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Nonlinear behavior of matrix-inclusion composites under high confining pressure: application to concrete and mortar

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Abstract

This paper is devoted to a micromechanics-based simulation of the response of concrete to hydrostatic and oedometric compressions. Concrete is described as a composite made up of a cement matrix in which rigid inclusions are embedded. The focus is put on the role of the interface between matrix and inclusion which represent the interfacial transition zone (ITZ). A plastic behavior is considered for both the matrix and the interfaces. The effective response of the composite is derived from the modified secant method adapted to the situation of imperfect interfaces. ***To cite this article: T.H. Le et al., C. R. Mecanique 336 (2008).***

Résumé

Comportement non linéaire de composites à phase inclusionnaire sous haute pression : application aux bétons et mortiers. On présente une approche micromécanique de la réponse d'un béton à des compressions œdométrique ou hydrostatique. Le béton est décrit comme un composite avec une matrice cimentaire et des inclusions rigides. L'accent est mis sur le rôle de l'interface entre matrice et inclusion qui représente la zone interfaciale de transition (ITZ). On se donne un comportement élastoplastique pour la matrice ainsi que pour les interfaces. Le comportement homogénéisé est obtenu à l'aide de la méthode sécante modifiée adaptée à la présence d'interfaces. ***Pour citer cet article : T.H. Le et al., C. R. Mecanique 336 (2008).***
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Mots-clés : Milieux continus ; Béton ; Mortier ; Interface ; Homogénéisation ; Nonlinéarité

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1. Introduction

The interfacial transition zone (ITZ) in concrete refers to a region of the cement paste surrounding the aggregates in which the mechanical properties of the paste are believed to be lower than in the bulk. The purpose of the present Note is to investigate the role of the ITZ in the effective response of concrete under compression. In particular, we aim at highlighting that the discrepancy of behavior between the hydrostatic and œdometric compression for high pressure values can be explained by an adapted constitutive law of the ITZ. The ITZ is replaced by a 2D interface the behavior of which is described by a constitutive equation relating the stress vector $\boldsymbol{T}$ acting on the aggregate and the jump $[\boldsymbol{\xi}]$ of the displacement vector $\boldsymbol{\xi}$ in the interface. Introducing the unit normal $\boldsymbol{n}$ to the interface and the normal and tangential stress components $T_n = \boldsymbol{T}\cdot\boldsymbol{n}$ and $\boldsymbol{T}_t = \boldsymbol{T} - T_n\boldsymbol{n}$, this constitutive equation reads:

$$\begin{cases} T_n = k_n[\boldsymbol{\xi}\cdot\boldsymbol{n}] \\ \boldsymbol{T}_t = k_t[\boldsymbol{\xi}]_t \end{cases} \tag{1}$$

where $[\boldsymbol{\xi}]_t = [\boldsymbol{\xi}] - [\boldsymbol{\xi}\cdot\boldsymbol{n}]\boldsymbol{n}$ is the tangential component of the displacement jump. k_n and k_t respectively represent the normal and tangential stiffnesses of the interface. The aggregates themselves are modelled as rigid spherical inclusions, with density N and radius R. Their volume fraction in the composite is denoted by $\phi_a = 4\pi NR^3/3$.

The work exposed hereafter focuses on the implementation of a homogenization scheme taking specifically into account the role of the interface. The impact of such an imperfect interface on mechanical properties at the upper scale has already been the subject of various contributions [1–3].

Notations. In the following, the deviatoric part of the strain (resp. stress) tensor $\boldsymbol{\varepsilon}$ (resp. $\boldsymbol{\sigma}$) is $\boldsymbol{\varepsilon}_d = \boldsymbol{\varepsilon} - \frac{1}{3}\operatorname{tr}\boldsymbol{\varepsilon}\mathbf{1}$ (resp. $\boldsymbol{\sigma}_d = \boldsymbol{\sigma} - \frac{1}{3}\operatorname{tr}\boldsymbol{\sigma}\mathbf{1}$). We also introduce the scalar $\varepsilon_d = (\frac{1}{2}\boldsymbol{\varepsilon}_d : \boldsymbol{\varepsilon}_d)^{1/2}$ (resp. $\sigma_d = (\frac{1}{2}\boldsymbol{\sigma}_d : \boldsymbol{\sigma}_d)^{1/2}$). $\bar{a}$ denotes the average of the field $a(z)$ in the composite while $\bar{a}^\alpha$ is the average over the phase α.

2. Linear homogenized behavior

We first model the cement paste as an isotropic linear elastic material (stiffness tensor $\mathbb{C}^c$, bulk and shear moduli k_c and μ_c, Poisson's ratio ν_c), the interface being characterized by the two constants k_n and k_t. We look for the effective behavior of the composite which is to be characterized by the homogenized stiffness tensor $\mathbb{C}^{\text{hom}}$.

In the latter, the aggregates together with the surrounding interface are considered as spherical inclusions in the generalized sense of morphological pattern (see [4]). The cement paste is regarded as a matrix in which the aggregate + interface (A + I) inclusions are embedded. The effective behavior is derived according to the generalized Mori–Tanaka scheme [4].

This requires one to solve the generalized Eshelby's problem in which a spherical A+I inclusion with radius R is embedded in an infinite medium with bulk and shear moduli k_c and μ_c. Uniform strain boundary conditions ($\boldsymbol{\xi} \to \boldsymbol{E}^\infty\cdot z$) are prescribed at infinity ($|z| \to \infty$). First an isotropic loading is considered ($\boldsymbol{E}^\infty = E^\infty\mathbf{1}$). In spherical coordinates with the center of the inclusion as a pole, the displacement in the medium surrounding the A + I inclusions takes the form:

$$\boldsymbol{\xi}(z) = \left(Ar + \frac{B}{r^2}\right)\boldsymbol{e}_r \tag{2}$$

Coefficients A and B are determined from the continuity of the stress vector at the interface and from the boundary condition at infinity:

$$A = E^\infty; \qquad \frac{B}{R^3} = \frac{3k_c - k_nR}{4\mu_c + k_nR}E^\infty \tag{3}$$

In the framework of the generalized Mori–Tanaka scheme, the average strain in the matrix $\bar{\boldsymbol{\varepsilon}}^c$ and in the A + I inclusion $\bar{\boldsymbol{\varepsilon}}^{A+I}$ read:

$$\bar{\boldsymbol{\varepsilon}}^c = E^\infty\mathbf{1}; \qquad \bar{\boldsymbol{\varepsilon}}^{A+I} = \left(A + B/R^3\right)\mathbf{1} \tag{4}$$

The auxiliary strain E^∞ is related to the macroscopic strain $\boldsymbol{E}$ by the average rule:

$$\boldsymbol{E} = (1-\phi_a)\bar{\boldsymbol{\varepsilon}}^c + \phi_a\bar{\boldsymbol{\varepsilon}}^{A+I} \tag{5}$$

Similarly, the stress average rule reads:

$$\boldsymbol{\Sigma} = (1-\phi_a)\bar{\boldsymbol{\sigma}}^c + \phi_a \bar{\boldsymbol{\sigma}}^{A+I} \tag{6}$$

with $\bar{\boldsymbol{\sigma}}^c = \mathbb{C}^c : \bar{\boldsymbol{\varepsilon}}^c$ and

$$\bar{\boldsymbol{\sigma}}^{A+I} = k_n(AR + B/R^2)\mathbf{1} \tag{7}$$

The condition $\boldsymbol{\Sigma} = \mathbb{C}^{\text{hom}} : \boldsymbol{E}$ eventually yields:

$$k^{\text{hom}} = \frac{3(1-\phi_a)k_c + \phi_a \alpha k_n R}{3(1-\phi_a + \alpha\phi_g)} \quad \text{with } \alpha = \frac{A + B/R^3}{E^\infty} = \frac{4\mu_c + 3k_c}{4\mu_c + k_n R} \tag{8}$$

In particular, in the case of an incompressible matrix:

$$k^{\text{hom}} = \frac{4(1-\phi_a)}{3\phi_a}\mu_c + \frac{R}{3\phi_a}k_n \tag{9}$$

In order to determine the homogenized shear modulus μ^{hom}, the solution of the generalized Eshelby's problem for a purely deviatoric strain $\boldsymbol{E}^\infty$ at infinity is due. We consider for instance

$$\boldsymbol{E}^\infty = E^\infty(\mathbf{e}_1 \otimes \mathbf{e}_1 - \mathbf{e}_2 \otimes \mathbf{e}_2) \tag{10}$$

where $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ define a Cartesian orthonormal frame. In spherical coordinates (r, θ, φ) ($\theta = 0$ corresponding to the direction of $\mathbf{e}_3$), the displacement field in the domain $r > R$ is sought in the form [5]:

$$\boldsymbol{\xi}(\mathbf{r}) = \xi_r(r)\sin^2(\theta)\cos(2\varphi)\boldsymbol{e}_r + \xi_\theta(r)\sin(\theta)\cos(\theta)\cos(2\varphi)\boldsymbol{e}_\theta + \xi_\varphi(r)\sin(\theta)\cos(\theta)\cos(2\varphi)\boldsymbol{e}_\varphi \tag{11}$$

with

$$\begin{aligned}
\xi_r(r) &= Ar + 3\frac{C}{r^4} + \frac{5-4\nu_c}{1-2\nu_c}\frac{D}{r^2} \\
\xi_\theta(r) &= Ar - 2\frac{C}{r^4} + 2\frac{D}{r^2} \\
\xi_\varphi(r) &= -\xi_\theta(r)
\end{aligned} \tag{12}$$

Coefficients A, C and D are again determined from the stress vector continuity at the interface and from the strain condition at infinity ($A = E^\infty$). Following the same steps as for the spherical loading, a Mori–Tanaka estimate for μ^{hom} is then derived. In the case of an incompressible cement matrix, the later reads:

$$\mu^{\text{hom}} = \frac{\mu_c}{2}\frac{10\mu_c k_n R + 48\mu_c^2 + 2k_t R^2 k_n + 12k_t R\mu_c + (12k_t R\mu_c + 6\mu_c k_n R - 48\mu_c^2 + 3k_t R^2 k_n)\phi_a}{5\mu_c k_n R + 24\mu_c^2 + k_t R^2 k_n + 6k_t R\mu_c - (4k_t R\mu_c + 2\mu_c k_n R - 16\mu_c^2 + k_t R^2 k_n)\phi_a} \tag{13}$$

It is worth recalling that the macroscopic moduli (9) and (13) have been obtained under the assumption of the interfacial law (1). The validity of the latter should obviously be restricted to compressive normal stress to avoid the nonlinear effect of the decohesion of a unilateral contact. Keeping in mind that the aim of this work is to model the nonlinear behavior of concrete, the linear scheme will be used as a tool in the nonlinear homogenization process. Nevertheless, the condition of compressive stress state will have to be satisfied in this linear scheme, which will be the case for the loadings considered hereafter.

3. Nonlinear homogenized behavior

3.1. Principle of nonlinear homogenization

A more realistic modelling should take into account irreversible strains in the cement matrix. We now assume that the matrix is a perfect elastoplastic von Mises material, whose plastic criterion takes the form:

$$\frac{1}{2}\boldsymbol{\sigma}_d : \boldsymbol{\sigma}_d = K^2 \tag{14}$$

No unloading being considered, we approach this behavior by nonlinear elasticity. The bulk modulus k_c is kept constant while the shear modulus μ_c is a decreasing function of the scalar deviatoric strain ε_d, chosen in such a way that the condition (14) is asymptotically satisfied for large ε_d [6,7]:

$$\mu_c(\varepsilon_d) = \frac{K}{2\varepsilon_0}\frac{1}{1+\varepsilon_d/\varepsilon_0} \tag{15}$$

The constant ε_0 is a reference deviatoric strain which is related to the initial elasticity $\mu_0 = \mu(0)$ of the matrix by $2\varepsilon_0 = K/\mu_0$. The cement-aggregate interfaces are still characterized by a constitutive equation of the form (1).

Due to the nonlinear behavior of the matrix, the shear modulus $\mu_c(\varepsilon_d(z))$ is now a function of the loading level and of the location in the cement paste. In order to deal with this nonlinearity, the modified secant method [8] is adopted for the derivation of the homogenized behavior. In short, secant methods propose to estimate the shear strain level in the matrix by a so-called "effective" value $\langle\varepsilon_d\rangle$, which is supposed to represent an average of the strain field. In turn, the shear modulus $\mu_c(\varepsilon_d(z))$ is then approximated by $\mu_c(\langle\varepsilon_d\rangle)$. The modified secant method introduces an original energy-based effective strain. More precisely, the later is the second order moment $\overline{\overline{\varepsilon_d}} = (\frac{1}{2}\overline{\boldsymbol{\varepsilon}_d : \boldsymbol{\varepsilon}_d}^c)^{1/2}$ of the deviatoric strain. $\overline{\overline{\varepsilon_d}}$ is related to the derivative of the homogenized stiffness w.r.t. μ_c [9]

$$2\phi_c\overline{\overline{\varepsilon_d}}^2 = \frac{1}{2}\boldsymbol{E} : \frac{\partial}{\partial\mu_c}\boldsymbol{C}^{\mathrm{hom}} : \boldsymbol{E} \tag{16}$$

If macroscopic properties are isotropic ($\mathbb{C}^{\mathrm{hom}} = 3k^{\mathrm{hom}}\mathbb{J} + 2\mu^{\mathrm{hom}}\mathbb{K}$), it yields:

$$2\phi_c\overline{\overline{\varepsilon_d}}^2 = \frac{1}{2}\frac{\partial k^{\mathrm{hom}}}{\partial\mu_c}E_v^2 + \frac{\partial\mu^{\mathrm{hom}}}{\partial\mu_c}\boldsymbol{E}_d : \boldsymbol{E}_d \tag{17}$$

where $\boldsymbol{E}$ is the macroscopic strain applied to the representative elementary volume (r.e.v.) ($E_v = \mathrm{tr}(\boldsymbol{E})$ and $\boldsymbol{E}_d = \boldsymbol{E} - \frac{1}{3}\,\mathrm{tr}\,\boldsymbol{E}\mathbb{I}$).

The composite made up of the matrix with shear modulus $\mu_c(\overline{\overline{\varepsilon_d}})$ together with the A + I inclusions is then homogenized in the framework of the generalized Mori–Tanaka scheme presented at Section 2. The effective behavior is finally estimated in the nonlinear form $\Sigma = \mathbb{C}^{\mathrm{hom}}(\boldsymbol{E}) : \boldsymbol{E}$. For simplicity, only the limit case of incompressible matrix ($k_c \to \infty$) is considered.

3.2. Compaction of concrete under hydrostatic compression

We investigate in this section the behavior of concrete under hydrostatic compression ($\boldsymbol{E} = E\mathbf{1}$). It is recalled by (9) that k^{hom} depends on the effective matrix shear modulus $\mu_c(\overline{\overline{\varepsilon_d}})$ and on k_n which is first regarded as constant. Combining this equation with (17) yields the following estimate for $\overline{\overline{\varepsilon_d}}$:

$$\overline{\overline{\varepsilon_d}} = -\frac{E_v}{\sqrt{3\phi_a}} \tag{18}$$

Hence, $\overline{\overline{\varepsilon_d}}$ increases simultaneously with the macroscopic volume strain $|E_v|$ whereas (15) and (9) indicate that both $\mu_c(\overline{\overline{\varepsilon_d}})$ and k^{hom} decrease. Asymptotically, k^{hom} tends toward the limit $Rk_n/(3\phi_a)$ as shown on Fig. 1. In contrast, the experimental results [10] on the behavior of concrete under high hydrostatic pressure plotted on the same figure reveal a stiffening of the material and a change of curvature in the $\Sigma_c(E_v)$ curve. It is believed that these features should be attributed to the stiffening of the cement-aggregate interfaces, as closure goes on. In addition, a constant value of k_n allows the normal displacement jump to reach any negative value and thus may not prevent possible interpenetrations. We therefore introduce a phenomenological dependence of the normal stiffness k_n of the interface on the normal component $\beta = [\boldsymbol{\xi}]\cdot\boldsymbol{n}$ of the displacement jump:

$$k_n = \frac{k_{n0}}{1+\beta/\beta_0} \tag{19}$$

The positive constant β_0 can be interpreted as the maximum possible closure of the interface. Due to the incompressibility of the cement matrix, the surface average of β can be directly related to E_v:

$$E_v = 3\phi_a\frac{\bar{\beta}}{R} \tag{20}$$

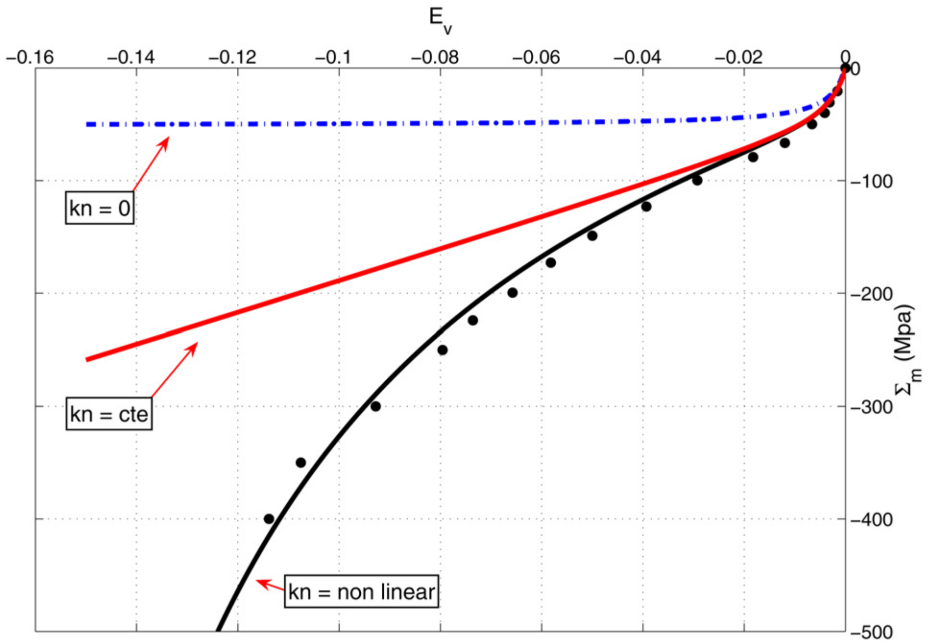

Fig. 1. Macroscopic homogenized behavior and stiffening effects – points: experimental results from Burlion et al. [10] – curves: models with the following parameters $Rk_{n0} = 2100$ Mpa, $\phi_a = 0.5$, $\epsilon_0 = 0.0027$, $\mu_0 = 11\,700$ Mpa for k_n constant and $\beta_0/R = 0.135$ for k_n nonlinear.

The homogenized behavior in hydrostatic compression is obtained by considering both μ_c and k_n as functions of E_v. As shown in Fig. 1, this simple small strain model with rigid aggregates and incompressible plastic matrix provides an excellent agreement with the experimental results. Interestingly, it reproduces the change of concavity of the experimental stress-strain curve and the existence of a vertical asymptote. Indeed, the maximum compaction corresponding to total interface closure ($\beta = -\beta_0$) is given by:

$$E_v^{\lim} = -3\phi_a \frac{\beta_0}{R} \tag{21}$$

It is emphasized that the average normal displacement jump is involved by means of a first order moment. Indeed, this choice allows to relate the latter to the macroscopic strain by the exact relationship (20) i.e. without resorting to any homogenization scheme. We could also have chosen a second order moment to interpret our nonlinear homogenization scheme in the framework of variational methods developed in [11]. This would have had the great advantage of providing a macroscopic potential. Nevertheless, these methods rely upon the existence of a microscopic potential defining the behavior of each constituent, which will not be the case anymore in the next section in which β_0 will depend on the shear strains in the interface.

3.3. Compaction of concrete under oedometric loading

In the framework of the model of Section 3.2, it should be observed that the above value of maximum compaction is also relevant under oedometric compression (uniaxial confined compression), that is, for a uniaxial macroscopic strain state. This is due to the fact that the maximum closure of the interface is assumed to be a material constant. In contrast, the macroscopic volume strain is known to be greater in oedometric compression than in a purely hydrostatic experiment [10]: it is believed that this is due to the fact that nonpure hydrostatic loading induces irreversible shear strains in the interfaces which enhance the compaction. Indeed, it should be emphasized that this behavior is specific to concrete and mortar. For instance, it does not occur in porous metal alloys in which the maximum volume strain corresponds to the closure of the porosity. This strongly suggests that it must be related to the existence of the ITZ.

In fact, the aggregates and the cement being modelled as incompressible materials, the volume strain observed at the macroscopic scale goes back to the pore collapse in the ITZ. The idea is that the amount of pore collapse depends on the shear strain applied to the ITZ. We therefore modify the phenomenological model (19) through the fact that β_0 now depends on the tangential component $\gamma = |[\boldsymbol{\xi}]_t|$ of the displacement jump:

$$k_n = \frac{k_{n0}}{1 + \beta/\beta_0(\gamma)} \tag{22}$$

where γ is the sliding of the interface. k_t is supposed constant. Moreover, we choose a simple linear law for β_0

$$\beta_0(\gamma) = \beta_0^0(1 + a_0\gamma/R) \tag{23}$$

In order to implement this model, an estimate of γ is due. For this purpose, we resort to the quadratic average of γ over the cement-aggregate interface. The later is related to the derivative of the homogenized stiffness tensor w.r.t. the tangential stiffness of the interface [12]. This result represents the counterpart in terms of displacement jump of Kreher's identity (16). More precisely, let us consider a r.e.v. Ω of the composite. The elastic energy density Ψ in the linear elastic problem is the sum of the contributions of the cement paste (domain Ω_c) and of the interfaces $\mathcal{I}_i$:

$$|\Omega|\Psi = \frac{1}{2}\int_{\Omega_c} \boldsymbol{\varepsilon} : \mathbb{C}_c : \boldsymbol{\varepsilon}\,\mathrm{d}\Omega + \sum_i \frac{1}{2}\int_{\mathcal{I}_i} \left(k_n\beta^2 + k_t\gamma^2\right)\mathrm{d}S = \frac{|\Omega|}{2}\boldsymbol{E} : \mathbb{C}^{\mathrm{hom}} : \boldsymbol{E} \tag{24}$$

Deriving this relation w.r.t. k_t, it can be shown that:

$$|\Omega|\frac{\partial\Psi}{\partial k_t} = \frac{|\Omega|}{2}\boldsymbol{E} : \frac{\partial\mathbb{C}^{\mathrm{hom}}}{\partial k_t} : \boldsymbol{E} = \frac{1}{2}\int_{\mathcal{I}} \gamma^2\,\mathrm{d}S \tag{25}$$

where $\mathcal{I} = \bigcup_i \mathcal{I}_i$. Note that this result is by no means trivial since both the strain field $\boldsymbol{\varepsilon}$ in the cement paste and the displacement jump $[\boldsymbol{\xi}]$ depend on k_t. The quadratic average $\bar{\bar{\gamma}}$ of the tangential jump is then defined as:

$$\bar{\bar{\gamma}}^2 = \frac{1}{|\mathcal{I}|}\int_{\mathcal{I}} \gamma^2\,\mathrm{d}S \tag{26}$$

We eventually derive $\bar{\bar{\gamma}}$ from (25):

$$\bar{\bar{\gamma}}^2 = \frac{R}{3\phi_a}\boldsymbol{E} : \frac{\partial\mathbb{C}^{\mathrm{hom}}}{\partial k_t} : \boldsymbol{E} \tag{27}$$

In particular, in the isotropic case, (27) reduces to

$$\bar{\bar{\gamma}}^2 = \frac{2R}{3\phi_a}\frac{\partial\mu^{\mathrm{hom}}}{\partial k_t}\boldsymbol{E}_d : \boldsymbol{E}_d \tag{28}$$

where the identity $\partial k^{\mathrm{hom}}/\partial k_t = 0$ (see (9)) has been used. In particular, under hydrostatic compression, we retrieve from (28) that $\bar{\bar{\gamma}} = 0$.

Returning now to the nonlinear homogenization problem, the spirit of the modified secant method suggests to estimate the tangential stiffness $k_t(\gamma)$ in the real r.e.v. by the uniform value $k_t(\bar{\bar{\gamma}})$. In the case of an oedometric loading, we have

$$\boldsymbol{E}_d : \boldsymbol{E}_d = \frac{2}{3}E_v^2 \tag{29}$$

The averages $\bar{\beta}$, $\overline{\overline{\varepsilon_d}}$ and $\bar{\bar{\gamma}}$ are related to the macroscopic strain respectively by (16), (20), (28), together with the expressions (9) of k^{hom} and (13) of μ^{hom}. Fig. 2 compares the prediction of the micromechanical model with experimental results. The parameters of the model are on the one hand those identified previously from the results of an hydrostatic compression test, and on the other hand the coefficient a_0 and the tangential stiffness k_t. Again, the agreement with the experimental data is excellent at high mean pressure Σ_m. The discrepancy between theory and experiment (dashed line part of the experimental curve) is most probably due to experimental problems to measure accurately low values of Σ_m [10].

It should also be recalled that the nonlinear homogenization scheme implemented here relies on the definition of a unique effective value of the strain state for each phase. The heterogeneity of the strain state within the matrix phase should be better captured by defining several concentric spheres centered on the inclusions and an effective strain in each zone. As shown in [13], this method could improve the accuracy of the macroscopic response.

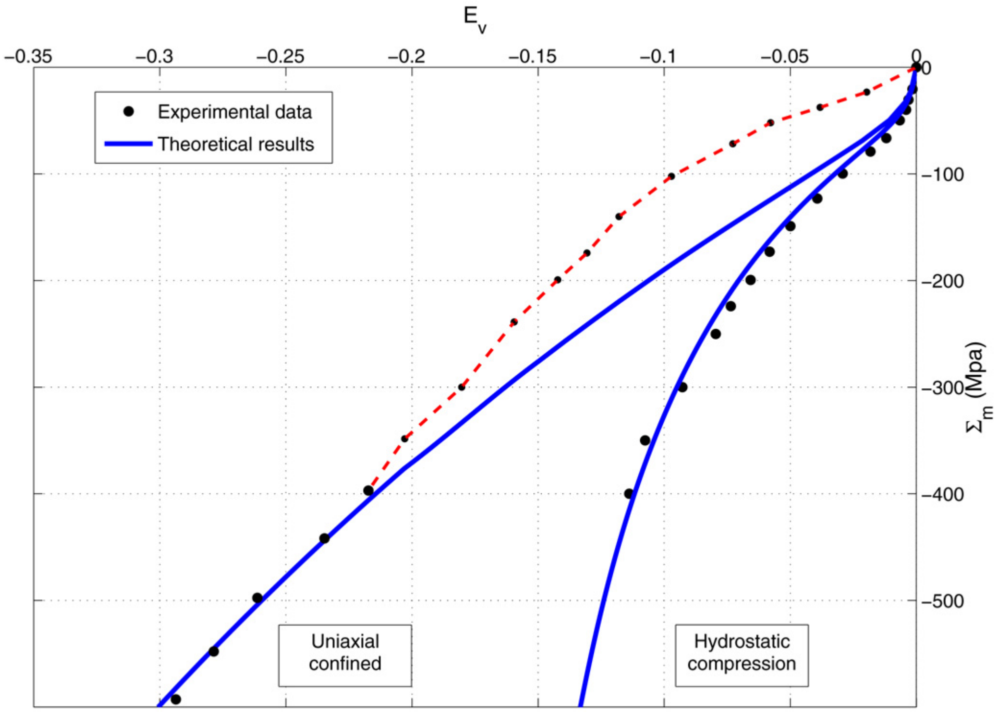

Fig. 2. Stress–strain response under hydrostatic compression loading and uniaxial confined loading with $a_0 = 160$, $k_t = k_{n0}$ and the same parameters as in Fig. 1.

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