistical elementary volumes (SEV) are generated while using a small enough number of DE to have acceptable computational times. However, these SEV (~µm) are several orders of magnitude smaller than the thickness of plasma sprayed ceramic coatings (~mm) and cannot be used to the direct simulation of dynamic experiments. Thus, quasi-static compressive loadings are applied on

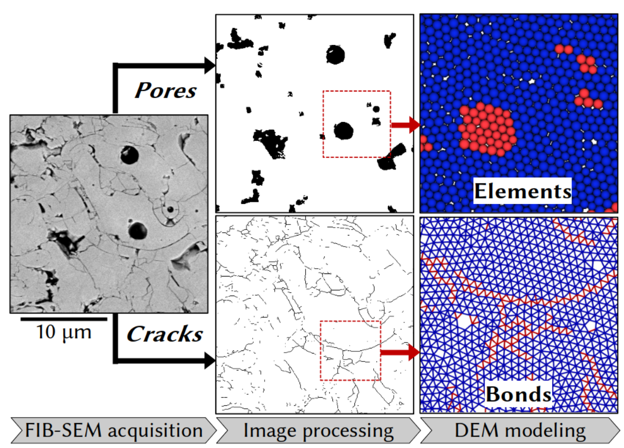

Fig.1 – 3D digital twins generation procedure: from FIB-SEM to DEM (described in 2D)

the SEV to predict the pressure-density relationships at macroscopic scale. These simulations successfully reproduce (i) the non-linear behavior induced by the closing of the initial cracks [7] (orange curve on Fig.2a) and (ii) the anisotropy due to the preferential cracks orientation. Besides, the digital model allows to investigate the macroscopic effect of each microstructural component independently: simulations can be performed on twins containing only cracks or only pores as shown on Fig.2a.
In order to simulate laser-induced shock waves experiments, such as described in the work of [7], the entire thickness of a coating (536 µm) is digitalized in 2D from several SEM images stitched together. An ablation pressure pulse is applied on one side of the 2D twin, and the evolution of the computed velocity profiles at different depth in the coating are monitored. As highlighted on Fig.2b, this simulation demonstrates the suitability of the model to capture the shock waves mitigation by introducing the microstructure morphology in a purely elastic material.
Finally, several fracture criteria adapted to DEM [5] are assessed in order to represent micro-cracking at the local scale, as shown on Fig.3b, and to study their influence on the macroscopic behavior.

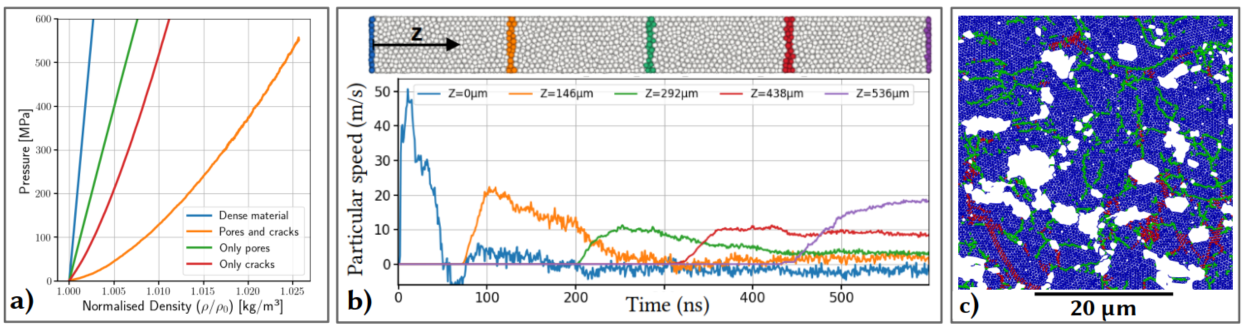

Fig.2 – a) Pressure-density relations obtained from quasi-static compressions on the 3D twin and simulation of a compressive wave propagation on the 2D twin: b) velocity profiles at different thickness (Z axis) and c) a focus in a part of the twin to visualize new micro-cracks (shown in red)

3. Conclusions

A discrete element modeling procedure has been set up to reproduce the real 3D microstructure of complex porous materials, like plasma-sprayed ceramics, with the help of FIB-SEM observations. Some dynamic and quasi-static simulations have shown the suitability of the proposed model to reproduce the specific behavior of these materials. Laser-induced shock waves experiments are planned to quantitatively validate the numerical results. Future works will be dedicated to the representation of other coatings microstructures, and to study the effect of local crack initiation and propagation on the macroscopic properties.

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