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# Nonsmooth fracture dynamics of functionally graded materials

F. Perales<sup>1</sup>, Y. Monerie<sup>1</sup> and A. Chrysochoos<sup>2</sup>

<sup>1</sup> *Institut de Radioprotection et de Sûreté Nucléaire, DPAM, SEMCA, LEC, BP. 3, 13115 St-Paul-Lez-Durance Cedex, France*

<sup>2</sup> *Laboratoire de Mécanique et Génie Civil, CC048, Place E. Bataillon, 34095 Montpellier Cedex 5, France*

**Abstract.** This paper presents a numerical framework for the simulation of dynamic fracture of heterogeneous material. It consists in a multibody approach based both on the concept of Frictional Cohesive Zone Model and on NonSmooth Contact Dynamics. The heterogeneities of the material are taken into account using a multiscale method. The microscopic scale corresponds to the scale of heterogeneities. The macroscopic scale corresponds to the structure where gradients of properties will be invoked. The ability of the framework is illustrated by the fracture of hydrided Zircaloy-4, constituting nuclear cladding tube, under transient loading.

## 1. INTRODUCTION

The core of a Pressurized Water Reactor (PWR) contains a stack of fuel pellets surrounded by a Zircaloy cladding tube. During nuclear reactor operation, the microstructure of these tubes evolves because of the migration/precipitation of hydrogen. The microstructure appears as a two phase material constituted of zirconium hydrides platelets embedded in a Zircaloy metal matrix. The hydride-induced embrittlement can lead to the failure of the fuel rods under accident conditions.

In the frame of the French “Institut de Radioprotection et de Sûreté Nucléaire” (IRSN) research program on nuclear fuel safety under accident conditions, a new numerical framework dedicated to the study of the dynamic fracture of heterogeneous and functionally graded materials has then been developed. The framework consists in a micromechanical approach, based on both the concept of Frictional Cohesive Zone Model (FCZM) and a multibody method in the context of the NonSmooth Contact Dynamics (NSCD).

The FCZM couples standard cohesive zone model, describing the vectorial traction – separation relationship in the fracture process zone, with nonsmooth surface behaviors such as frictional contact. Since dynamic problems involving unilateral constraints are not regular (velocity can become discontinuous), the NSCD approach is used in order to solve the equations of the frictional contact without any regularization nor penalization. These modelings are developed in a total lagrangian finite deformation formulation, implicit dynamics and periodic homogenization.

The associated software is composed of three libraries, each dealing with a part of the mechanical problem. The ability of the numerical framework and of the associated platform are illustrated by two examples. The first one quantifies the weakening effect of brittle inclusions in an elastoplastic matrix. The second one deals with the dynamic fracture of a functionally graded material at the scale of the structure.

## 2. MULTIBODY APPROACH AND FRICTIONAL COHESIVE ZONE MODEL

To analyse the effects of the microstructure heterogeneity on the material behavior, a micromechanical modeling based on a multibody concept and FCZM is proposed. The multibody system consists in

independant meshes connected one to each other with FCZM-type interface relationship. The bulk volumic behaviors inside the meshes as well as the surface properties of the FCZM vary with the position in space. This variation is related to the phases of a composite material, for example at the microscale, or to continuous properties such as graded properties, at the macroscale.

The FCZM concept represents the physics of the fracture process at the crack tip, from crack initiation to post-fracture unilateral contact and friction. The present model [7] is inspired by the adhesive-friction law of Raous et al. [9] and by the surface damage law of Michel et al. [4]. A cohesive stress, denoted by  $\mathbf{R}^{\text{coh}}$ , is added on the Signorini-Coulomb complementary problem (1)-(2) and related to the displacement jump  $[\mathbf{u}]$  across the crack lips (3) :

$$0 \leq (R_N + R_N^{\text{coh}}) \leq 0, \quad (1)$$

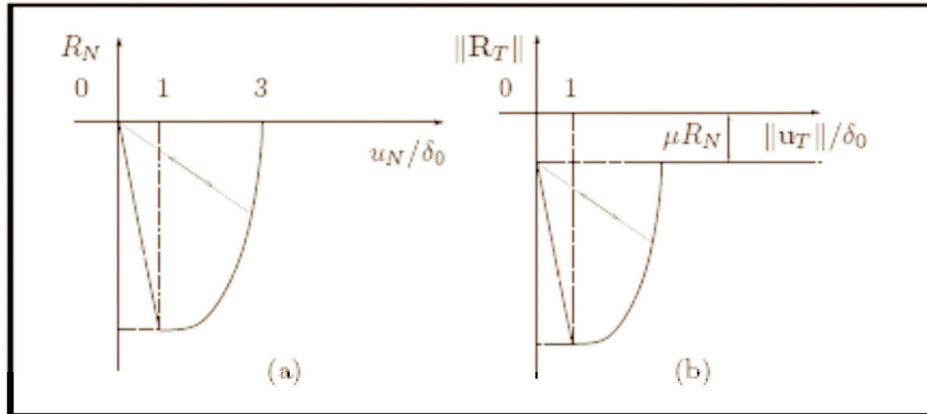
$$\begin{cases} \|R_T + R_T^{\text{coh}}\| < \mu |R_N + R_N^{\text{coh}}| & \dot{u}_T = 0 \\ \|R_T + R_T^{\text{coh}}\| = \mu |R_N + R_N^{\text{coh}}| & \dot{u}_T = -\lambda (R_T + R_T^{\text{coh}}) \end{cases} \quad \text{such as } \dot{u}_T = -\lambda (R_T + R_T^{\text{coh}}) \quad (2)$$

$$\mathbf{R}^{\text{coh}} = \beta \left( C_N \mathbf{n} \otimes \mathbf{n} + C_T \frac{\mathbf{u}_T \otimes \mathbf{u}_T}{\|\mathbf{u}_T\|^2} \right) \cdot [\mathbf{u}] \quad \text{and} \quad \beta = \min(g(\|\mathbf{u}\|), g(\|\mathbf{u}_{\max}\|)). \quad (3)$$

Subscripts  $N$  and  $T$  respectively denote the normal and tangential components ( $\mathbf{R} = R_N \mathbf{n} + R_T \mathbf{t}$ ,  $\mathbf{R}^{\text{coh}} = R_N^{\text{coh}} \mathbf{n} + \mathbf{R}_T^{\text{coh}}$  and  $[\mathbf{u}] = u_N \mathbf{n} + \mathbf{u}_T$ ),  $\mathbf{n}$  is the unit normal vector of the cohesive zone,  $C_N$  and  $C_T$  denote respectively the initial normal and tangent stiffness of the perfect interface (MPa/m),  $\mathbf{u}_{\max}$  is the maximum value reached by  $\mathbf{u}$  during the fracture process,  $g$  is a decreasing function of  $\|\mathbf{u}\|$  (progressive softening),  $\mu$  is the Coulomb friction and  $\beta$  is a surface variable ( $\beta = 1$  : the interface is undamaged,  $0 < \beta < 1$  : the interface is partially damaged and  $\beta = 0$  : the interface is fully damaged). The damage evolution is governed by :

$$g(x) = \beta_0 \text{ if } x \leq \delta_0, \quad g(x) = 0 \text{ if } x \geq \delta_c, \quad g(x) = \frac{\beta_0(\delta_c - x)}{\delta_c - 2\delta_0 + x} \text{ if } \delta_0 < x < \delta_c, \quad (4)$$

where  $\delta_0 = \sqrt{\frac{w}{(9-4\ln 4)} \left( \frac{1}{C_N} + \frac{1}{C_T} \right)}$ ,  $\delta_c = 3\delta_0$ ,  $0 \leq \beta_0 \leq 1$ , is an initial surface damage and  $w$  is a reference fracture energy ( $\text{J/m}^2$ ). In a 2D case, Fig. 1 shows the normal and the tangential behavior associated to the FCZM (1)-(4).



**Figure 1.** The 2D FCZM : (a) normal behavior ( $u_T = 0$ ) - (b) tangent behavior ( $R_N$  constant,  $u_N = 0$ ).

### 3. NONSMOOTH CONTACT DYNAMICS AND FCZM

Denoting  $M$  the mass matrix,  $\mathbf{q}$ ,  $\dot{\mathbf{q}}$  and  $\ddot{\mathbf{q}}$  respectively the discrete displacement, the velocity and the acceleration,  $F(\mathbf{q}, \dot{\mathbf{q}}, t)$  the internal and external forces and  $\mathbf{r}$  the representative of local reaction forces, the investigated dynamic problem is composed of equations (1)-(4) and the discrete dynamic equation:

$$M\ddot{\mathbf{q}} = F(\mathbf{q}, \dot{\mathbf{q}}, t) + \mathbf{r} \quad (5)$$

The equation (5) is treated without any regularization nor penalization techniques using the frame of the NSCD approach [3] and the functional framework defined by Moreau [6]. In particular, the derivatives are written in the sense of the distribution and the time integration scheme is *implicit*.

Using linear mappings between global unknowns (velocity  $\dot{\mathbf{q}}$  and impulse  $h\mathbf{r}$ ) and their relative counterparts ( $\dot{\mathbf{U}}$  and  $h\mathbf{R}$ ), and previous formulation of Monerie and Acary [5], the three dimensional system to solve for each contact  $\alpha$  writes [3]:

$$\dot{\mathbf{U}}^\alpha = \dot{\mathbf{U}}_f^\alpha + \mathbf{W}^{\alpha\alpha} h (\mathbf{R} - \mathbf{R}^{\text{coh}})^\alpha, \quad \mathbf{R}_N^\alpha = \text{proj}_N + (R_N^\alpha - \rho U_N^\alpha), \quad \mathbf{R}_T^\alpha = \text{proj}_D + (\mathbf{R}_T^\alpha - \rho \dot{\mathbf{U}}_T^\alpha) \quad (6)$$

where  $\rho > 0$  and  $D$  is the section of Coulomb's cone for contact  $\alpha$ ,  $\mathbf{U}_f^\alpha$  is the velocity at the contact in the absence of contact  $\alpha$  and  $h$  is the length of the time step. The system is solved using the generalized Newton method of Alart and Curnier [1].

### 4. NUMERICAL SOFTWARE

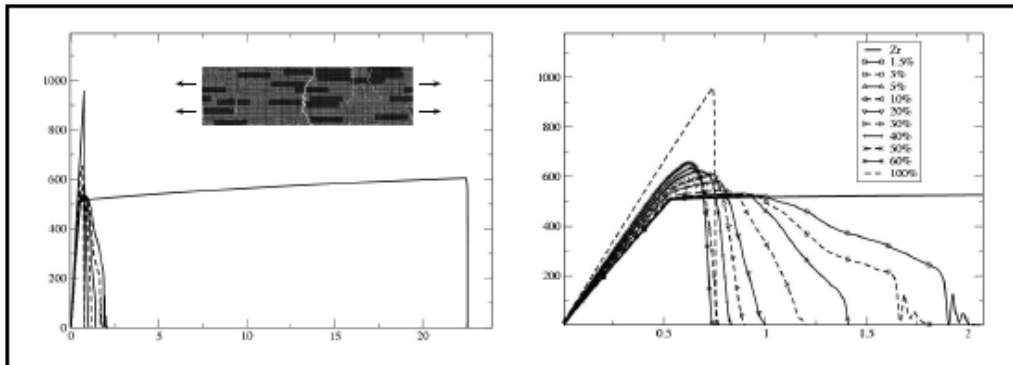
The application software, called 'X-per', is written using Object Oriented and Mixed Programming. The conception rests on three libraries having a clear mechanical meaning : 1) a library dedicated to contact problems using NSCD approach (LMGC90, [2]), 2) a Finite Element library (PELICANS, [8]), and 3) a material constitutive models library (MatLib, [10]).

The software allows to simulate, in finite deformation, the dynamic fracture of heterogeneous materials from the crack initiation to post-fracture behavior.

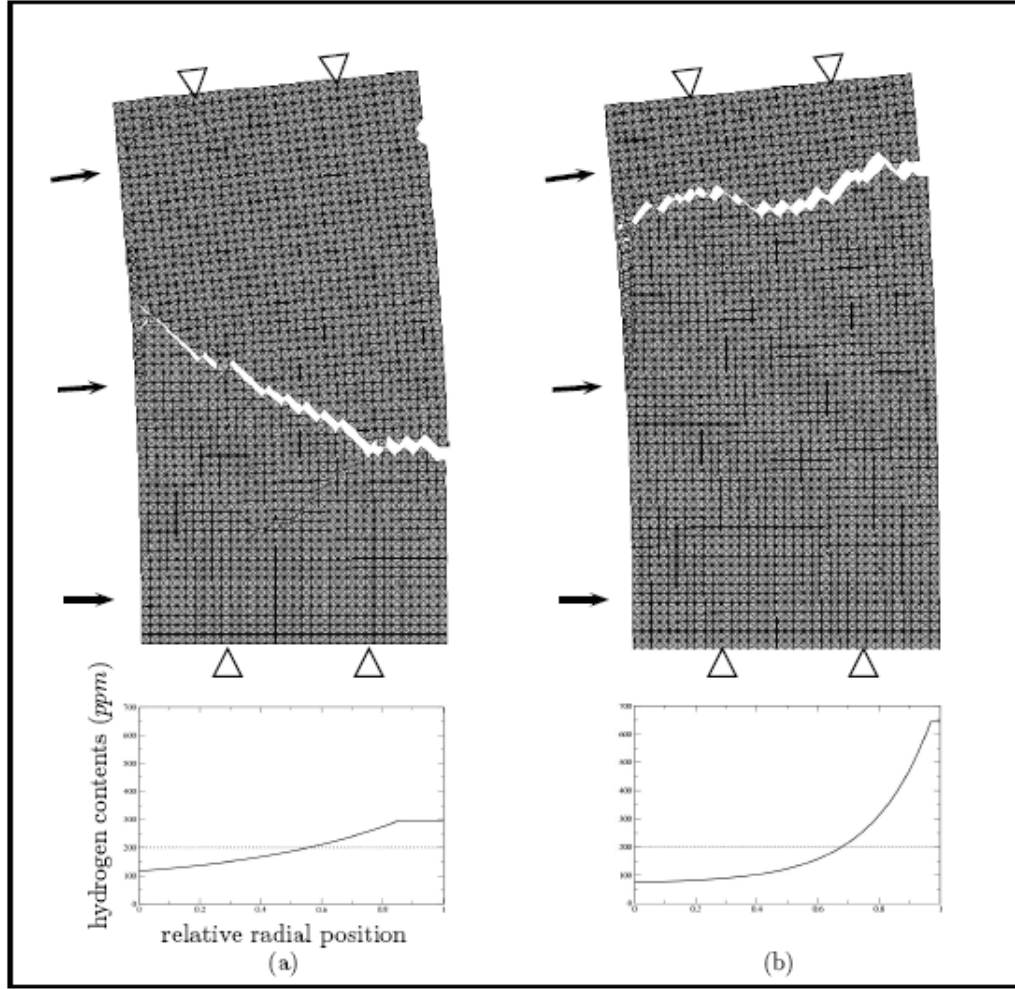
### 5. APPLICATIONS

#### 5.1 Influence of brittle phase on the fracture of an elastoplastic material

This application deals with the numerical simulation of the damage elastoplastic behavior of the Zircaloy-4. At the microscale, the numerical simulations have been made using periodic Representative



**Figure 2.** Overall stress (MPa)/strain (%) curve of the hydrided Zircaloy-4 for various hydrogen contents, with a zoom at small strains (right).



**Figure 3.** Influence of the profile gradient of hydrogen contents on the dynamic rupture features of a part of cladding tube : (a) low gradient ( $p = 0.5$ ) : crack branching along shear band ; (b) high gradient ( $p = 0.8$ ) : quasi-brittle fracture.

Volume Elements for various volume fractions of inclusions. Each microstructure is composed of a metal matrix (Zircaloy-4) and rectangular aligned inclusions randomly distributed (zirconium hydrides). The Zircaloy-4 behavior is assumed to be elastoplastic (J2 plasticity,  $E = 99 \text{ GPa}$ ,  $\nu = 0.325$ ,  $\sigma_0 = 450 \text{ MPa}$ ,  $H_Y = 850 \text{ MPa}$ ) and hydrides to be elastic ( $E = 135 \text{ GPa}$ ,  $\nu = 0.32$ ). The FCZM coefficients of Zircaloy-4, zirconium hydrides and Zircaloy-hydride interface are respectively:  $C_N^{Zr} = 2 \times 10^{18} \text{ Pa/m}$  and  $w^{Zr} = 1 \text{ J/m}^2$ ,  $C_N^{ZrH} = 2C_N^{Zr}$  and  $w^{ZrH} = 0.8w^{Zr}$ ,  $C_N^{Zr-ZrH} = 2C_N^{Zr}$  and  $w^{Zr-ZrH} = 0.8w$ .

Moreover, we assume a low friction coefficient  $\mu = 0.05$  and same compliance for the normal and tangential behaviors  $C_N = C_T$ . A macroscopic strain gradient rate is prescribed along the direction of the aligned inclusions ( $\dot{\bar{F}}_{xx} = 10^6 \text{ s}^{-1}$ ) and the resulting stress/strain curves are plotted on Fig. 2 for various volume fraction of inclusions.

A key feature of these simulations is that the overall elastoplastic and damageable behaviour of the Zircaloy matrix is conveniently described by the dynamic multibody approach without any viscous regularization, neither in the bulk behaviors (in the meshes), nor in the interfaces (in the FCZM). In

addition, the Fig. 2 shows the deleterious influence of the hydride on the material ductility: the ultimate tensile elongation decreases rapidly with hydrogen contents.

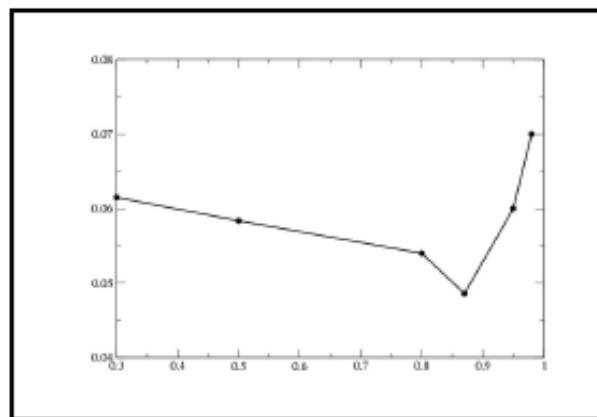
## 5.2 Dynamic fracture of an heterogeneous cladding tube

This second application deals with the macroscopic fracture of an hydrided Zircaloy-4 cladding tube with a gradient of hydrogen contents. At this scale, the volumic bulk behaviors are derived with the help of some analytical homogeneization techniques in a separate work [11] and surfacic behaviors of the FCZM are given by the results of the previous section. These volumic and surfacic behaviors depend on hydrogen contents and are respectively introduced at the Gauss points and at the contacts node where the FCZM is integrated.

The simulations are performed on a part of a cladding tube in two dimensions and in a plane perpendicular to the axis of the tube. Various mean hydrogen contents  $[\bar{H}]$  and various profile gradients are investigated. The hydrogen gradients are characterized by a parameter  $p$  ( $p = 0$  : no gradient,  $p = 1$  : limit case of a bimaterial microstructure). A radial velocity  $v_r = 20 \text{ ms}^{-1}$  is imposed on the inner side of the tube. Precracks are present in an outer layer, corresponding to some highly brittle zirconia.

Fig. 3 shows the rupture features for  $[\bar{H}] = 200 \text{ ppm}$  and two gradients  $p = 0.5$  and  $p = 0.8$ . Crack propagates rapidly from the outer side to the inner side in the high hydrogen concentration area. If this area is small enough ( $p = 0.5$ ), the crack velocity decreases progressively and a crack branching can appear along some shear bands. Otherwise ( $p = 0.8$ ), the precrack is long enough to go through the entire structure leading to a brittle failure of the cladding tube.

Fig. 4 shows the importance of the profile gradient in the fracture toughness. Below  $p = 0.9$ , the higher the gradient, the lower the fracture energy: the gradient acts as a precrack whose length grows with  $p$ . Above this value, the gradient becomes beneficial for the fracture toughness: the microstructure tends to a bimaterial which can accomodate a part of the shear strain at its interface.



**Figure 4.** Energy ( $\text{Jm}^{-2}$ ) vs profile gradient for 200 ppm of hydrogen.

## 6. CONCLUSION

This paper has presented a numerical framework for the dynamic fracture of heterogeneous materials. The framework consists in a multibody approach based on the concept of Frictional Cohesive Zone Model and NonSmooth Contact Dynamics approach. The associated numerical platform is developed by coupling libraries with Object Oriented and Mixed Programming. The efficiency of this numerical

framework was underlined on the multiscale simulation of a functionally graded metal matrix composite from the nuclear industry. In particular, the intensity of heterogeneity profile gradient minimizing the dynamic fracture toughness of this tubes was qualified.

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