A multi-scale coupling method to simulate the silica glass behavior under high pressures.

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Abstract. *The response of glasses subjected to high pressures can be classif ed into three classes : normal, anomalous and intermediate depending on the deformation mechanism and the cracking pattern. The silica glass which is the scope of this work is a typical anomalous glass. The numerical study of this behavior with continuum methods (e.g. FEM, CNEM) presents several diff culties and drawbacks. Because, this requires a very small scale analysis. The discrete methods (e.g. MD, DEM) represent a good choice to simulate this behavior. However, these methods are very time consuming (CPU-wise). In this work, a discrete-continuum coupling method is proposed to study the behavior of this brittle material subjected to high pressures. The coupling results, obtained in this work, compare favorably with past experimental results.*

Keywords: Coupling ; silica; Vickers indentation.

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1 INTRODUCTION

The discrete element method (DEM) [2] presents an alternative way to study physical phenomena requiring a very small scale analysis or those which cannot be easily treated by continuum mechanics, such as wear, fracture and abrasion problems. In the past decades, an increasing interest in the discrete element method has led to the development of many interesting variations of this method. The most recent variation involves modelling the interaction between particles by cohesive beams [2]. This method correctly simulates the 3D linear elastic behavior of the continua. However, numerical simulations are very time consuming (CPU-wise). Furthermore, a very great number of particles are required to discretize small domains. This method does not consider large structure simulations. However, in most situations, the effects that must be captured by DEM are localized in a small portion of the studied domain. Thus, the use of a specif c multi-scale method to treat the phenomena at each scale appears to be advantageous. In this work a discrete-continuum coupling method between the discrete element method (DEM) [2] and the constrained natural element method (CNEM) [7] is proposed for dynamic simulations. This coupling method is then applied to study the Vickers indentation and the laser induced damage in silica glass. Compared with experimental results, good numerical results are obtained.

2 DEM-CNEM COUPLING

The coupling method developed in this work is based on the Arlequin approach [6] which gives a f exible framework to couple dissimilar methods. This approach consists of :

1. A superposition of mechanical states in the given subdomains Ω_C and Ω_d with an overlapping zone Ω_O (Fig. 1).

2. A weak coupling (based on the weak formulation):

   (a) Def nition of the gluing zone Ω_G:

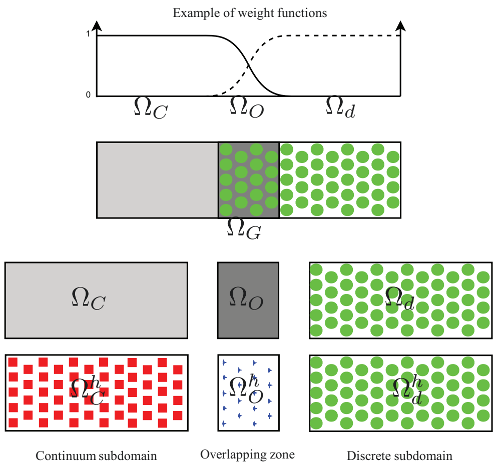


Figure 1: Global domain decomposition

In this study, the gluing zone Ω_G is the same as the overlapping zone Ω_O. Hereafter, the term "overlapping zone" will be used to design the overlapping zone or the gluing zone.

(b) Mediator space $\mathcal{M}$:

To ensure the correct dialogue between the models, the control quantities in the overlapping zone must be chosen carefully. Here, the velocity coupling, in a weak sense in Ω_O, is chosen. The mediator space denoted by $\mathcal{M}$ is defined as the space of the velocities defined in Ω_O.

(c) Projection operator and junction model:

The projection operator Π projects the continuum and discrete velocities on the mediator space. The junction model defines the linking conditions between the two models in the overlapping zone. To project the velocities on $\mathcal{M}$, an interpolation, whose shape functions will be defined later, is used. The junction model used in this work is the $H^1(\Omega_O)$ scalar product defined by Equation 1:

$$< \boldsymbol{\lambda}, \boldsymbol{q} >_{H^1(\Omega_O)} = \int_{\Omega_O} \boldsymbol{\lambda} \cdot (\Pi \dot{\boldsymbol{u}} - \Pi \dot{\boldsymbol{d}}) + l^2 \boldsymbol{\varepsilon}(\boldsymbol{\lambda}) : \boldsymbol{\varepsilon}(\Pi \dot{\boldsymbol{u}} - \Pi \dot{\boldsymbol{d}}) \, d\Omega \tag{1}$$

where $(\Pi \dot{\boldsymbol{u}} - \Pi \dot{\boldsymbol{d}})$ is the difference between the projected continuum and discrete velocities on Ω_O, $\boldsymbol{\lambda}$ is the Lagrange multiplier field and l, the junction parameter, is an H^1 coupling parameter. If $l = 0$, the $H^1(\Omega_O)$ scalar product becomes equivalent to the $L^2(\Omega_O)$ scalar product (2) known as the Lagrange multiplier model.

$$< \boldsymbol{\lambda}, \boldsymbol{u} >_{L^2(\Omega_O)} = \int_{\Omega_O} \boldsymbol{\lambda} \cdot (\Pi \dot{\boldsymbol{u}} - \Pi \dot{\boldsymbol{d}}) \, d\Omega \tag{2}$$

The displacement and velocity fields in Ω_C and Ω_d do not have the same nature. Indeed, Ω_C is a continuum whereas the Ω_d is a discrete subdomain. The discrete field associated with Ω_d is defined only at the particle positions. To be able to compute the junction models (1) and (2), an interpolation is defined on the DEM particles in Ω_O using shape functions.

3. The energy partition between the DEM and CNEM media in the overlapping zone:

As shown in Figure 1, the two models coexist in Ω_O. Therefore, the energies in this zone must be weighted, and, a kind of partition of unity in terms of energy is performed. Three weight functions, $\alpha(\boldsymbol{x})$, $\beta(\boldsymbol{x})$ and $\gamma(\boldsymbol{x})$, are introduced for the internal energy, the kinetic energy and the external work of the continuum subdomain, respectively. All of the functions verify the following:

$$\begin{aligned} f(\boldsymbol{x}) : \quad \Omega \quad &\rightarrow \quad [0,1] \\ \boldsymbol{x} \quad &\rightarrow \quad \begin{cases} 1 & \text{in } \Omega_C \backslash \Omega_O \\ [0,1] & \text{in } \Omega_C \cap \Omega_O \\ 0 & \text{otherwise} \end{cases} \end{aligned} \tag{3}$$

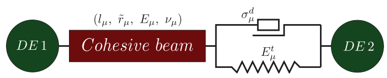


Figure 2: Densif cation model

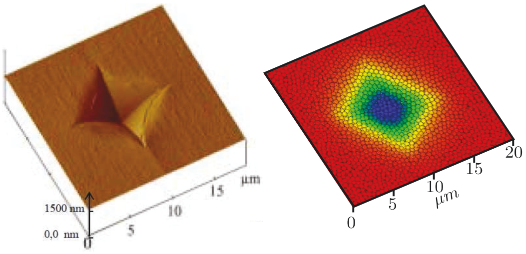


Figure 3: Indentation print compared with experimental result [**?**]

In a complementary manner, the internal energy, the kinetic energy and the external work of the discrete subdomain are weighted by $\bar{\alpha}(\boldsymbol{x}) = 1 - \alpha(\boldsymbol{x})$, $\bar{\beta}(\boldsymbol{x}) = 1 - \beta(\boldsymbol{x})$ and $\bar{\gamma}(\boldsymbol{x}) = 1 - \gamma(\boldsymbol{x})$, respectively.

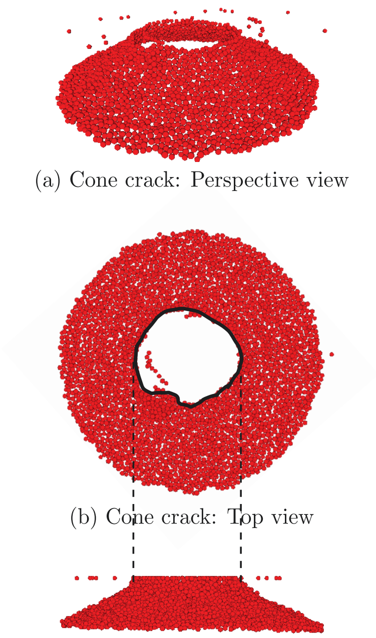
This coupling approach involves several coupling parameters which must be carefully studied to ensure a correct wave propagation between the continuum and discrete models. A complete study can be found in Reference [4].

3 SILICA GLASS MODELING

The CNEM-DEM coupling method is applied to study the silica glass response under high pressures. The discrete element method is applied in the zones of high stress concentration and the continuum method (CNEM) is applied in the rest of the studied domain. Because the CNEM domain is far from the high loaded zones, only the elastic behavior is modeled in this subdomain. Whereas, a new model taking into account the permanent deformation and the fracture of silica glass is applied in the DEM subdomain. This model which is developed in this work is brief y reviewed here. A "spring-slider" system is connected in series with each cohesive beam linking two particles, as shown in Figure 2. When the compression stress in the associated beam σ^c_{beam} reaches the microscopic densif cation threshold σ^d_μ, the slider activates and the densif cation mechanism takes place. The densif cation level beyond σ^d_μ is controlled by the microscopic tangential modulus E^t_μ, which is adjustable. Finally, to model the saturation stage, the slider stops slipping above a certain limit controlled by the maximum microscopic permanent deformation of cohesive bonds $\varepsilon^{p\,max}_\mu$. To model the fracture, a new criterion based on the computation of an equivalent of Cauchy stress in each discrete element is used [3]. When the hydrostatic pressure exceeds a breaking limit, determined by calibration, the discrete element in question releases from its neighbors. For more details, the reader can refer to [3, 5].

4 APPLICATIONS

This method is applied to study the silica glass response under high pressures. In this section, the Vickers indentation in silica glass is brief y reviewed. In the case of low indentation force ($F_{indent} = 500\,mN$), the response of silica glass is characterized by the absence of fracture and only permanent deformation set up. Figure 3 presents the indentation print compared with experimental result [1]. When high indentation force is applied, silica glass has a strong tendency to form a cone crack, even when indented with a Vickers tip. Because of its important densif cation behavior, a spherical densif ed zone is formed beneath the Vickers indenter which in turn operates as a spherical indenter, so that a cone crack is set up that can accompany median, radial and lateral cracks. Figure 4 presents the numerical cracking response of silica glass indented with a Vickers tip at the beginning of fracture (before the cracking becomes unstable). In this f gure, only the discrete elements where the fracturing criterion is reached are shown.



(a) Cone crack: Perspective view

(b) Cone crack: Top view

(c) Cone crack: Side view

Figure 4: Cracking pattern of silica glass indented with a Vickers tip

5 CONCLUSIONS

A new 3D coupling method based on the Arlequin approach adapted for dynamic simulations is developed in this paper . After studying its different coupling parameters, this method is applied to study the silica glass behavior under high pressures. The first application preformed in this work is the Vickers indentation. Good numerical results are obtained in this application which compare favoraly with experimental ones. Another application which is currently under way concerns the laser-induced damage in silica glass.

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