CALIBRATION AND NUMERICAL VALIDATION OF A MICROMECHANICAL DAMAGE MODEL

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ABSTRACT : The mechanical behaviour of brittle geomaterials is strongly determined by the growth and nucleation of microcracks. In the present work, a micromechanical damage model is numerically implemented and calibrated on a sandstone. First we present the general framework and the physical features assumed for the anisotropic damage. Then, the model is used to simulate the mechanical behaviour of the material under triaxial and proportional compression. The results show good agreements between the experience and the model predictions, and allow to give more insight on the dominant mechanisms of deformation.

1 INTRODUCTION

Since two decades, Continuum Damage Mechanics (CDM) has been the subject of tremendous researches (Krajcinovic, 1989 ; Lemaître, 1990). The conventional phenomenological approach of damage modelling is based on the use of internal variables (scalar, vectorial or tensorial). This variable is supposed to represent the salient features of the microcracking which generates the brittle damage. In Kondo et al. (1992) such modelling approach was used for a britlle sandstone. In spite of its efficiency in some situations, the phenomenological approach lacks to describe precisely some specific features of brittle damage : stress - induced anisotropy, unilateral effects due to microcracks closure (see Chaboche, 1992). On the other hand, micromechanical models, by using informations at mesoscopic level, try to give more insight on the damage phenomenon. The main purpose of the present study is to calibrate and validate a three-dimensional micromechanical constitutive theory inspired from Fanella and Krajinovic (1988) and Ju and Lee (1991). An outline of the paper is as following. First, we summarize the mechanical behaviour of the material characterized by a stress-induced anisotropy and the dilatant deformations. Then, the general framework of the micromechanical model is presented. Calibration on triaxial tests and numerical simulations allow to demonstrate the strong capabilities of the model to reproduce the experimental data. More particularly, the comparisons of the numerical predictions with the damaged moduli (experimentally determined by cyclic tests) show good agreements.

2 SUMMARY OF EXPERIMENTAL RESULTS

Experiments have been conducted on a brittle sandstone (Fontainebleau sandstone). This material is constituted mainly by quartz grains (98%), the rest being clay minerals. The average quartz grains size is about 250 µm and the initial relative porosity is low (about 10%). The average specific density is $23.7\ (\pm 0.2)\ kN.m^{-3}$. The specimens (cylinders) measured 37.5 mm in diameter by 75 mm in length. They are tested under the same boundary conditions and the current laboratory environment conditions. Great care has been taken in the design and sequences of the experimental frame to warrant uniform loading of samples.

Hydrostatic and Triaxial compressive tests

Hydrostatic compressive tests are first performed. Stress-strains (axial and lateral) curves indicate that Fontainebleau sandstone is initially isotropic. The experimental results for triaxial tests are presented in terms of deviatoric stress $(\sigma_1 - \sigma_3)$. σ_1 is the axial stress and σ_3 is the confining pressure. Figure 1 shows the stress-strain curves for triaxial tests with different confining pressures. These curves correspond to a typical brittle behaviour with stress induced anisotropy and a large dilatancy in deformation (related to the strong non linearity of the lateral strains). Proportional compression tests are also performed and will serve as validation of the modelling (see section 4).

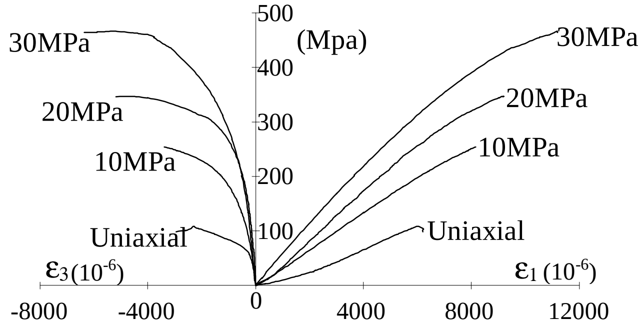


Figure 1 : Stress-strain curves for monotonous triaxial compression tests

3 BRIEF PRESENTATION OF THE 3-D MICROMECHANICAL DAMAGE MODEL

3.1 General framework

Consider a representative elementary volume (REV) containing a great number of microcracks (see for example Nemat-Nasser and Horii (1993 for conditions on REV). It is assumed that the solid matrix (brittle) is homogeneous and has a linear elastic behaviour, with a initial compliance denoted $\bar{S}^0$. The constitutive relations of the microcracks-weakened solid, linking the macroscopic stress $\bar{\sigma}$ and the macroscopic strain $\bar{\varepsilon}$ is described through the overall compliance matrix $\bar{S} = \bar{S}^0 + \bar{S}^d$. $\bar{S}^d$ is the inelastic part of the compliance due to microcracks present in the REV. Such constitutive relations can be summarised as follow (Ju, 1991) :

complementary free energy :

$$\psi^*(\bar{\sigma}, \bar{S}) = \frac{1}{2}\bar{\sigma}{:}\bar{S}{:}\bar{\sigma} = \frac{1}{2}\bar{\sigma}\ (\bar{S}^0 + \bar{S}^d)\bar{\sigma} \quad (1)$$

state laws : $$\bar{\varepsilon} = \frac{\partial \psi^*}{\partial \bar{\sigma}} = \bar{S}{:}\bar{\sigma} = (\bar{S}^0 + \bar{S}^d)\bar{\sigma} \quad (2)$$

The damage dissipation inequality which is $\frac{1}{2}\bar{\sigma}\,\dot{\bar{S}}\,\bar{\sigma} \geq 0$ depends strongly on the rate of the overall compliance.

Voigt's notations are used in all the study.

$$\begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \\ e_6 \end{bmatrix} = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix} \text{ et } \begin{bmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \\ \tau_4 \\ \tau_5 \\ \tau_6 \end{bmatrix} = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} \text{ with } e_i = S_{ij}\tau_j.$$

The development of the damage micromechanical model requires :

i) evaluation of the overall compliance for the elastic brittle material weakened by numerous interactive microcracks
ii) use of precise kinetic equations for microcracks growth.

We examine now these two points

3.2 Overall compliance of the microcracked solid

The inelastic part of the compliance $\bar{S}^d$ is estimated from the displacement discontinuities field (cracks opening displacements, COD) b_i'. The general form of the solution for penny-shapped cracks in anisotropic medium loaded in compression (figure 2) is as given by Lee and Ju, (1991) and Ju and Lee (1991) (see Horii and Nemat-Nasser, 1983 for 2-D solutions) :

$$b'_i(x', y') = 2a\sqrt{1 - x'^2 - y'^2}\, C'^{-1}_{ik}\, \bar{\sigma}'_{1k} \quad (3)$$

Matrix C'^{-1} is a tensor which relates COD to the applied (macroscopic) stress tensor. It depends on material properties (anisotropic elastic parameters). The prime indicates that COD are calculated in the local frame of each microcracks. Contribution of all microcracks to inelastic compliance is given by :

$$\bar{\varepsilon}^{d} = \bar{S}^{d}\bar{\sigma} = \frac{1}{2V}\sum_{k}\left[\int_{A_k}(b\otimes n + n\otimes b)dA\right]^{(k)} \quad (4)$$

V is the volume occupied by the RVE. A_k is the area of k-th microcrack. n is the normal to the microcrack surface.

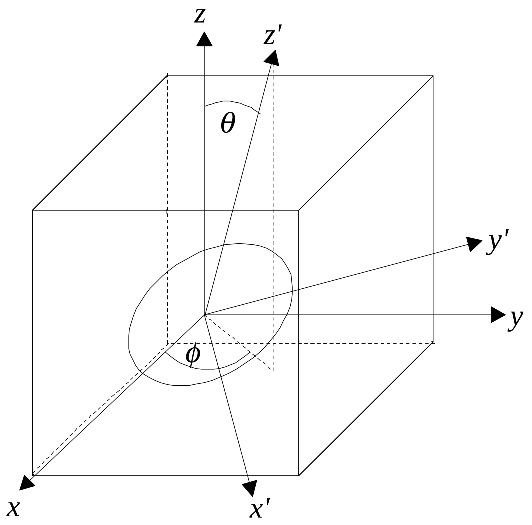


Figure. 2 : 3-D penny shaped microcrack geometry and definition of axes

In fact, the summation in expression (4) is semi analytically evaluated by average techniques. For this, microcracks distribution is supposed to be spatially continued and their location and orientation are random : the initial radius and orientation of defects are randomly distributed on $\left[a_{0_{\min}}, a_{0_{\max}}\right]$ for radius, on $\left[0, \frac{\pi}{2}\right]$ for θ , and on $[0, 2\pi]$ for ϕ . Microcracks interactions are taken into account by use of the Self Consistent Method (SCM). In this method each defect is assumed to be already in the unknown effective medium. Since the SCM is used, an iterative algorithm is needed for the calculation of the overall compliance.

3.3 Microcracks growth mechanisms and Kinetic equations

Based on the previous statistical assumptions, the initial microstructure is determined by the minimum and maximum grain size and by the microcrack density. Pre-existing microcracks are supposed to be at grains-matrix interfaces (the material can be viewed as a composite aggregate). The progressive damage is the result of microcracks growth when the solid is loaded. Under tensile load, cracks may propagate in mode I (opening mode), whereas the propagation is more complex under compression. Based on works of Nemat-Nasser and Horii, (1982) and Zaitsev (1983) the kinetic equations of microcrack growth under compressive loading is summarised as follow (figure 3).

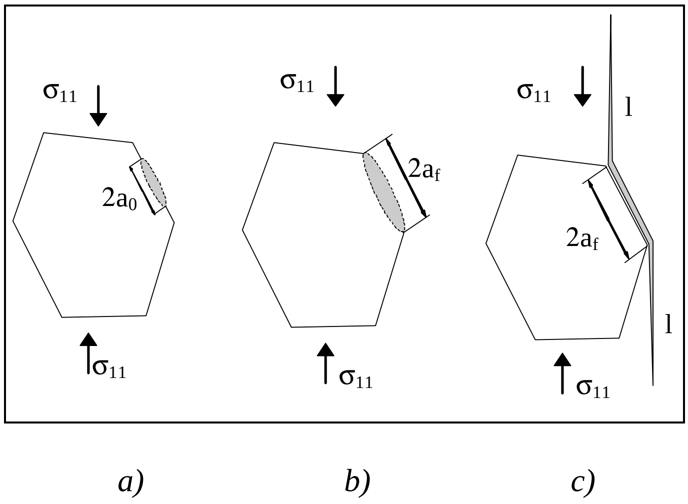


Figure 3 : Mechanisms of microcracks growth under compressive load - a) sliding without propagation ; b) propagation in unstable mode II ; c) Kinking in mixed mode

Case b) corresponds to instantaneous crack growth at the interface ; such growth is temporarily stopped by the matrix energy barrier. The crack begins to kink (case c) when the stress intensity factor attains the critical mode I value K_{Ic}^{m} in the matrix. Propagation conditions are obtained from classical fracture mechanics analysis. Details of such analysis can be found in Fanella and Krajcinovic (1988) or in Ju and Lee (1991).

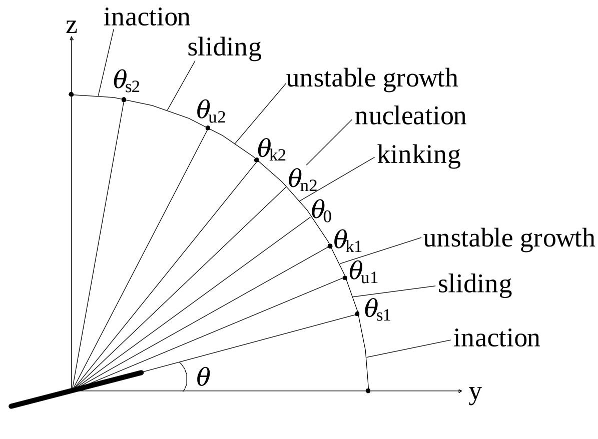


Figure 4 : 3-D compressive active damage domain

At each load step a domain of active damage (sliding, unstable growth, kinking and opening) depending on microcracks orientation is determined (see figure 4).

For completeness, note that microcracks nucleation mechanism is integrated in the analysis via the classical Zener-Stroh model based on a critical debonding shear stress.

4 CALIBRATION OF THE MODEL AND NUMERICAL PREDICTIONS

4.1 Constitutive parameters and calibration of the model

The 3-D micromechanical model requires 9 parameters which have physical meanings and then are easy to be identified. These parameters can be divided in two distinct classes :

Macroscopic parameters :

These parameters are the Young modulus E, the Poisson's ration ν, the friction coefficient, the interfacial fracture toughness K_{Ic}^{if} and the matrix fracture toughness K_{Ic}^{m}

Mesoscopic parameters :

The precise description of the initial microstructure requires parameters such as the minimum and maximum grain size $D_{\min}$ and $D_{\max}$, the initial microcracks density w_0 and the critical debonding stress τ_c^0 (for nucleation mechanism).

We intend here to show the capabilities of the micromechanical damage model. The calibration is done using the set of triaxial compression tests presented at figure 1. Note that, except for E and ν, a single set of parameters is used for all the triaxial tests. Figure 5 shows two examples of comparisons of the numerical results and the experimental data. The computed results correlate well these data and confirm the efficiency of the model.

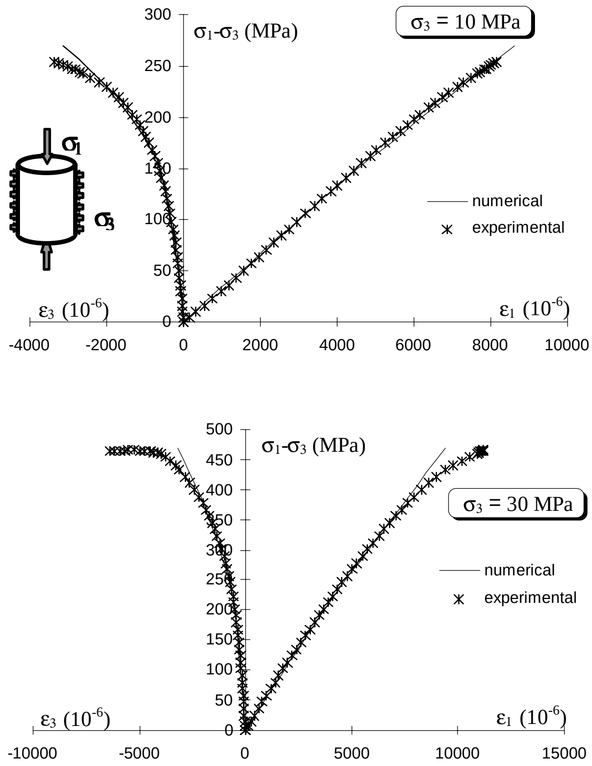


Figure 5 : Triaxial compressive tests - Comparisons between experiments data and numerical results

4.2 Numerical predictions of damaged moduli : comparisons with experimental data

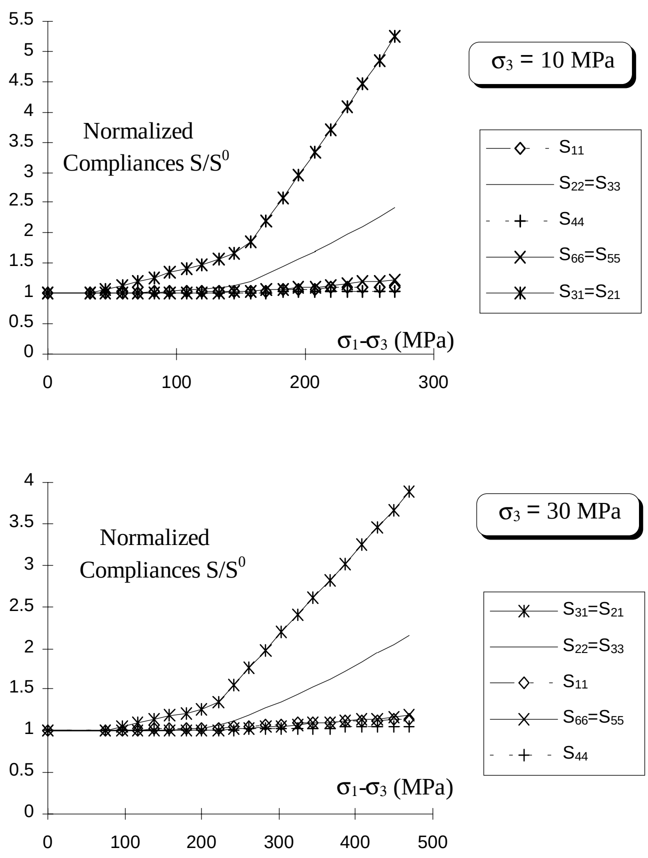
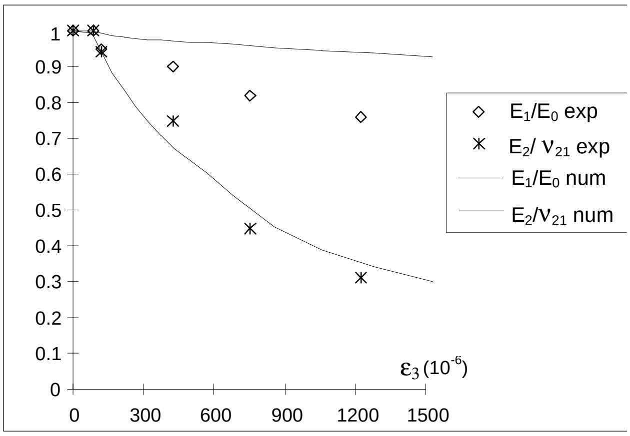


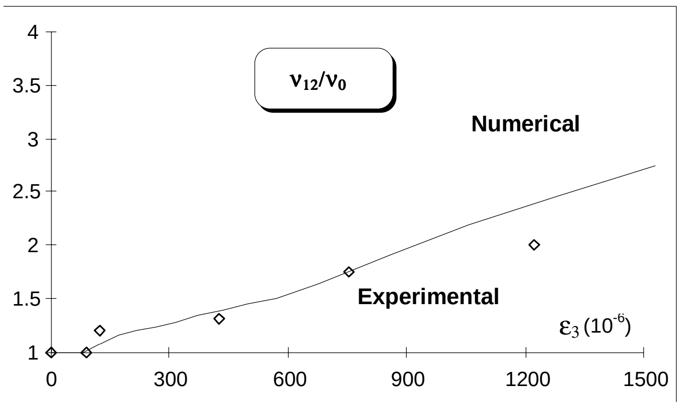
Figure 6 : Normalised compliances variation in triaxial compression

The detailed analysis of the results shows that the dilatancy is essentially due to microcracks kinking (axial opening mode). In order to show the importance of damage anisotropy, we have plotted at figure 6 the variation of the normalised components of the compliance tensor. Variation of the lateral compliance $\bar{S}_{22}$ is observed to be much larger than for the axial one $\bar{S}_{11}$. The more important increase of $\bar{S}_{21} = \bar{S}_{31}$ explains the strong non-linearity of lateral strain and then the dilatancy.

These results are interpreted in term of the moduli and Poisson's ratio variation (see figures 7 for test with $\sigma_3 = 10\text{MPa}$). Comparisons of predicted values with experimental data (obtained from cyclic compression tests) give good agreements. Note however that the model underestimates slightly the decrease of axial modulus.



a)

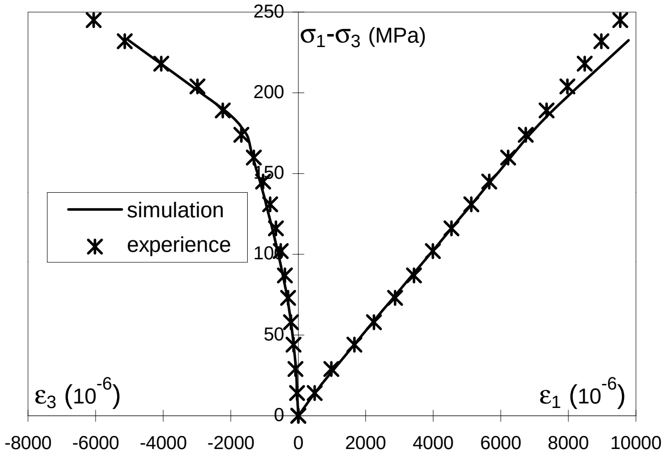


b)

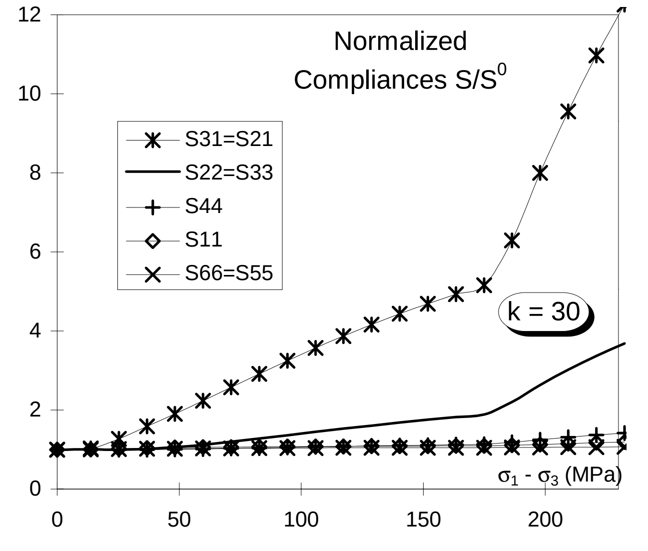
Figure 7 : Predictions of the moduli decrease
a) Axial and lateral moduli b) Poisson's ratio

4.3 Proportional stress path test :

On the basis of the preceding calibration, numerical simulations are conducted on proportional stress path tests (experimental results are available for this test). We present on figure 8a the predictions for a test performed at a ratio $k = \dfrac{\sigma_1}{\sigma_3} = 30$. It is observed that the numerical predictions are in accordance with the tests data. In comparison with the triaxial data $(\sigma_3 = 10\text{MPa})$, damage in the present case is more pronounced for similar deviatoric stress (see figure 8b).



a)



b)

a) Comparisons between experiments data and numerical results b) Normalised compliances variation under proportional compression
Figure 8 : Proportional compressive tests (k = 30) -

4.4 Influence of parameters :

A study of the influence of some parameters has been done. We present here some illustrations for the initial microcracks density w_0 (figure 9) and for nucleation mechanism (figure 10) in a triaxial test $(\sigma_3 = 10\text{MPa})$. From figure 9 we note that the material response depends strongly on its initial damage state. The material is more dilatant when the initial density w_0 is more important. Finally the nucleation mechanism appears to be important in the anisotropic damage process. We observe that the simulation without generation of new microcracks (0 pn on figure 10) leads to non negligible differences with experimental data.

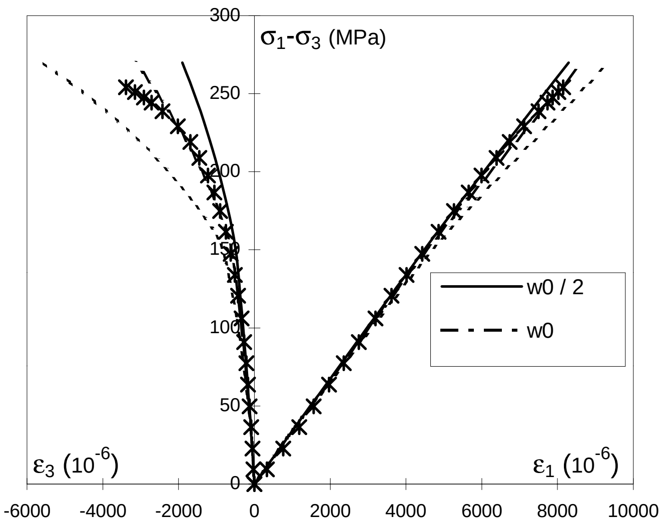


Figure 9 : Uniaxial compression - Effect of initial microcracks density (ω_0 is the reference density)

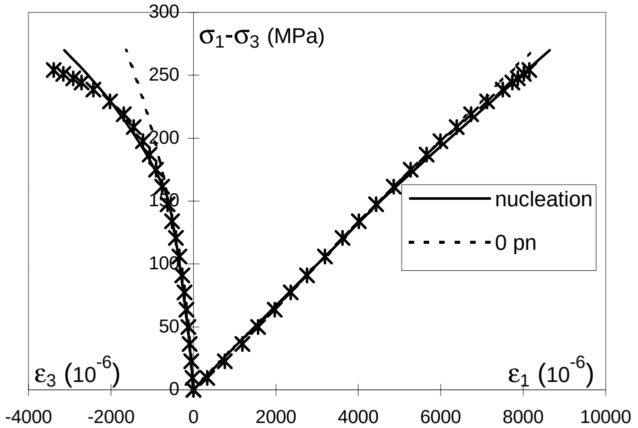


Figure 10 : Influence of nucleation mechanism

5 Conclusions

A 3-D micromechanical damage model is implemented and used for simulate the behaviour of a sandstone under triaxial and proportional loadings. The numerical results confirm the capabilities of the modelling approach and the salient features of the brittle damage are well reproduced by the model. Furthermore, the numerical simulations give some information on the importance of the various mesoscopic mechanisms involved in the brittle damage process. More complex stress paths are under investigation in order to check cracks closure effects on damage (damage desactivation). Finally, in order to study the effect of damage on stability of structures, we plan to introduce the model in a Finite Element code.

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