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Three-dimensional modeling and numerical predictions of multimodal nonlinear behavior in damaged concrete blocks.

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2 Abstract

3

In this paper, the multimodal nonlinear elastic behavior of concrete, which is representative of 4 a consolidated granular material, is modeled numerically. Starting from a local three-5 dimensional softening law, the initial stiffness properties are re-estimated according to the local 6 strain field. The experiments deal with samples of thermally damaged concrete blocks 7 successively excited around their first three modes of vibration. The geometry of these samples 8 9 cannot be described by a one-dimensional approximation in these experiments where 10 compressional and shear motions are strongly coupled. Despite this added complexity, the nonlinear behavior for the three modes of vibration of the samples is well captured by the 11 simulations using a single scalar nonlinear parameter appropriately integrated into the elasticity 12 equations. It is shown that without sufficient attention payed to the latter, the conclusions would 13 have brought erroneous statements such as nonlinearity dispersion or strain type dependence. 14

1 I. Introduction

2

Geomaterials exhibit mechanical softening under dynamic loading, usually combined with 3 hysteresis and slow-dynamics effects (Johnson et al., 1996; TenCate et al., 2000). These effects 4 are reversible and deterministic. From a micro-structure standpoint, a recent study has 5 6 established a correlation between micro-crack density and softening effects (Payan et al., 2014a,b). From an energy balance point of view, it means that some potential energy disappears 7 8 when the material is loaded dynamically and is slowly recovered when the material is at rest. These properties are relevant to various natural processes and industrial applications including 9 the onset of earthquake and avalanches in geophysics (Johnson and Jia, 2005), the aging of civil 10 11 infrastructure (Eiras et al., 2016; Payan et al., 2007; Vu et al., 2016), the design of acoustic meta-materials with extreme stiffness (Diani et al., 2009; Wang and Lakes, 2004), or the 12 13 assessment of bone fragility in the medical field (Haupert et al., 2014).

14

15 The dynamic response of these materials has been first modeled by Guyer et al. (1995) using the Preisach formalism, which is a phenomenological description borrowed from the field of 16 17 electromagnetics. This model has then been refined to include slow-dynamics effects through thermally activated random transitions between the open and closed states of the hysteretic 18 19 elements of the Preisach system (Delsanto and Scalerandi, 2003; Nobili and Scalerandi, 2004). 20 More recently, Pecorari (2015) proposed a hysteretic model sharing some features with the Jiles-Atherton model (also borrowed from the field of electromagnetics), which he enhanced to 21 22 capture the slow-dynamics effects. It is also worth mentioning the soft-ratchet model of slowdynamics originally proposed by Vakhnenko et al. (2004) and recently modified by Favrie et 23 al. (2015) to include classical nonlinearity and viscoelasticity. All these models, however, have 24 been derived in the one-dimensional (1D). Three-dimensional (3D) effects are an essential part 25 of the dynamic response observed in geomaterials and cannot be ignored (Egle and Bray, 1976; 26 Payan et al., 2007, 2009; Tournat et al., 2004). Lyakhovsky et al. (2009) proposed a two-27 dimensional continuum damage rheology model capturing hysteretic nonlinearity and some of 28 29 the features observed in nonlinear resonance experiments. A similar model was used by Hamiel 30 et al. (2009) to describe stress-induced anisotropy in damaged geomaterials. Note that in these models, damage is not recoverable and slow-dynamics effects are not considered. The recent 31 32 modeling work of Berjamin et al. (2017) includes slow-dynamics effects, but although it can be naturally extended to 3D analysis, the simulations are carried out only for a 1D case. 33

2 Attempting to develop a predictive tool to link the microstructural properties of the material to the nonlinear elastic response observed experimentally is a challenging task. Despite a high 3 sensitivity to microstructures, amorphous condensed matter arrangement, and environmental 4 conditions (e.g., temperature, pressure) (Lott et al., 2016; Pavan et al., 2009; TenCate et al., 5 6 2000), the elastic nonlinear parameters seem to depend on the choice of the experimental setup 7 in much of the previous work reported in the literature. For instance, Renaud et al. (2013) 8 showed that material softening effects in Berea sandstone may vary by up to an order of 9 magnitude depending on the probing direction while the material is isotropic. In the work of Payan et al. (2014a,b) on concrete, two techniques were used to estimate a parameter of 10 nonlinearity. The two techniques showed the same trends but the magnitudes of the measured 11 parameter differ by an order of magnitude. These experimental data where derived using the 12 13 most common 1D approximation. However, a complex strain field leads to a 3D problem from a mechanical point of view and using a 1D approximation to describe this problem may lead to 14 15 erroneous conclusions.

16

17 Recently, Lott et al. (2016, 2017) show that conditioning can be properly accounted in 3D using a single scalar nonlinear parameter into the appropriate set of elasticity equations using 18 uncoupled single mode resonance type of experiments, i.e., shear and compressional. The aim 19 20 of this paper is to study the validity of this model to nonlinear resonance experiments, involving strong coupling between shear and compressional motion types. Numerical simulations are 21 22 compared to experimental data from nonlinear resonances in gradually thermally damaged concrete blocks. Using a single scalar nonlinear parameter appropriately introduced in elasticity 23 equations, the validity of the model is demonstrated and discussed. 24

25

26 **II. Theoretical framework**

27

In continuum mechanics, the parameters needed to compute the linear dynamic response of an elastic body are the mass density, the linear elastic tensor, and the damping parameters. If the geometry of the sample is complex and/or the material is heterogeneous, numerical techniques (e.g., finite-element method) should be used and the distribution of these parameters should be known for all computation cells discretizing the sample. In this paper, we study consolidated granular materials, which may be described as a disordered network of mesoscopic-sized "hard"

elements (e.g., grains with characteristic lengths ranging from tens to hundreds of microns) 1 cemented together by a "soft" bond system (e.g., amorphous silica, calcite) (Guyer and Johnson, 2 1999). Despite the complexity of the structure, the linear elastic response of these materials at 3 macroscopic scale is well captured by the model of a continuum. This continuum may have 4 heterogeneous properties under dynamic loading as a combined result of the complex spatio-5 6 temporal distribution of the strain field in the sample and the strain-induced material softening 7 (Payan et al., 2007; Remillieux et al., 2015; Renaud et al., 2013). Material softening is thought to originate from the microscopic-sized defects (e.g., micro-cracks) in the "soft" subsystem and 8 at the interfaces between the "hard" and "soft" subsystems (Payan et al., 2014a). To incorporate 9 these defects in the macroscopic continuum model, we consider a volume dV that is small 10 enough to satisfy the requirements of the numerical schemes but large enough to ensure a 11 12 constant micro-crack density from one volume to the next. Furthermore, we assume that the 13 defects are randomly distributed and oriented within the volume dV, with a length-scale much smaller than the typical acoustic wavelengths used in this study. With dV being on the order of 14 1mm³, the above criteria are satisfied. 15

16

17 The approach used in this paper is similar to the one used by Zubelewicz (1990) in transient 18 numerical simulations of rock fractures. Each contact within the medium brings softening 19 effects through nonlinear cohesive mechanisms. These effects are then integrated over an 20 elementary volume dV and used for a mesoscopic mechanical implementation within a 21 continuum with possible heterogeneous properties.

22

Recently, the authors (Lott *et al.*, 2016, 2017) proposed a general formulation to include material-softening effects in the equations of elasticity. This formulation is an extension of that proposed by Hughes and Kelly (Hughes and Kelly, 1953). The tensorial product between the strain and stress vector bases, $\delta_{ij}=n_i^{stress} \otimes n_j^{strain}$, is the natural basis for the elastic tensor and should now include softening effects as,

29
$$\Lambda_{ij} = \delta_{ij} (1 - \alpha \Delta \varepsilon_{ij}^*), \qquad (1)$$

30

31 or equivalently in matrix form as,

32

33 $\Lambda = I_3 - \alpha \varepsilon^*,$ (2)

where n_i is the principal strain direction, $\Delta \varepsilon_{ij}^*$ the strain amplitude, the star symbol denotes the basis formed by the principal strain axes, and α is a scalar quantifying the softening effect. The stiffness tensor is then expressed as,

- 7 $C_{ijkl}^{*} = [\lambda + 2(l \lambda m)Tr(\varepsilon) + 2(\lambda + m)(\varepsilon_{i}^{*} + \varepsilon_{k}^{*}) 2\mu\varepsilon_{i}]\Lambda_{ij}\Lambda_{kl} +$ $8 \qquad [\mu + (\lambda + m - \mu)Tr(\varepsilon) + 2\mu(\varepsilon_{i} + \varepsilon_{j} + \varepsilon_{l})](\Lambda_{ik}\Lambda_{jl} + \Lambda_{il}\Lambda_{jk})$ $6 \qquad + \frac{1}{2}n\sum_{\nu} (\Lambda_{j\nu k}^{i\nu l} + \Lambda_{j\nu l}^{i\nu k})\varepsilon_{\nu}$ (3)
- 9

1

5

where λ and μ are the Lamé constants and *l*, *m*, *n* are the Murnaghan constants (Murnaghan, 10 1937). Practically, the material-softening law is applied in the basis formed by the principal 11 strain axes. This basis is obtained from an eigen decomposition of the strain field ε measured 12 in the geometric basis. This decomposition, $\varepsilon = \mathbf{P} \varepsilon^* \mathbf{P}^{-1}$, is always possible because the strain 13 tensor is always real and symmetric. Once the softening law has been applied to the stiffness 14 tensor in the basis formed by the principal strain axes, the following transformation is used to 15 express the conditioned stiffness tensor in the geometric basis: $C_{ijkl} = P_{ir}P_{js}P_{kt}P_{lu}C^*_{rstu}$. This 16 result is equivalent to classical acoustoelasticity theory when the term quantifying softening is 17 18 equal to the identity matrix.

19

In this study, the validity of the model will be assessed using nonlinear resonance experiments 20 or more commonly referred to in the literature as nonlinear resonant ultrasound spectroscopy 21 (NRUS). In these experiments, a sample is subjected to sequences of periodic signals at various 22 frequencies around a resonance frequency and at increasing amplitudes while, for each periodic 23 signal, data are recorded when the sample vibrates at or near a steady state. Under these 24 conditions, the effects of the first-order term of nonlinearity in the classical description, i.e., 25 terms involving β in 1D and (l, m, n) in 3D, average to zero over one cycle of the harmonic 26 27 excitation. This is not the case with the second-order term of nonlinearity δ but the proposed model does not go beyond the first order. As a result, Eq. (3) can be simplified by removing the 28 terms involving third-order elastic constants (i.e., only the linear version of the elastic tensor is 29 30 used to apply the softening law),

31

32
$$C_{ijkl}^* = \lambda \Lambda_{ij} \Lambda_{kl} + \mu \left(\Lambda_{ik} \Lambda_{jl} + \Lambda_{il} \Lambda_{ijjk} \right).$$
 (4)

Finally, each cell (dV) of the sample can be conditioned by the strain amplitude at that cell. This means that the stiffness tensor is no longer uniform over the volume of the sample but depends on the local strain tensor. The sample experiences softening with a complex distribution (i.e., that of the strain field), which in turns lowers its resonance frequencies. Because of the heterogeneity, the resonance frequencies have to be computed numerically.

- 6
- 7

8 III. Numerical application to experimental data

9

The validity of the model is examined against experimental data collected during resonance 10 11 experiments. The samples are those described by Payan et al. (2014b). The three samples used in this study consist of concrete blocks with dimensions $6 \times 10 \times 10$ cm³. One sample is kept 12 intact and used as a reference. The other two samples are thermally damaged at 120 and at 13 250°C using a slow increase then decrease in temperature to prevent from eventual mechanical 14 15 damage induced by thermal gradients. Thermal damage allows the density of micro-cracking within the concrete samples to be increased as needed. Below 300° C, microcracks are 16 17 essentially caused by drying as well as differential thermal dilatation between cement paste and aggregates. In concrete the most brittle zone is the interface between the aggregates and the 18 19 cement paste. This zone, commonly referred to as Interfacial Transition Zone (ITZ), is the most 20 porous and crystallized region. It is thus quite natural to assume that most of the thermal damage will occur in the ITZ. With an arbitrary grain distribution, thermal damage of concrete can 21 reasonably be considered as isotropic. 22

23

24 A. Experimental protocol and results

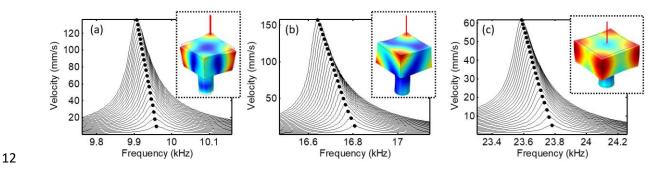
25

The samples are excited with an ultrasonic cleaning transducer (Ultrasonics World, DE, USA) powered by a function generator (National Instrument PXI-5406 function generator) coupled to a voltage amplifier (TEGAM 2350). The vibrational responses of the samples are recorded by a Polytec laser vibrometer (OFV 5000, 1.5 MHz bandwidth) using a digitizer (National Instrument PXI-5122). Both generation and acquisition lines are managed by the NRUS module of the Resonance Inspection Techniques and Analysis (RITA) software designed and implemented by T. J. Ulrich and Pierre-Yves Le Bas at Los Alamos National Laboratory. More details about the signal processing for these experiments may be found in the paper of Payan et
 al. (2014b).

3

Three resonant modes are then considered for NRUS. The mode shapes, source, and receiver positions are shown in Fig.1 for the sample thermally damaged at 120°C. Two of the modes are dominated by a bending motion and require the source and receiver to be located near the corners of the sample, where the amplitude is the highest, to enhance the signal to noise ratio. The third mode studied here consists of a "bulk/breathing" motion which is excited by placing the source transducer at the center of one large face and recorded by pointing the laser beam at the center of the opposite face.

11



13

FIG. 1. (Color online) Experimental (a) first, (b) second and (c) third NRUS curves for the
120°C damaged sample. Insets are the corresponding modal shapes.

16

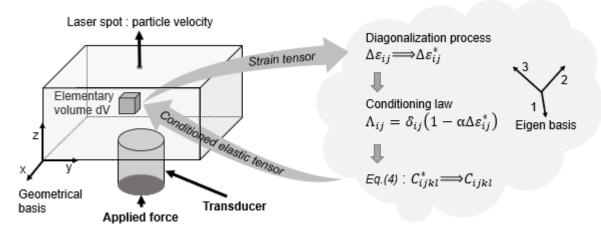
17 **B. Numerical protocol**

18

The relatively large mass added by the transducer is accounted for in the model by an aluminum cylinder with a perfect contact between the transducer and the sample. The following protocol is applied (Fig.2) to describe the numerical process. The simulations are carried out using the "Structural Mechanics" module of the commercial finite-element software package Comsol® Multiphysics.

Step 1 : A first eigenvalue problem is solved to compute the resonance frequencies of the samples with linear elastic properties (before the material-softening law is applied), which were already measured by Payan *et al.* (2014b) in previous work. The predicted and measured resonance frequencies of the systems with linear elastic properties that are reported in Table. I are in excellent agreement. Having a representative and accurate linear model is essential to the numerical protocol in this problem because the maximum values

- of strain amplitudes in the samples are recovered from the linear model, based on the laser
 measurement at a single point.
- Step 2 : In the second step of the numerical protocol, a frequency-domain simulation is
 conducted by imposing a normal force on the free flat surface where the transducer is
 mounted. The amplitude of the normal force is tuned to match the particle velocity at the
 measured position on the sample.
- Step 3 (Fig.2): The strain tensor is extracted at all nodes of the mesh discretizing the sample and used for the conditioning step. As the media is initially considered isotropic and homogeneous, the initial local stiffness is independent of the choice of basis and usually written C_{ijkl} = λ δ_{ij}δ_{kl} + μ (δ_{ik}δ_{jk} + δ_{il}δ_{jk}). Using Eq. (1) and Eq. (4), the material softening effect is applied to the stiffness tensor C_{ijkl}* trough the tensors Λ_{ij} in the eigen basis.
- Step 4 (Fig.2) : The conditioned elastic tensor is then transposed back to the "geometrical"
 basis. After this numerical procedure, the sample, initially homogeneous and isotropic,
 becomes heterogeneous and anisotropic.
- Step 5 : A final eigenvalue problem is solved to compute the resonance frequencies of the samples with conditioned elastic properties. Steps 2 to 5 are repeated for several amplitudes
 to provide a curve of the relative shift of the resonance frequency.
- 18



- 19
- 20 FIG. 2. Scheme of the numerical and experimental protocols.
- 21

Resonance frequencies f_0 (kHz)						
Sample	e Mode 1 N			Mode 2	Mode 3	
	Exp	Num	Exp	Num	Exp	Num
Ref	10.16	10.09 (-0.7%)	17.33	17.36 (+0.2%)	24.02	24.43(+1.7%)

Ī	120°C	9.95	9.96 (+0.1%)	16.86	16.81 (-0.3%)	23.30	23.79 (+2.1%)
Ī	250°C	9.43	9.53 (+1%)	15.97	14.739 (-7.7%)	22.31	22.30 (-0.1%)

1 Table. I. Resonance frequencies obtained experimentally and numerically with linear RUS.

2

3 IV. Results and discussion

4

5 Predicted and measured material softening in NRUS are shown in Fig.3 for the three samples.
6 The values of *α*₀ used in the simulations to match the experimental data are reported in Table.
7 II.

8

Sample	α0
Reference	300
120°C	520
250°C	1000

9 Table. II. Values of the parameter α_0 used in the NRUS simulations for the three concrete 10 samples.

11

12 Note that this value increases by more than 300% between the reference sample and the most damaged sample, which seems to be consistent with the evolutions of the nonlinear parameters 13 14 reported in the literature. To highlight the efficiency of the present model, the "apparent" nonlinear parameters are measured by linear regression of the relative frequency shift as a 15 function of the strain amplitude for the three modes studied. This apparent nonlinear parameter 16 changes with the mode order and the type of strain (e.g., volumetric and deviatoric) used in the 17 18 analysis. For each mode and each sample, the apparent nonlinear parameters obtained with volumetric and deviatoric strains are reported in Fig.4. Tying this apparent nonlinear parameter 19 to a 1D description will lead to erroneous conclusions including that the nonlinearity is 20 dispersive (i.e., depends on the order of the mode) or is dependent on the type of strain involved 21 22 (e.g., shear or compressional components). It is important to stress that the nonclassical nonlinearity should be handled by a local parameter appropriately integrated within the 23 24 elasticity equations.

25

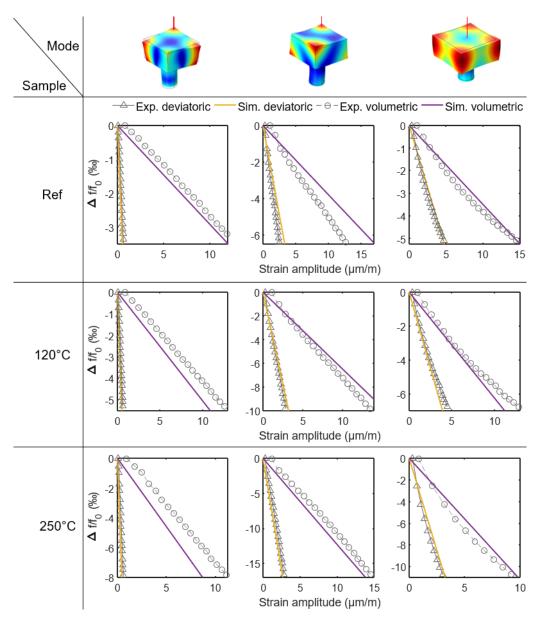
Numerical simulations using a single scalar parameter α_0 reproduce well the experimental observations, independently from the type of strain used or the mode order employed in the nonlinear analysis. There are some discrepancies between numerical simulation and experiments for some cases, but it does not seem to be consistent with the type of mode or a particular sample. Discrepancies are most likely due to the complexity of the experiment and the presence of a large transducer mounted at various positions on the sample to excite the various modes. Also, the sample do not have the perfect parallelepiped geometry used in the model. Even if the sample size was precisely measured using a caliper, parallelisms deviations are not accounted for in the simulations.

8

9 For the third mode, all the frequency shifts flatten a little bit at increasing amplitude (Fig.3).
10 This behavior may be induced by some hidden resonant peaks which could appear at high
11 amplitude. This can happen especially at "high" frequency when the resonance frequency
12 density becomes high. Even if the location of the transducer was chosen so as to favor a given
13 mode shape, other nearby resonances may alter these curves.

14

More importantly, the simulation results indicate that, in the case of concrete the nonlinear behavior of the material for both compressional and torsional motions is well captured by a single local scalar parameter. These results are in agreement with the fact that the distribution of defects in the thermally damaged concrete samples is isotropic.



2 FIG. 3. (Color online) Experimental and numerically predicted resonances curves for the whole

³ set of samples and modal shapes.

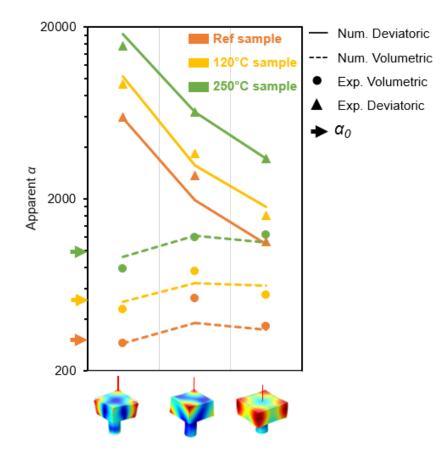


FIG. 4. (Color online) Experimental and numerically derived apparent nonlinear parameters. *α*₀
is also reported for comparison.

4

5 V. Conclusion

6

7 A tensorial interpretation of the softening effects under dynamic stress was integrated in a 8 numerical scheme using a single scalar parameter. The key feature of the model relies on locally applying a softening law to the elastic tensor in the eigenbasis of the strain field and 9 10 transforming this tensor back to the geometrical basis once the softening has been applied. 11 Numerical simulation results were compared to nonlinear multi-modal resonance experiments on thermally damaged concrete samples. In these samples, it was well adapted to predicting 12 nonlinear behavior of their complex mode shapes involving coupling between shear and 13 14 compressional components. This is in good agreement with the fact that an isotropic distribution of defects is expected in these materials. 15

16

17 It also shown that without accounting for these issues, the derived apparent nonlinear parameter 18 can lead to erroneous interpretations. In this study, one could conclude to frequency dispersion

1	or strain type dependences of nonlinearity. However, none of these statements are supported by
2	the appropriate description of nonlinearity in the elasticity equations.
3	
4	Future improvements of the model will aim at accounting for textured type of microcracking
5	using the more general framework of a vectorial nonlinear parameter. Indeed, experimental data
6	reported in the literature (Remillieux et al. 2016; Lott et al. 2017) show that many sedimentary
7	rocks (e.g., Berea sandstone) exhibiting preferred oriented micro cracking features would
8	require such a description.
9	
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13	program (Grant No. FE-634-15-FY15).
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TABLES

Resonance frequencies f_0 (kHz)						
Sample	Mode 1		Mode 2		Mode 3	
	Exp	Num	Exp	Num	Exp	Num
Ref	10.16	10.09 (-0.7%)	17.33	17.36 (+0.2%)	24.02	24.43(+1.7%)
120°C	9.95	9.96 (+0.1%)	16.86	16.81 (-0.3%)	23.30	23.79 (+2.1%)
250°C	9.43	9.53 (+1%)	15.97	14.739 (-7.7%)	22.31	22.30 (-0.1%)

4 Table. I. Resonance frequencies obtained experimentally and numerically with linear RUS.

Sample	α0
Reference	300
120°C	520
250°C	1000

7 Table. II. Values of the parameter α_0 used in the NRUS simulations for the three concrete

8 samples.

1 FIGURE CAPTION

- 2
- FIG. 1. (Color online) Experimental (a) first, (b) second and (c) third NRUS curves for the
 120°C damaged sample. Insets are the corresponding modal shapes.
- 5
- 6 FIG. 2. Scheme of the numerical and experimental protocols.
- 7
- 8 FIG. 3. (Color online) Experimental and numerically predicted resonances curves for the whole
- 9 set of samples and modal shapes.

- 11 FIG. 4. (Color online) Experimental and numerically derived apparent nonlinear parameters. α_0
- 12 is also reported for comparison.