WORKSHOP PROGRAM

and

BOOK OF ABSTRACTS

Department of Civil, Environmental and Mechanical Engineering

University of Trento

Via Mesiano, 77 – TRENTO (ITALY)

March 20, 2015

Workshop Chair

Francesco Dal Corso

WORKSHOP OBJECTIVES

The workshop will bring together international experts in the field of ceramic science and material modelling and representatives from research institutes and industry.

The aims of the workshop are: (i) to set-up the state of the art of the constitutive modelling in ceramics, (ii) to assess the possibilities of improving efficiency and safety in industrial processes of refractories and (iii) to define the current challenges in the engineerization of the liquid steel technology as related to the use of ceramic components.

GENERAL INFORMATIONS

Workshop Chair

Francesco Dal Corso, University of Trento

Scientific Committee

Willi Pabst, Institute of Chemical Technology, Prague, Czech Republic
Marco Paggi, IMT Lucca, Italy
Severine Romero-Baivier, VESUVIUS, Belgium
Anna Tampieri, ISTEC-CNR, Italy
John R. Willis, University of Cambridge, UK

Organizing Committee

Francesco Dal Corso, University of Trento, Italy
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CONGRESS VENUE

The workshop venue is the Department of Civil, Environmental and Mechanical Engineering of the University of Trento (via Mesiano, 77). The Department is located on a beautiful hill, 10 minutes far from Trento's city center by taking bus N.5 at the train station.

SUPPORTERS

HOTBRICKS IAPP EU PROJECT

MARIE CURIE ACTIONS

UNIVERSITY OF TRENTO Italy

VESUVIUS

UNDER THE PATRONAGE OF

PROVINCIA AUTONOMA DI TRENTO

STATE OF THE ART AND CHALLENGES IN THERMAL AND MECHANICAL MODELLING OF CERAMIC MATERIALS

Program Overview

Friday 20 March 2015

8:15-8:45	Registration
8:45-9:00	Opening
9:00-10:40	Session 1
10:40-11:10	Coffe break + Poster Session
11:10-12:40	Session 2
12:40-14:00	Lunch
14:00-15:15	Session 3
15:15-15:45	Coffe break + Poster Session
15:45-18:00	Hotbricks Session

Friday 20 March 2015

8:15 - 8:45 Registration

8:45 - 9:00 Opening (Room R2)

9:00 - 10:40 SESSION 1 (Room R2 - Chair: M. Paggi)

9:00 - 9:20 Pabst, Gregorová, Uhlířová
L1 **Porosity dependence and temperature dependence of elastic properties of oxide ceramics, silicate-based ceramics and silica refractories**

9:20 - 9:40 Tampieri, Sandri, Panseri, Sprio
L2 **Self-assembling hybrid nano-composites with multi-scale organization for smart multifunctional applications**

9:40 - 10:00 Cologna, Tyrpekl, Wangle, Somers
L3 **Spark Plasma Sintering at JRC-ITU: an overview of the ongoing activities**

10:00 - 10:20 Sorarù, Zera, Jana
L4 **Ultra-High Temperature Polymer Derived Ceramics Aerogels and Foams**

10:20 - 10:40 Mazzalai, Kratzer, Muralt
L5 **Piezoceramics thin films for microelectromechanical systems: The in-situ growth of perovskite PZT thin films by PVD techniques**

10:40 - 11:10 Coffee Break + Poster Session (Room R1)

P1 Bordignon, Piccolroaz, Dal Corso, Bigoni
Numerical modelling for the strain localization and shear banding in materials

P2 Bortot, Springhetti, Gei
A universal curve for the design of optimal dielectric elastomer generators: benefits of ceramic filler addition

P3 Broseghini, Ricardo, Gelisio, Pugno, Scardi
A multibody model for planetary ball-milling

P4 Cecinato, Gajo
Analysis of dynamical effects in the formation of compaction bands

P5 Misseroni
Ultrasonic tests on green bodies: forming pressure and evolution of the elastic characteristics

P6 Morini, Piccolroaz, Mishuris
Cracks propagation in ceramic materials: a singular integral formulation

P7 Shahzad, Dal Corso, Bigoni
Stress magnification and Notch Stress Intensity Factors for composite materials containing polygonal inclusions

P8 Tommasini, Bigoni, Misseroni
Mechanical models for instabilities induced by dry friction

P9 Pisano, Royer-Carfagni
Critical issues in the coaxial double ring test for ceramics and glass

Friday 20 March 2015

11:10 - 12:40 SESSION 2 (Room R2 - Chair: A. Tampieri)

11:10 - 11:25 Argani, Misseroni
L6 **Numerical experiments for determination of stiffening laws for ceramic compaction**

11:25 - 11:40 Sprio, Ruffini, Dapporto, Tampieri
L7 **New strategies to develop reinforced bioceramics for load-bearing applications**

11:40 - 11:55 Falope, Lanzoni,Radi
L8 **Partially coated ceramic layer under thermal stress**

11:55 - 12:10 Paggi, Lenarda
L9 **A geometrical multiscale numerical method for coupled hygro-thermo-elastic problems in layered materials**

12:10 - 12:25 Gei, Bortot, Springhetti
L10 **Mechanical to electrical energy conversion with ceramic particle-reinforced soft materials**

12:25 - 12:40 Benvenuti, Sevostianov
L11 **A computational approach based on the integration of the equivalent-eigenstrain concept with the eXtended Finite Element Method for general-shaped inclusions embedded in ceramic materials**

12:40 - 14:00 Lunch (Room R1)

14:00 - 15:15 SESSION 3 (Room R2 - Chair: G. Soraràù)

14:00 - 14:15 Noselli, Deshpande, Fleck
L12 **Toughening mechanisms in particulate and layered solids**

14:15 - 14:30 Rambaldi, Prete, Timellini, Bignozzi
L13 **Acoustic and thermal performances of ceramic tiles and tiling systems**

14:30 - 14:45 Radi, Morini
L14 **Thermal stress fields between two unequal circular holes in a ceramic medium**

14:45 - 15:00 Bardella, Panteghini
L15 **On the compressive strength of glass-microballoons/thermoset-matrix syntactic foams**

15:00 - 15:15 Swan, Piccolroaz, Bigoni
L16 **Green Body Production from Alumina Powder:Constitutive Theory, Implementation, and Experimental Validation**

15:15 - 15:45 Coffee Break + Poster Session (Room R1)

15:45 - 18:00 HOTBRICKS SESSION (Room R2 - Chair: W. Pabst)

15:45 - 16:00 Romero Baivier, Gregoire
L17 **Modelization of a ladle cyclelife**

16:00 - 16:15 Papathanasiou, Dal Corso, Gourgiotis
L18 **Finite element simulation of thermal shock in micro-structured solids with applications to refractories**

16:15 - 16:30 Penasa, Piccolroaz, Bigoni, Dal Corso, Romero Baivier
L19 **Computational modelling of refractory materials at high temperature**

16:30 - 16:45 Poly, Romero Baivier
L20 **Challenges in thermal and mechanical modelling of ceramic refractories involved in the continous casting process of steel**

16:45 - 17:00 Madaschi, Gajo, Cecinato, Romero Baivier
L21 **Effect of 'local' strain rate on the determination of elastic modulus during crush tests at high temperature in rock-like materials**

17:00 - 17:15 Godin, Madaschi, Romero Baivier
L22 **Experimental tests use to study the ceramic material behavior**

17:15 - 17:20 Bigoni, Dal Corso, Gregoire, Romero Baivier
L23 **Thermoplasticity towards the design of ceramics for high-temperature applications**

17:20 - 17:25 Gajo, Cecinato
L24 **Some considerations about thermomechanical and thermophysical modelling of ceramic refractory materials**

17:25 - 17:30 Leoni, Shovkun, Godin, Romero Baivier
L25 **Phase composition of high-temperature refractories**

17:30 - 17:35 Cecinato, Gajo, Romero Baivier
L26 **A review of thermomechanical and thermophysical properties of ceramic refractory materials**

17:35 - 17:40 Dal Corso, Zisis, Gourgiotis
L27 **Contact regimes during heat conduction through a microstructured solid**

17:40 - 18:00 Final discussion

Abstracts of

Lectures

L1

Porosity dependence and temperature dependence of elastic properties of oxide ceramics, silicate-based ceramics and silica refractories

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Elastic constants are the most important basic properties that must be known not only for assessing the room-temperature mechanical behavior but also the high-temperature performance and thermal shock resistance of high-temperature engineering ceramics and refractories. This contribution reports on theoretical predictions and experimental measurements of elastic constants for oxides (alumina, zirconia, silica), two-phase composites (alumina-zirconia) and multiphase silicate-based ceramics (kaolin-mullite- and mullite-alumina-based ceramics). The dependence of Young's moduli on phase composition, porosity and temperature is discussed. One- and two-point bounds (Paul bounds and Hashin-Shtrikman bounds) as well as model relations are used for the prediction of effective properties and compared with experimental data obtained by impulse excitation measurements. With regard to porosity it is shown that for all materials investigated so far – except for highly porous cellular ceramics (with more than 70 % porosity) – our exponential relation provides more realistic predictions for the effective Young's modulus of porous ceramics than the commonly used power-law relation [1-3]. Concerning the temperature dependence of elastic moduli it is shown that not all ceramic materials used in high-temperature applications exhibit a decrease of Young's modulus with temperature and that some of them exhibit complicated hysteresis effects and other elastic anomalies. In particular, the temperature dependence of the Young's modulus of silica refractories is discussed in great detail. Silica refractories in the form of silica bricks are irreplaceable for certain applications, e.g. electro-steel kilns or hot blast air heaters (Cowper heaters) for blast furnaces. In this contribution we report on new results concerning silica refractories with tridymite contents of 47–63 % and porosities of 13–17 % that have been characterized by impulse excitation up to 1200 °C and by dilatometry up to 1300 °C. During heating, Young's moduli start to decrease from their room temperature values (9–12 GPa) to about 5–7 GPa at 200 °C, followed by a very steep increase at around 230 °C to values higher than the room temperature values and a nonlinear increase to their final high-temperature values. During cooling, Young's moduli increase even further, exhibit a maximum and a nonlinear decrease that does not follow the heating curve, a very steep decrease at around 200 °C and a final increase to the initial room temperature values, so that a closed loop results during thermal cycling. Dilatometric measurements confirm that this behavior correlates closely with the phase transitions between low- and high-temperature silica subpolymorphs. Microcracks are identified as the primary cause of the low Young's moduli and their increase with temperature [4,5].

Acknowledgements: This work is part of project P108/15-18513S (GAČR).

References:

[1] Pabst W., Gregorová E., Sedlářová I., Černý M.: *J. Eur. Ceram. Soc.* **31**, 2721-2731 (2011).
[2] Pabst W., Gregorová E., Malangré D., Hostaša J.: *Ceram. Intern.* **38**, 5931-5939 (2012).
[3] Pabst W., Gregorová E., Černý M.: *J. Eur. Ceram. Soc.* ***33**,* 3085-3093 (2013).
[4] Pabst W., Gregorová E., Kutzendörfer J.: *Ceram. Intern.* **40**, 4207-4211 (2014).
[5] Gregorová E., Černý M., Pabst W., Esposito L., Zanelli C., Hamáček J., Kutzendörfer J.: *Ceram. Intern.* **41**, 1129-1138 (2015).

L2

Self-assembling hybrid nano-composites with multi-scale organization for smart multifunctional applications

Anna Tampieri[1], Monica Sandri[1], Silvia Panseri[1], Simone Sprio[1]
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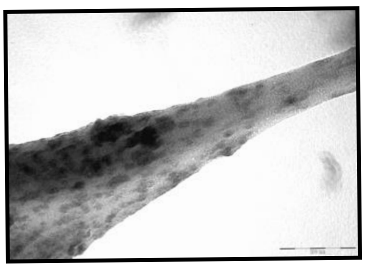
The formation of human bones is governed by self-assembling and organization of collagen molecules in a complex 3-D structure, acting as a template for simultaneous mineralization with nanocrystalline, ion-substituted apatite. Since a decade, the reproduction of the conditions of bone formation allowed to settle a biomimetic synthesis process generating hybrid constructs where the mineral phase, i.e. a biomimetic, nanosized hydroxyapatite, is heterogeneous nucleated on Type I collagen. This process is directed and controlled by the chemical features and physical confinement imposed by the self-organizing polymeric matrix, so that the mineral phase has physical, chemical and ultra-structural resemblance with mineral bone[1,2]. Moreover, the possibility of tailoring the mineralization extent also enabled the synthesis of graded constructs mimicking different areas of multifunctional joint regions[3]. It was demonstrated that these unique features can trigger, in vivo, the cascade of events leading to regeneration of bone and multifunctional anatomical areas, such as osteochondral and periodontal regions.

The same biomineralization process can be applied on blends of polymeric matrices by imposing synthesis conditions yielding chemical or physical interaction between the different components and simultaneous mineralization, thus opening the way to achieve new devices with enhanced mechanical strength and wider potential applications.

The mechanical and structural modeling of such hybrid composites requires a deep knowledge of the interaction, at the molecular level, between: i) the various polymeric components of self-assembling matrices as well as ii) the organic matrix and the apatite nanoparticles that heterogeneously nucleate under specific physical, chemical and structural constraints. These interactions determine the assembling and 3D organization of nanosized hybrid building blocks into complex, hierarchically organized constructs with specific mechanical and functional properties.

To elucidate the ultra-structural properties of these complex devices, deep spectroscopic and microscopic investigation has to be performed in association with techniques based on nano-indentation that shall be specifically designed to evaluate space-dependent mechanical properties at various size scales, up to the level of the nanosized inorganic phase, i.e. a biomorphic apatite phase the properties of which are strongly influenced by its strong chemical and topotactic interaction with the polymeric matrix.



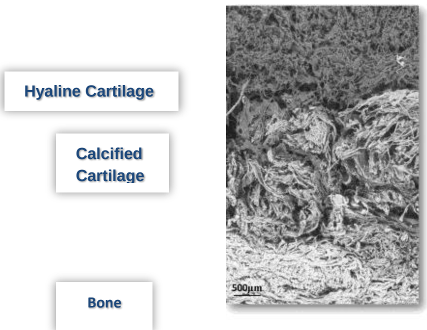


Figure 1. Left: TEM image of a collagen fibre presenting heterogeneously nucleated apatite nanophase; Right: SEM image of a 3D graded device for osteochondral regeneration.

References:
[1] A. Tampieri, et al. J. Biomed. Mater. Res., **67A**; 618 (2003).
[2] S. Sprio, M. Sandri, S. Panseri, C. Cunha C, A. Tampieri. J Nanomater. **2012**, 418281(2012).
[3] A. Tampieri et al. Biomaterials **29(26)**; 3539 (2008).

L3

Spark Plasma Sintering at JRC-ITU: an overview of the ongoing activities

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Spark Plasma Sintering (SPS) is an electric field assisted technique, currently being widely investigated in industrial and academic ceramic materials research communities. It allows fast and low temperature material densification and thus enables the synthesis of materials with unique microstructures and properties. Very recently JRC-ITU integrated a unique downscaled version of a SPS device in a glovebox, opening a new realm of opportunities for the synthesis of ceramics bearing transuranic elements. First results on the sintering of actinide dioxides will be presented along with a study on the incorporation of elements and compounds, hitherto impossible due to their high vapour pressure or low melting points. An outlook of the future developments, with a focus on safety of nuclear fuels, will be presented.

L4

Ultra-High Temperature Polymer Derived Ceramics Aerogels and Foams

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Polymer-Derived Ceramics, PDCs, represent a new family of ceramic materials which can be made directly from polymers by pyrolysis. These PDCs embody remarkable nanostructural, chemical and mechanical stability at temperatures approaching 2000°C, even though they are processed at much lower temperatures. In this presentation we report on the novel synthesis and characterization of highly porous aerogels and foams made of β-silicon carbide PDCs.

The aerogels are obtained through crosslinking, via hydrosylilation reaction, a Si-H-containing polycarbosilane with a vynil-containing crosslinker in a highly diluted solution. The wet gel is then supercritically dried with CO_2 and pyrolyzed in inert atmosphere to induce the organic-to-inorganic transformation. Accordingly we produced monolithic β-SiC aerogel having a colloidal microstructure with SSA up to 200 m^2/g, pore volume up to 95% and whose nanostructure is stable up to 2000°C.

The ceramic β-SiC foams are produced using the template method starting from suitable polymeric foams. SiC foams have open cell structure with cell and window sizes of 500 and 170 μm respectively. The foams are stable in air up to 1550 °C and in inert atmosphere up to 2000°C. Density of the SiC foams spans from 0.035 to 0.3 g/cc.

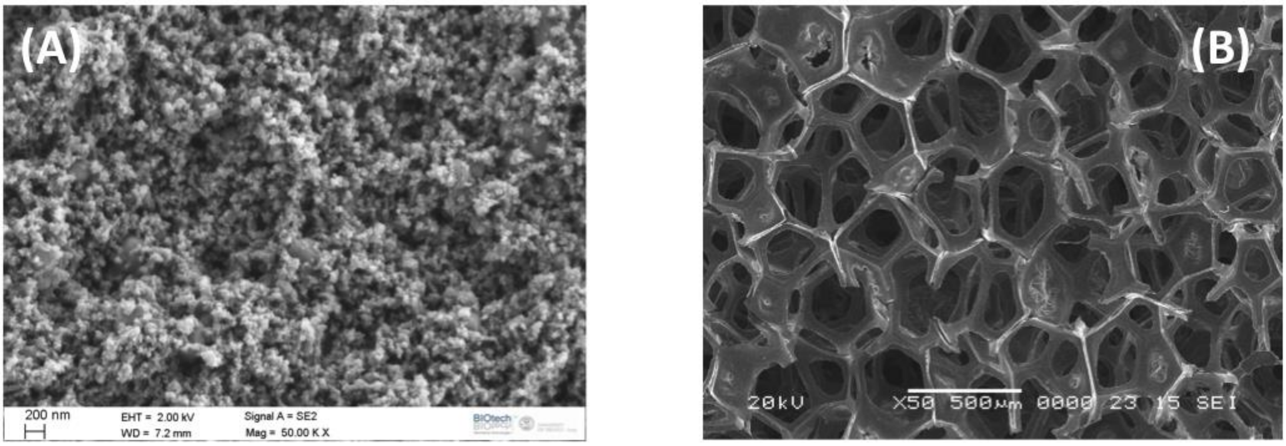

Figure 1. Microstructure of the: (A) SiC aerogel and (B) SiC foams produced at 1200°C.

Both aerogels and foams can find application as high temperature insulation materials, filters, catalyst supports or sensors, to mention only few of them.

References:

[1] 1] P. Colombo, G. Mera, R. Riedel, G. D. Soraru, "Polymer-Derived Ceramics: 40 Years of Research and Innovation in Advanced Ceramics", J. Am. Ceram. Soc., **93** [7] 1-32 (2010).

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[3] E. Zera, R. Campostrini, P.R. Aravind, Y.D. Blum, G. D. Sorarù, "Novel SiC/C Aerogels through Pyrolysis of Polycarbosilane Precursors", Adv. Eng. Mater., **16** (6), 814-819 (2014).

L5

Piezoceramics thin films for microelectromechanical systems: The in-situ growth of perovskite PZT thin films by PVD techniques

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The recent progress in synthesis and integration of highly piezoelectric lead-zirconate-titanate (PZT) ceramics thin films onto silicon substrates are paving the way for new, more efficient and faster devices in micro electro-mechanical systems (MEMS). Very promising markets are predicted for these piezo-MEMS devices, which include ink-jet printheads, micro-pumps, microphones, micromotors, micromachined ultrasound transducers for medical applications, energy harvesters and many others. The high piezoelectric activity of PZT allows indeed to generate large forces and to convert a high fraction of mechanical energy into electricity. In comparison to competing principles, piezo-MEMS devices need less power and are faster than thermally actuated devices and work with lower voltage than electrostatic actuators.

Magnetron sputtering is a large-throughput and reliable technology, but high-performing PZT thin films were not straightforward to achieve, due to the difficulties related with the vacuum processing and the physics of perovskite films nucleation and growth. We defined a high-quality high throughput sputtering process, directly on an industrial machine suitable for large silicon substrates. We show how the film orientation can be tuned between highly- (100) textured and (111), simply by playing with the thickness of an ultrathin seed layer. With an optimized process, this route results in films characterized by a remarkable transverse effective piezoelectric coefficient ($e_{31,f} = -23$ C/m^2) on samples showing very low dielectric losses and leakage currents.

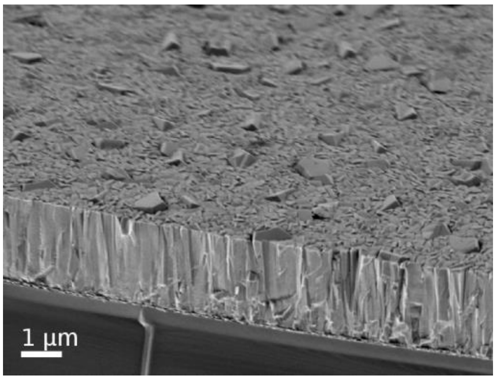

Fig. 1. SEM of a highly piezoelectric PZT thin film in-situ grown by RF magnetron sputtering.

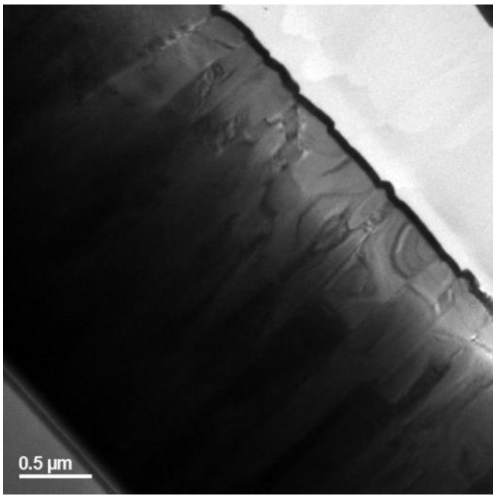

Fig. 2. TEM cross-section of a typical film: the microstructure is very compact.

L6

Numerical experiments for determination of stiffening laws for ceramic compaction

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Piccoloraz et al. [1,2,3] proposed a constitutive model to simulate the forming and the compaction of ceramic powders, taking into account the transition from a granular powder to a dense green body. The model is based on a non-linear relation between plastic deformation and elastic properties [4]. The influence of plastic deformation on elastic characteristics has been observed on uniaxial strain compression tests on aluminum silicate powders performed at the Instabilities Lab of the University of Trento, showing that the elastic modulus is related to the forming pressure. The constitutive model developed in [1,2,3] is based on 21 material parameters, but only some of these can be calibrated through specific experimental tests [5], while those related to the plastically-related elastic stiffening do not admit a direct experimentation.

Elastic stiffening is investigated in this presentation through a numerical analysis on a single powder grain by means of particle packing and contact problem. A powder particle is assumed to obey an elastic-perfectly plastic constitutive law of von Mises type; the material properties used in the simulations take into account the fact that the grain of ceramic powder is usually a porous solid (as illustrated in [6]). The simulations show that stiffness is a function of the forming pressure similar to that observed experimentally.

Acknowledgements: Financial support from the European FP7–Intercer2 project (PIAP-GA-2011-286110-INTERCER2) is gratefully acknowledged.

References:

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New strategies to develop reinforced bioceramics for load-bearing applications

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The regeneration of load-bearing bone parts is particularly relevant since such bones are destined to sustain critical body functions such as deambulation and manipulation. In this respect, the current approaches for bone repair are prevalently based on substitution of missing or diseased bone parts with inert devices that do not enable bone regeneration and recovery of the original functionality.

Calcium phosphates are elective biomaterials for bone regeneration; however they are characterized by intrinsic weakness that limits potential applications in regeneration of load-bearing bone parts. Moreover the sintering process required for consolidation of ceramic materials reduces the surface activity and bioactivity. In this respect new strategies can be adopted to develop new regenerative devices with improved biologic and mechanical competence.

Bioactive ceramic composites can synergistically associate osteogenic character and mechanical strength. In this respect titanium dioxide is a very promising material, with good biocompatibility, mechanical strength and relative density close to that of inorganic bone that can be associated to apatite phases to form new composites exhibiting higher osteogenic character than HA as well as enhanced compressive and flexural strength, and potential bio-resorbability in vivo[1,2].

Different approaches enable the achievement of solid implants without recurring to any thermal treatment of sintering. For the regeneration of vertebral bodies, injectable ceramic pastes based on metastable calcium phosphates can be developed, to take advantage of their ability to self-harden in vivo by physical entanglement of nanosized apatite elongated particles. These new cements can provide early sustain to bone tissue weakened by trauma or metabolic diseases such as osteoporosis. The bone-like composition and porosity can drive bone cells to fast tissue regeneration, and progressively increase the bio-competence of damaged bone until complete regeneration.

Regeneration of long segmental bones is probably the most challenging clinical issue to be addressed: to induce regeneration of well-organized bone it is required the implantation of scaffolds with bone-like composition, complex 3-D structure, open porosity conducive to extensive angiogenesis and sufficient mechanical strength to withstand early physical stimulation and stimulate mechanotransduction processes at the cell level. The convergence of all these requirements is hard to achieve, due to intrinsic limitation in the conventional manufacturing techniques. In this respect a promising approach is to take inspiration from Nature and develop biomorphic transformation processes to convert native wood structures into biomimetic bone scaffolds with hierarchically organized structure[3]. This new approach can pave the way to a new generation of devices for regeneration of long segmental bones.

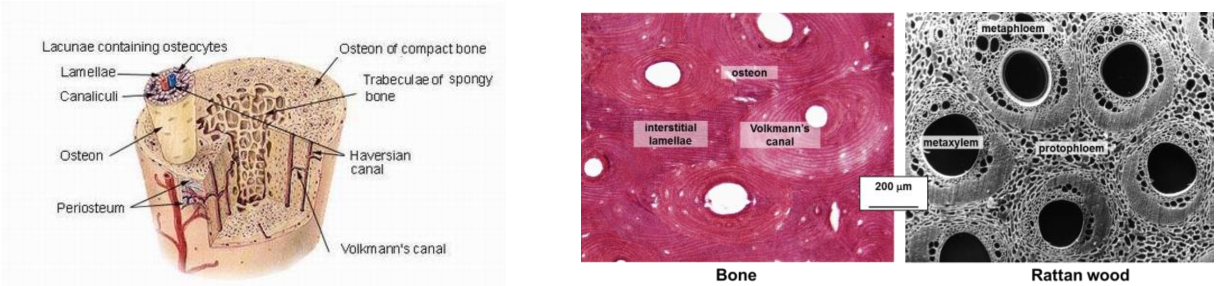

Figure 1. Left: Hierarchical Organization of bone; right: similarity between structure of bone and Rattan wood.

References:
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2. C. Cunha, S. Sprio et al. *J Biomed Mater Res: Part A.* **101A(6)**, 1612. (2013)
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L8

Partially coated ceramic layer under thermal stress

F. Falope[1], L. Lanzoni[1], E. Radi[2]

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Thin films and coatings technology has known a large development in the last decades due to the large number of devices involving thin films employed in high-tech industries, mainly in microelectronics, electrochemistry, semiconductors and optical electronics. Indeed, realization of MEMS and NEMS used into biomedical components, chemical reactors, integrated circuit, solar cells, flat panels displays, sensors, insulator and protection systems, transducers, high-precision measuring instruments, etc. are examples of important applications having significant commercial implication. Recently, many theoretical and experimental studies have been focused on the feasibility of a crystalline undulator (CU), that is a special kind of MEMS realized by covering a ceramic substrate. This micro-device can be used to produce a coherent beam of X-ray at high energy levels by exploiting the channelling phenomenon [1]. The substrate generally consists of a Silicon or Germanium crystalline plate covered by a thin film deposed on both surfaces by a proper chemical process (e.g. LPCVD) at high temperature. Through a suitable photolithographic process, the film is properly patterned in order to impart a periodic deformation to the crystalline substrate, suitable to produce coherent interaction with a beam particles. The system adopts a periodic curvature as a result of the misfit strain due to the different thermal expansivities of the layer and the film

The present work provides an extension of the paper [2] by taking into account the anisotropy of the substrate and coatings. The substrate is modelled as a 2D orthotropic elastic layer under plane strain conditions, whereas the film is assumed to behave like a membrane, thus neglecting its flexural stiffness. The problem is formulated by imposing perfect adhesion between the film and the substrate, thus leading to a singular integral equation. The problem can be reduced to a linear algebraic system by using a series expansion of Chebyshev polynomials for the interfacial shear stress and Fourier series expansion for the displacement field. The effects of anisotropy of the materials are then examined and discussed.

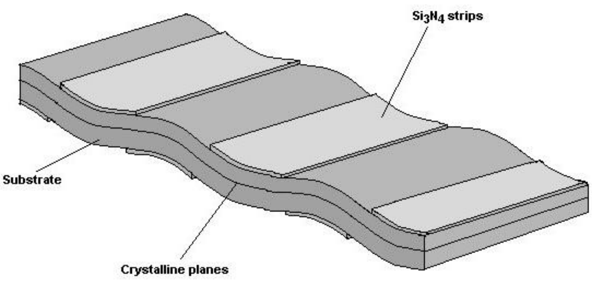

Figure 1: Crystalline undulator

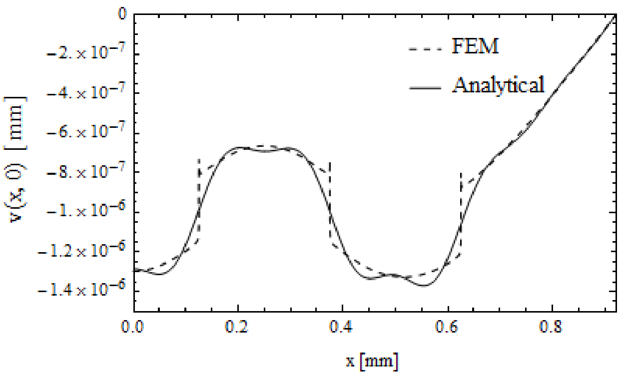

Figure 2: Transversal displacement in crystalline undulator

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L9

A geometrical multiscale numerical method for coupled hygro-thermo-elastic problems in layered materials

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Devices for energy applications, such as photovoltaic modules and solid oxide fuel cells, are composite structures obtained by assembling layers of various materials. Some have the role to guarantee protection from the environment by a suitable sealing of the device, others have specific electric or chemical features to produce energy. The durability of these devices is a serious concern due to fracture events promoted by the mismatch between the thermo-mechanical properties of the material constituents, often amplified by the severe working conditions they are exposed. Moreover, their modelling is very complex and it requires a multi-physics framework to gain an accurate picture of their overall working conditions and performance.

In the present contribution we propose a numerical method for the solution of coupled hygro-thermo-elastic problems involving thin layers with thermo-viscoelastic properties. Examining a stack of a photovoltaic module we have a glass cover for environmental protection, two layers of an epoxy material used to encapsulate a layer of brittle silicon solar cells, and finally a backsheet. Heat and stress transfer is taking place across the thickness of the epoxy layers and it is essentially a 2D (if a cross-section of the module is examined) or a 3D (if the whole module is simulated) problem. On the other hand, moisture diffusion takes place within a domain of one dimension lower, by permeating the same encapsulant from the edges or from the backsheet and diffusing along a direction parallel to the average plane of the module.

We therefore propose a computational geometrical multiscale approach where the 3D (or 2D for a cross-section) thermoelastic problem and the 2D (or 1D for a cross-section) moisture diffusion problem are solved using a staggered scheme. More specifically, for heat conduction and stress transfer we discretize the encapsulant layer by zero-thickness interface elements whose constitutive response is governed by a novel cohesive zone model (CZM) for thermo-visco-elasticity. All the other layers are discretized by continuum finite elements. The stiffness of the CZM is function of time and temperature according to the model based on fractional calculus proposed in [1] and validated by experiments. The thermal part of the CZM is described by a Fourier type constitutive equation dependent on crack opening. For the problem of moisture diffusion, on the other hand, a finite element mesh of one dimension lower is used for the sole epoxy layers. In each time step, after solving the thermo-mechanical problem, the diffusivity of the epoxy is updated based on the temperature and on the relative opening displacements available from the thermo-mechanical solution. Then, the moisture diffusion problem is solved. Comparison with experiments is provided.

Acknowledgements: The research leading to these results has received funding from the European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013) / ERC Grant Agreement n. 306622 (ERC Starting Grant "Multi-field and multi-scale Computational Approach to Design and Durability of PhotoVoltaic Modules" - CA2PVM).

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L10

Mechanical to electrical energy conversion with ceramic particle-reinforced soft materials

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An outstanding issue in the field of dielectric elastomers is the design of materials with enhanced electromechanical coupling able to improve the mechanical-to-electrical energy conversion in soft generators. To this aim, an interesting option is represented by random composites, where ceramic fillers with a high dielectric constant are dispersed in a silicone matrix. At the moment the most promising reinforcing materials to be employed as a disperse phase, already tested for soft dielectric actuators, are lead magnesium niobate-lead titanate (PMN-PT) and lead zirconate-titanate (PZT). In particular, two different composites based on a poly-dimethyl-siloxane (PDMS) matrix are here taken into consideration. The first one is PDMS reinforced with a 10% in volume of PMN-PT powder, the second one is reinforced with a 1% in volume of PZT.

The performance of a soft dielectric generator is computed employing a typical four-step cycle, where nominal load and electric charge are alternately held constant [1]. The amount of energy extracted during this cycle is limited by various mechanisms of failure, namely electric breakdown, ultimate stretch, loss of tension and electromechanical instability. The optimal cycle is identified by solving an optimization problem with electromechanical constraints associated with these limits. In this way we estimate the performance improvement achieved by the composite device with respect to the homogeneous one. In comparison with pure PDMS, the PDMS-10%PMN-PT allows an increase of more than 60% in the harvested energy per unit volume, while PDMS-1%PZT shows a minor improvement, in the range of 23.5-37.4%.

Acknowledgements: MG and EB acknowledge financial support from the EU FP7 project PIAP-GA-2011-286110-INTERCER2. RS acknowledges financial support from the EU FP7 project PIRSES-GA-2013-610547-TAMER.

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L11

A computational approach based on the integration of the equivalent-eigenstrain concept with the eXtended Finite Element Method for general-shaped inclusions embedded in ceramic materials

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Tempering and firing practices decrease the strength of ceramic materials such as those used for traditional pottery, due to thermal expansion mismatch between temper particles and ceramic matrix [1]. We study stress concentration around sharp temper inclusions where damaged zones have a toroidal shape (Figure 1) [2]. For this purpose, a variational formulation based on Eshelby's equivalent eigenstrain approach [3] is developed. In this approach, the toroidal damaged zone is treated as an inclusion surrounded by a "regularized" layer of finite width simulating an imperfect interface. The regularized layer is treated as an equivalent eigenstrain [4]. The associated numerical formulation is obtained by means of the regularized eXtended Finite Element Method. This method is suitable for general shaped inclusions because it describes interfaces implicitly through the level set method, while making discretization independent of the interface geometry. In the present work, three-dimensional simulations have been performed on a specimen with a toroidal inclusion for variable Young moduli and Poisson coefficients of the matrix and the inclusion. Figs. 1 e 2 show the stress σ_{zz} for a tensile specimen with a hard and a soft torus inclusion, respectively, subjected to a tensile pressure p_z of 1MPa applied over the top, with Poisson coefficient of 0.2 for both matrix and inclusion. In Fig.1 and 2, a perfect interface between torus and matrix has been assumed. One fourth of the specimen has been studied because symmetries of loading and geometry have been exploited.

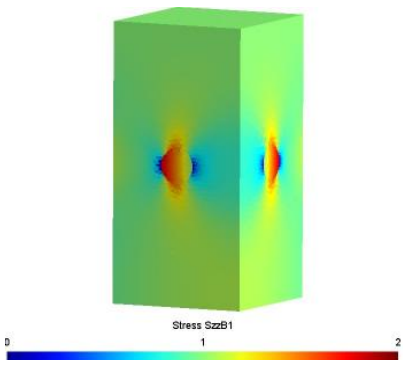

Fig. 1 stress σ_{zz} (MPa) for hard toroidal inclusion

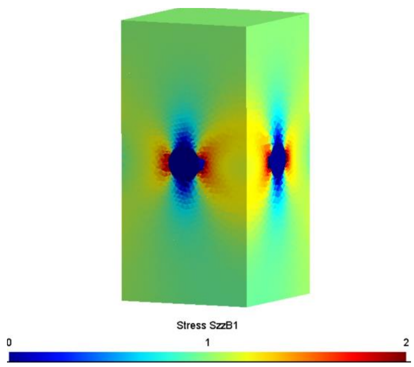

Fig. 2. stress σ_{zz} (MPa) for soft toroidal inclusion

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L12

Toughening mechanisms in particulate and layered solids

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Layered and particulate solids are commonly employed as engineering materials, with applications ranging from lightweight structural parts to high strength coatings. Commonly, high strength composites are brittle, and there is a need to improve their macroscopic toughness by suitable tailoring of topology and interfacial properties. A number of toughening strategies are available and a major thrust of our study is to compare, via finite element computations, the potency of toughening for some of these strategies. First, the enhancement in toughness due to a parallel array of cracks in an elastic solid is explored and the stability of co-operative cracking is quantified. Second, toughening by crack kinking is analyzed for a layered solid containing a pre-existing crack. The asymptotic problem of continued crack advance versus symmetric kinking is considered. The two competing crack paths involve rupture of cohesive zones, and each crack is endowed with a uniform strength and a critical displacement. Third, the evolution of the crack path (and associated crack growth resistance curve) is determined for a regular array of elastic, hexagonal grains bonded together by cohesive zones of finite strength and finite work of separation. Regardless of the initial configuration of a semi-infinite parent crack, with varying degrees of initial crack tip branching, we find that a single dominant crack ensues. The study concludes with the analysis of a mode I crack in a multi-layer stack of elastic and elastic-plastic solids. Plastic dissipation in the ductile layers conveys macroscopic toughening but the degree of toughening is sensitive to the relative height of the layers. In summary, the study demonstrates that multiple cracking is typically a difficult mode to activate under quasi-static conditions and the kinking mechanism, when activated, is the most potent in enhancing the toughness of a solid.

Acknowledgements: GN gratefully acknowledges the support by SISSA through the excellence program SISSA NOFYSAS 2012.

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Acoustic and thermal performances of ceramic tiles and tiling systems

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Acoustic and thermal performances of floating floor and/or radiant floor can be improved by using suitable ceramic tiles with tailored porosity and microstructure. Porcelain stonewares are still the most widespread typology of tiles, due to their high physical and mechanical performances coming from a very low level of open porosity and water absorption (≤0.5wt%) [1]; but it is noteworthy that the closed porosity can be significantly different among commercial porcelain stonoware tiles. As a consequence, the properties directly dependent on the total porosity, such as thermal and acoustic ones, may be strongly diverse among commercial tiles.

Several commercial porcelain stoneware tiles having different composition, microstructure and porosity, were selected for the research work. These tiles and the tiling systems (tiles coupled with resilient underlayer materials such as glass fibre, cork and rubber) were studied on the basis of dynamic stiffness (UNI EN 29052-1). Their acoustic and thermal properties were investigated in terms of walking noise reduction (UNI EN ISO 10140-3) and thermal conductivity (ASTM E 1530).

It was observed that the choice of the method to determine the total porosity is fundamental to correlate this characteristic to other properties. Results showed that, for this type of ceramic, an accurate image analysis is more reliable than the real density determination by following a standardized method (ASTM C329-88) that is needed to estimate the closed porosity.

The dynamic stiffness can be considered a useful tool to estimate the acoustic performance of tiles or tiling system. Especially when a huge number of ceramic samples has to be tested, dynamic stiffness can give an indication of which samples deserve to be deepen studied by specific and more expensive acoustic tests.

The commercial porcelain stoneware tiles showed rather different acoustic and thermal properties depending on their total porosity and pores pore size distribution, confirming that microstructural characteristics should be considered in floor designing [2].

In tiling systems, both the acoustic and thermal insulating properties are improved, especially when rubber is used as resilient underlayer material.

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L14

Thermal stress fields between two unequal circular holes in a ceramic medium

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Thermal stresses play a significant role in a number of engineering problems ranging from the design of heat engines, nuclear plants and aircrafts to the enhancement of electronic devices and MEMS performance. In particular, the determination of stress concentrations due to thermal loadings is a main issue for the accurate design of many electronic devices, where a large number of conductive electric wires are embedded in a ceramic or Silicon matrix at a small distance from each other. In this case, the heat production due to the Joule effect may create high enough thermal stresses to cause cracking and rupture of the insulating ligament between the wires [1], thus reducing the performance of the device. Since cracks often initiate and propagate from the locations of stress concentration, such as holes and inclusions, then, an accurate evaluation of the stress concentration factor (SCF) in proximity of these defects is a prerequisite to assure the structural integrity of a number of ceramic components and to guarantee the proper functionality of many electronic devices.

An analytic solution is presented here for thermal stresses in an infinite thermoelastic medium with two unequal circular cylindrical holes held at different temperatures, under steady-state heat flux. The most general representation for a biharmonic function in bipolar coordinates [2] has been used. The stress field is decomposed in the sum of a particular stress field induced by the steady-state temperature distribution, which does not satisfy the conditions of vanishing tractions on the surfaces of the holes and vanishing remote stress field, and an auxiliary stress field required to satisfy these boundary conditions, which has been obtained for isothermal elasticity. The corresponding variations of the stress concentration factor, are determined in terms of the holes geometry and temperatures. Moreover, the J_k-integral vector and the *M*-integral are first generalized for steady state thermoelasticity and then calculated on a closed contour encircling one or both holes. Results are then presented for varying geometry of the holes (Fig. 1).

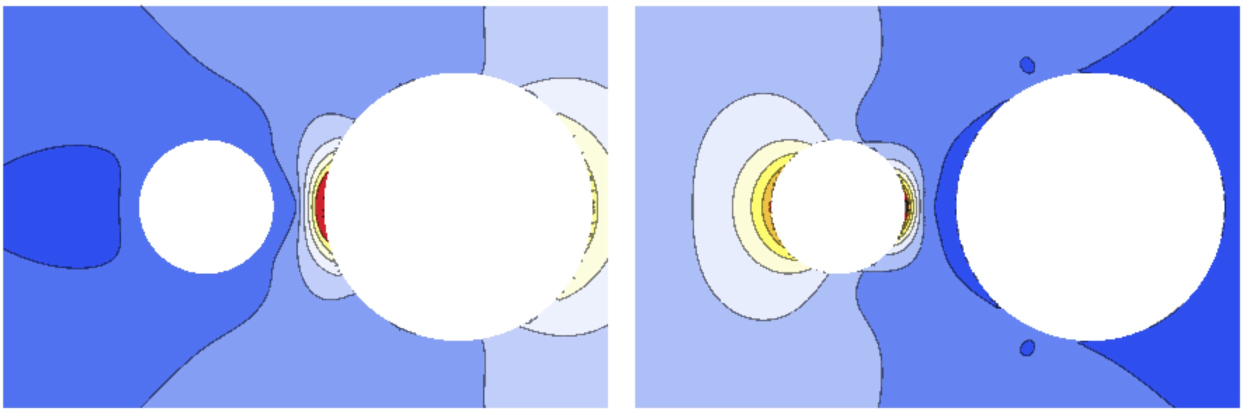

Fig. 1. Distribution of the maximum principal stress for $R_1 = 2R_2$, when $T_2 < T_1$ or $T_2 > T_1$.

Acknowledgements: Financial suopport from "Fondazione Cassa di Risparmio di Modena" is gratefully akowledged.

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On the compressive strength of glass-microballoons/thermoset-matrix syntactic foams

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This work is concerned with syntactic foams, that are particulate composites filled with hollow spherical inclusions. We propose a micromechanical model [1] to evaluate the uniaxial compressive strength for the most relevant case of glass inclusions of wall thickness of few micrometers (such particles are usually called *microballoons*) filling a thermoset matrix. The studied failure modality is experimentally characterised by shear bands inclined of about 45 degrees with respect to the loading axis, and a prominent softening behaviour. We develop a three-dimensional Finite Element modelling which extends and improves that proposed by our group in [2,3]. Different microstructures are described by cubic unit cells containing fifty hollow spheres accounting for different filler polydispersions and filler volume fraction up to 60%. Each microballoon is assumed to undergo brittle failure according to the structural criterion proposed in [3]. Here, we account for the matrix nonlinear behaviour and, in a phenomenological way, for the detriment of its mechanical properties, proportional to its *defectiveness*, which increases with the filler content and becomes extremely relevant at filler volume fraction larger than 50%. Our findings agree with experimental observations from the literature (see, e.g., [4]) and reveal room for improvement in the effective mechanical properties, possibly by acting on the manufacturing process.

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L16

Green Body Production from Alumina Powder: Constitutive Theory, Implementation, and Experimental Validation

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The production of green bodies is a crucial first step in the production of ceramics. The final properties of the piece are directly related to the uniformity of compaction, the residual-stress distribution, and particle cohesion. Because of the difficulty in mould production and setup costs, virtual prototyping can accelerate the development of new ceramics while decreasing costs and waste.

The numerical simulation of green body production combines many aspects of constitutive modeling such as: nonlinear elasticity, pressure-dependent plasticity, elasto-plastic coupling, Lode-angle dependence, and hardening. The proposed granular compaction model builds upon previous work[1] and incorporates the above-mentioned phenomena in a single continuum-level model that aims to predict residual stress fields as well as density heterogeneity in the green body in preparation for sintering.

This presentation will cover the theoretical underpinnings of the constitutive model, some aspects of the numerical implementation, parameterization method for alumina powder, and simulations of experiments for validation.

Acknowledgements: The authors gratefully acknowledge financial support from the European Union's Seventh Framework Programme FP7/2007-2013/ under REA grant agreement number PITN-GA-2013-606878-CERMAT2.

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L17

Modelization of a ladle cyclelife

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In the framework of the energy consumption saving in the steelmaking process, the ladle is one of the key elements where a huge quatitie of energy (gas or electricity) is involved. The ladle is a vessel allowing the transfer of molten steel from the melting furnace to the tundish at the continuous casting. It is of high importance to master the molten steel temperature during transfers to have the lowest temperature variation at the tundish and then to enhance steel quality and increase productivity.

The ladle is composed of a steel shell (blue part, Fig. 1.) inside which a refractory stack-up (lining) is masoned (red, white and black parts, Fig. 1.). The refractory stack-up is composed of several layers which could be:

- the working lining which is directly into contact with the molten steel,
- the safety lining which isolates the steel shell and prevents from break throughs,
- the insulation lining which either limits molten steel temperature drops and steel shell temperature increases.

First, the ladle is masoned with a new lining to be then preheated (Fig. 2.). The preheating allows reducing the thermal shock at the first molten steel tapping. After a metallurgical treatment of the steel, ladle is sent to the caster for teeming in the tundish. Empty ladle is then transfered to the ladle preparation area for inspection and cleaning and sent for a new cycle (tapping, treatment…). Ladle life could reach 100 cycles at least.

During each cycle, a huge quantity of energy is spent either to maintain molten steel temperature or to prevent from heat losses during empty ladle stand-bys. Improving the customer practice (i.e.: decreasing molten steel temperature variation at the tundish) would pass through a better knowledge of how the ladle temperature evolves during the process. Reaching that goal could be done via a numerical simulation. The development of the numerical model representing the ladle thermal cycle could by possible after choosing the accurate thermal boundary conditions. Comparing with measurements coming from the field during a ladle follow-up campaign contributed to the validation of the numerical model.

Fig. 1. Fınite element model of a ladle

Fig. 2. Ladle on the reheat area

Acknowledgements: The authors gratefully acknowledge support from the European Union FP7 project "HOTBRICKS - Mechanics of refractory materials at high– temperature for advanced industrial technologies" under contract number PIAPP–GA–2013–609758.

L18

Finite element simulation of thermal shock in micro-structured solids with applications to refractories

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Materials functioning at high temperature environments, such as refractories or thermal barrier coatings, are typically subjected to thermal shock conditions during their operation phase. Thermal stresses, induced by severe variations in the temperature field during sudden heating or cooling, are a key quantity for strength analysis [1]. Another significant design parameter is the material selection. Ceramic materials are a common choice due to their excellent heat resistance properties (low thermal diffusivity). The amorphous, grain dominated, micro-structure of ceramic materials, along with the possible existence of micro-cracks and porosity, introduces a high degree of complexity in simulation and a plausible field for the use of enhanced continuum theories [2].

In this study, Initial-Boundary Value Problems (IBVP) of thermoelasticity, in the framework of classical, micropolar and first strain gradient theory are treated numerically by means of the finite element method. After briefly revisiting the governing equations, appropriate time and length scales are introduced for specific applications (ceramics, alloys). The variational form of the resulting IBVP is studied and Galerking Finite Elements (FE) are introduced for the approximation of the solution.

Two different applications are presented. The first one examines the thermal stresses induced in a thin rectangular elastic body when subjected to a sudden change of its temperature due to convective heat exchange with a surrounding medium. This problem is relevant to the thermal shock of brittle materials such as refractories. The solution is derived in the framework of micropolar elasticity as an attempt to introduce the effects of microstructural characteristics (e.g. grain size), absent from the classical elasticity model. A second application refers to the thermoelastic response of a first strain gradient elastic half-space subjected to a uniform, sudden, temperature change on its free surface. The FE solution, as a function of the nondimensional spatial variable ξ (along the depth of the half-space) and temporal variable η, is presented in Fig. 1 for selected values of the microstructural parameters λ_A, λ_B.

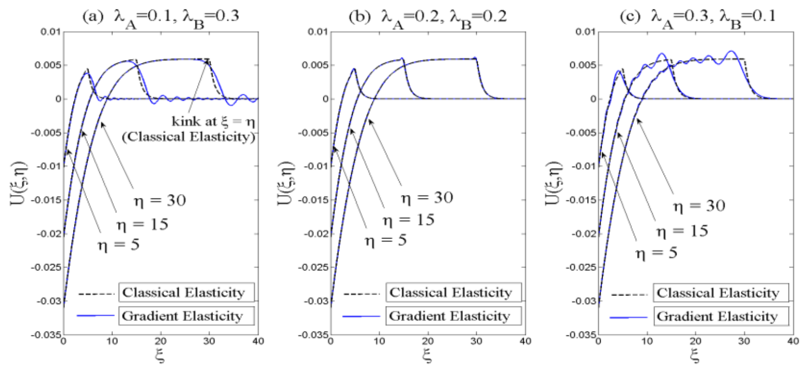

Fig. 1. Displacement field in a half-space subjected to thermal shock on its boundary.

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Computational modelling of refractory materials at high temperature

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Thermo-mechanical constitutive modelling is the key issue in the design of refractory devices in metal flow engineering, but routines taking into account the correct thermoplastic behaviour of these materials, to be used in advanced finite element softwares, are still not available.

The yield function recently proposed by Bigoni and Piccolroaz [1] is well-suitable to analyze elastoplasticity in refractory materials. Unfortunately, this flexible criterion is not defined outside the elastic domain, so that standard return mapping integration cannot be efficiently performed. Therefore, our research group developed two algorithms: a finite-step integration scheme based on a forward Euler technique with a 'center-of-mass-return' correction and a cutoff-substepping gradient-based integration [2].

The effects of high-temperature has been considered in the further developement of the constitutive model. Some consequences of thermal loads, such as the piezocaloric effect, are usually neglected in the most common FEM Software. For this reason non-standard finite elements, based on the fully coupled thermoelastic equations, have been efficiently implemented. The element performance has been tested comparing analytical solutions and numerical simulations of some simple examples. The wide range of experimental tests performed by our industrial partners allow us accuracy investigation and model fitting.

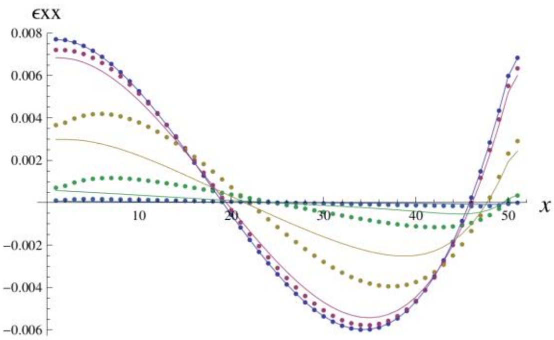

Fig. 1. Comparison of thermoelastic finite elements with and without piezocaloric effect.

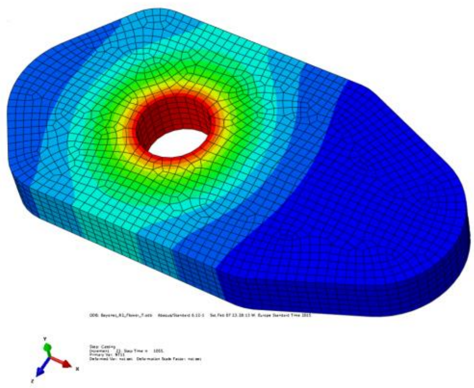

Fig. 2 . Thermal analysis of a refractory sliding plate during casting process

Acknowledgements: The authors gratefully acknowledge financial support from European Union FP7 project under contract number PIAPP-GA-2013-609758- HOTBRICKS.

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L20

Challenges in thermal and mechanical modelling of ceramic refractories involved in the continous casting process of steel

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Computational models are widely used in the industry for the development of new products. Their integration in the product development process allows engineers to have a better understanding of the products in their operating conditions. This shortens development times and also, as a consequence, results in products being optimized within their set working conditions.

However, for many reasons, the thermo-mechanical modelling of ceramic refractories used in the continous casting process of steel is still a great challenge. The main problem the computational model has to face is the complexity of their mechanical behaviour: pressure sensitivity [1], scattering and size effects on strength. Temperature and time dependency also has to be taken into account.

Furthermore, the harsh environment of the continous casting process of steel makes the field experiments difficult [2], which complicates the accurate definition of the various heat transfers between the product and its surrounding environment. We must also consider these difficulties during the modelling validation phase where innovative methods have to be used to verify the validity of the assumptions made throughout the model development.

Fig. 1. Operator manipulating a Ladle Shroud

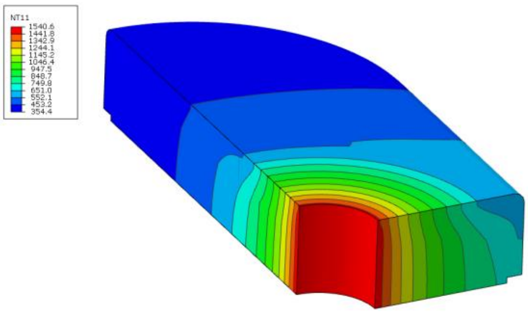

Fig. 2. Predicted temperature distribution inside a Slide Gate Plate

Acknowledgements:
The authors gratefully acknowledge support from the European Union FP7 project "HOTBRICKS - Mechanics of refractory materials at high– temperature for advanced industrial technologies" under contract number PIAPP–GA–2013–609758.

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L21

Effect of 'local' strain rate on the determination of elastic modulus during crush tests at high temperature in rock-like materials

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In iron and steel production, the materials directly in contact with the metal flow are subjected to extreme temperatures (1000 ÷ 1500 °C). The most common experimental set-up to determine the compression strength of rock-like materials is the 'crush' or unconfined compression (UC) test. With a special equipment, it is possible to perform UC tests whilst controlling the temperature of the specimen, up to about 1400 °C. From UC tests the Young's modulus of elasticity can also be measured, by determining the slope of the initial part of the $\sigma - \varepsilon$ curve. Measurements of Young's modulus of a rock-like material at high temperature are in general rather scattered, and it is difficult to identify a clear trend in the results.

Since the material behaviour at high temperature is deeply affected by creep deformations, the strain rate effect can be crucial in the determination of the material properties. The general set-up of a UC test consists of applying the load with a constant rate of strain until rupture of the specimen is attained. Despite the external strain rate applied by the press being constant, the local strain rate measured at the center of the specimen changes considerably in the tested specimens.

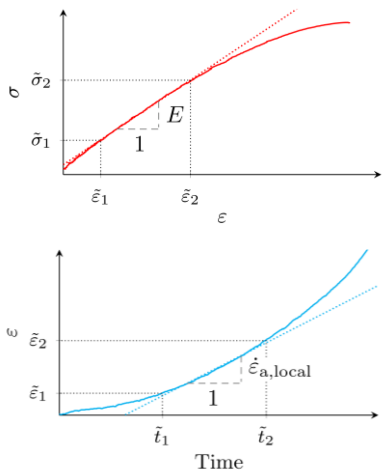

Fig. 1. Example of determination of the Young modulus and of the relevant local strain rate from UC tests.

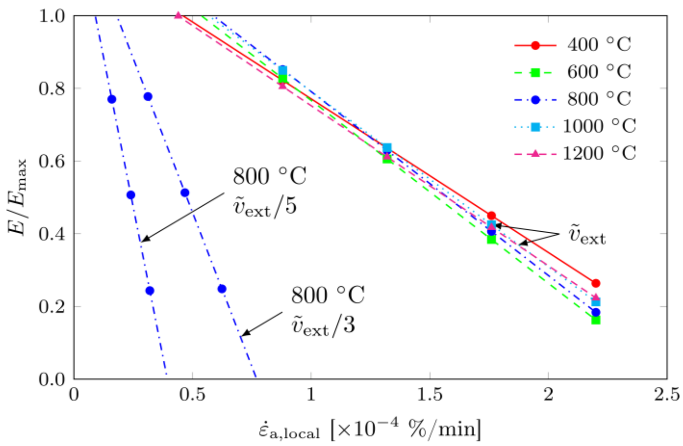

Fig. 2. Local strain rate vs. Young modulus for crush test at constant external strain rate for rock like materials.

Fig. 1 shows the procedure to determine Young's Modulus and the related local strain rate from UC tests. The interval of strain used to calculate Young's modulus is the same one also used to determine the local strain rate. The latter is defined as the best fitting overall slope of the time vs strain curve in the selected strain range. In Fig. 2, normalized values of Young's modulus obtained from a series of homogeneous UC tests are plotted versus local strain rate. It can be observed that trends relevant to tests performed at the same external strain rate are essentially the same for a very wide range of temperatures. However, carrying out UC tests at smaller external strain rates lead to a shift in the E vs local strain rate curve. This phenomenon could be related to the occurrence of viscous effects in the materials at hand, and should be studied in detail with further laboratory investigation.

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L22

Experimental tests use to study the ceramic material behavior

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The steel industry uses an important quantity of refractory ceramic to contain, guide and protect the molten metal during the different stages of its elaboration and its casting. This refractory ceramic is submitted to thermochemical and thermo-mechanical very intense stresses which limits the life cycle of these elements.

The experimental phase is necessary to understand the behavior of our materials and allows to reach the characteristic quantity of these. We thus developed within our laboratory different kind of trial (uniaxial and multiaxial) [2] allowing the characterization of our materials. In addition to, our materials being used at very high-temperature, we also adapted our bench tests to highlight the various present mechanical phenomena in the material with the evolution of the temperature (1500°) [1]. In that event, different trial protocol were developed: the cut of samples, the dimension measurement, the test as well as the post-treatment of the results.

The experimentation is also essential for a correct modelling and allows us to carry out our simulations by finite elements. It is the basis of the development of our materials laws at room temperature and high temperature.

The purpose being to obtain a greater reliability, to increase the life cycle of the material and to reduce production costs.

Fig. 1. Development of lab tests.

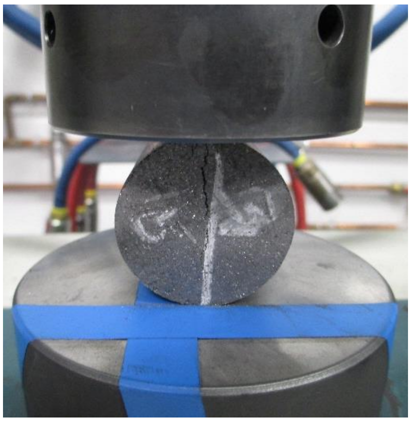

Fig. 2. Brazilian test

Acknowledgements: The authors gratefully acknowledge support from the European Union FP7 project "HOTBRICKS - Mechanics of refractory materials at high– temperature for advanced industrial technologies" under contract number PIAPP–GA–2013–609758.

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L23

Thermoplasticity towards the design of ceramics for high-temperature applications

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Although ceramics are usually considered brittle materials evidencing only traces of inelasticity prior to failure, there are situations in which inelastic strain strongly determines their mechanical behaviour. One of these situations is when a ceramic structural element is exposed to a high temperature environment, as is the case of the liquid steel technology. Indeed in metal casting, refractories are used in ladle/tundish slide gate systems, and for nozzles, moulds, and tubes, so that their design has to be optimized to improve their mechanical performances at high temperature, as well as thermal efficiency, in order to meet strict safety and functionality requirements.

Starting from results of experimental tests performed at high temperature, a thermoplastic mechanical modelling is developed for the design of refractory materials for the liquid steel industry. The model is based on a damage surface for ceramic materials [1], extended with a temperature dependent yield and thermoinelastic hardening laws capable of describing the behaviour of ceramics at high temperature.

Acknowledgements: Support from the European Union FP7 project "*Mechanics of refractory materials at high–temperature for advanced industrial technologies*" under contract number PIAPP–GA–2013–609758 is gratefully acknowledged.

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L24

Some considerations about thermomechanical and thermophysical modelling of ceramic refractory materials

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The elastic stiffness of refractory materials is tipically very high (ranging between 10 and 200 GPa) and their thermal expansion coefficient usually ranges between 3 and 6x10^{-6} (1/°K). As a result, when subjected to temperature variations of nearly 1500° K, the thermal strains are very large (0.45 - 0.90 %) which, if prevented, would lead to very high thermally induced stresses (45 - 1800 MPa). Although refractory pieces in operating conditions are not usually constrained at the external boundaries, to permit their thermal expansion, they may be subject to large thermal gradients, both during transient conditions and at the steady state. As a result, extreme self-equilibrated thermal stresses are induced by thermal gradients in these materials, due to their typical high stiffness. This is why, for a reliable modelling of the thermo-mechanical behaviour of refractory materials, it is very important to evaluate and simulate accurately the evolution of elastic stiffness and of thermal expansion coefficient under different stress and thermal conditions.

Refractory materials typically have thermo-mechanical properties which are usually very dispersed, depending on the chemical composition, forming process and curing temperature. In some refractory materials the elastic stiffness increases with increasing temperature, whereas in other materials it decreases. Some refractory materials have a reversible thermal behaviour, thus if heated at very high temperatures and then cooled, they do not show any permanent change of their thermo-mechanical properties. In contrast, some other materials exhibit an irreversible behaviour when subjected to a heating/cooling cycle.

Due to the dispersion of thermo-mechanical properties, it is not possible to formulate a general constitutive model that can simulate all typical aspects of refractory materials' response. Any thermo-mechanical constitutive model must be formulated and calibrated with reference to the given composition and forming process employed for the specific refractory material under examination, and it will consequently have a limited validity.

Some of the typical aspects of material responses, that can be applied to broad families of refractory materials, will be considered in this presentation. A simple thermodynamic potential will be presented and the implications involved in the simulations of the thermo-mechanical properties under complex thermo-mechanical loading conditions will be illustrated. Unfortunately, some simulated properties cannot be validated with regards to experimental results. Experimental tests in fact can be performed only under simple thermal and mechanical loading conditions. Anyway, these considerations will draw attention to the hidden assumptions involved in thermo-mechanical modelling of refractory materials and will stimulate discussion on the possible improvements of the experimental analyses.

Acknowledgements: The authors gratefully acknowledge financial support from European Union FP7 project under contract number PIAPP-GA-2013-609758-HOTBRICKS.

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L25

Phase composition of high-temperature refractories

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Real materials can be very different from their ideal counterpart. When produced in laboratory from chemically pure powders, a specimen is usually well reproducible. This concept can be very slack when dealing with industrial specimens, as different sets obtained from different raw materials batches can differ in composition and, possibly, in microstructure. A difference in composition can influence the mechanical properties both at room temperature and in exercise. If the composition and the microstructure is known, it can be possible to obtain the information on the mechanical behaviour starting from the mechanical properties of the component phases and of the knowledge of the grain-grain coupling. The composition of the specimens, in terms of component phases, can be obtained non-destructively by means of X-ray powder diffraction. The analysis was conducted on some of the high-temperature refractories, pointing out a complex composition that might change with the temperature, possibly affecting the behaviour of the component in service.

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L26

A review of thermomechanical and thermophysical properties of ceramic refractory materials

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To establish a reliable modelling framework providing a consistent insight into the thermomechanical behaviour of ceramic refractory materials, attention should be firstly given to the characterization of material thermoelastic and thermophysical properties. In other words, any dependency on temperature of the elastic (e.g. Young's and shear moduli) and thermophysical (e.g. specific heat capacity and thermal conductivity) properties should be experimentally established, to be consequently accounted for in an as accurate as possible manner in constitutive modelling.

In an attempt to corroborate and generalise the outcome of a set of existing thermomechanical experimental tests carried out on a limited range of refractory materials, a broad literature review was carried out including both casted and pressed ceramic materials with a wide range of compositions and target application.

Particular attention has been given to identifying trends with temperature (in the maximum range 20-1500 °C) of Young's modulus E, specific heat capacity at constant pressure c_p and thermal expansion coefficient α. It emerges that while c_p and α exhibit characteristic trends that are common to all material types, E shows a much wider variety of trends with temperature. Somewhat counter to engineering intuition, the elastic modulus of certain refractories (both measured with frequency techniques or by means of mechanical testing) does not exhibit a steady decrease with increasing temperature, but an initial nonlinear increase, sometimes followed by an abrupt drop beyond a threshold temperature (e.g., see Fig. 1). This could be due to the formation of low viscosity phases, i.e. the partial melting of some components before reaching the final temperature (Joliff et al. 2008).

After an illustration of the above mentioned experimental behaviour types, a discussion follows on the possibility of generalising the observed trends, to lay the foundations for a consistent thermomechanical modelling framework.

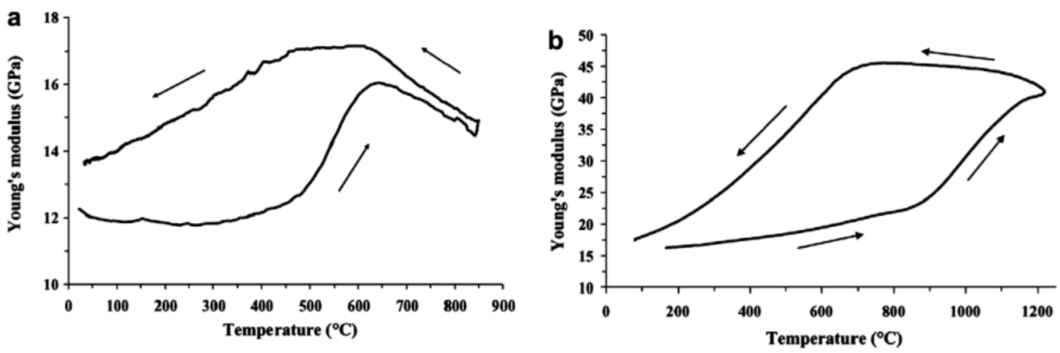

Fig. 1. Sample experimental plots illustrating the cyclic variation of Young's modulus with temperature, for two different types of ceramic refractories (Joliff et al. 2008).

Acknowledgements: The authors gratefully acknowledge financial support from European Union FP7 project under contract number PIAPP-GA-2013-609758-HOTBRICKS.

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L27

Contact regimes during heat conduction through a microstructured solid

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It is well known, that thermo-elastic effects may have significant results upon the macroscopic response in the mechanics of contact. On the other hand, as the scales in the contact system reduce progressively (micro to nano–scales), the internal material lengths become important and their effect upon the macroscopic response cannot be ignored.

We extend the classical contact solution for a punch indenting a homogeneous elastic half–plane, where heat conduction is permitted [1,2], to the analogous case of an indented microstructured solid. The behavior of the indented material is modelled through the couple–stress elasticity theory [3], which introduces characteristic material lengths and is appropriately modified in order to incorporate the thermal effects.

Similarly to the indentation problem in classical elasticity, depending on ratio between the total heat flux Q and the applied load P on the indenter, three different contact regimes can occur: perfect, separation, and imperfect contact. The obtained results show that the macroscopic conditions (essentially Q/P) for which the type of contact changes is strongly affected by the presence of internal microstructural length.

Acknowledgements: Support from the European Union FP7 project "*Mechanics of refractory materials at high–temperature for advanced industrial technologies*" under contract number PIAPP–GA–2013–609758 is gratefully acknowledged.

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Abstracts of

Posters

P1

Numerical modelling for the strain localization and shear banding in materials

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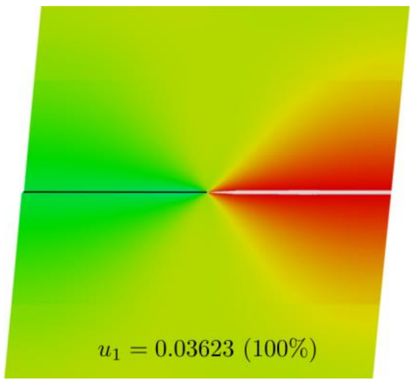
Strain localization and shear banding are investigated by means of a shear band model as a zero-thickness nonlinear interface. This model is implemented in Abaqus through user subroutine UMAT and tested through finite element simulation in elasto-plasticity [1]. The simulations are performed using an imperfection approach, where a shear band (present from the beginning of loading) is described as a region in which the yielding occurs at smaller values than in the rest of the matrix.

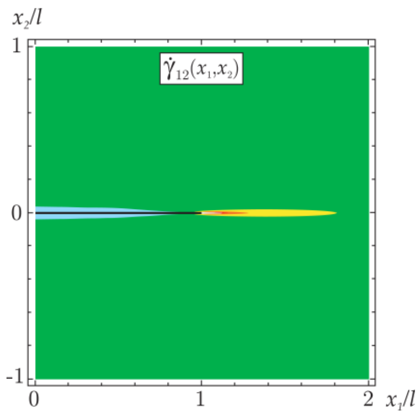
The presented approach is contrasted with a perturbative one [2], developed for a J2-deformation theory material, in which the shear band is modeled to emerge at a certain stage of a uniform deformation and the homogeneous prestress state is perturbed.

Both approaches confirm that the shear bands propagate rectilinearly under shear loading and that a strong stress concentration should be expected to be present at the tip of the shear band. These two features represent key concepts in the understanding of failure mechanisms of ductile materials.

Numerical approach:



Perturbative approach:



Acknowledgements: D.B., N.B. and F.D.C. gratefully acknowledge financial support from the ERC Advanced Grant 'Instabilities and nonlocal multiscale modelling of materials' FP7-PEOPLE-IDEAS-ERC-2013-AdG (2014-2019). A.P. thanks financial support from the FP7-PEOPLE-2013-CIG grant PCIG13-GA-2013-618375-MeMic.

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A universal curve for the design of optimal dielectric elastomer generators: benefits of ceramic filler addition

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The main goal in the field of dielectric elastomer generators (DEGs) is the optimization of these devices, undergoing a typical four-step load-driven cycle, where applied load and electric charge are alternately held constant. The amount of energy extracted during this cycle is limited by various mechanisms of failure, namely electric breakdown, ultimate stretch, loss of tension and electromechanical instability. Indeed, the optimal cycle complying with these limits is identified by solving a constrained optimization problem [2].

The outcome of the optimisation process is a universal curve, in the plane dielectric strength $\overline{E}_{eb}$ – ultimate stretch λ_U, defining an upper bound on the amount of energy harvested in function of the ultimate stretch ratio [2]. In order to extract the maximum energy form the DEG it is important that the pair of electromechanical properties of the material ($\overline{E}_{eb}$, λ_U) lie as close as possible to the universal curve.

To this end, composite materials with improved electromechanical coupling could be employed in the realization of enhanced electromechanical transducers. Promising materials, already tested for dielectric elastomer actuators [1], are random composites, where ceramic fillers with a high dielectric constant are dispersed in a silicone matrix. In the realization of dielectric elastomer generators (DEGs), among ceramics, the most adequate dispersed reinforcements are lead magnesium niobate-lead titanate (PMN-PT) and lead zirconate-titanate (PZT).

Two different composites are here taken into consideration, both based on a matrix of poly-dimethyl-siloxane (PDMS). The first one is reinforced with a 10% in volume of PMN-PT powder, the second one is reinforced with a 1% in volume of PZT. The electromechanical properties of both these composites lie very close to the universal curve, allowing to leverage the material obtaining a better performance with respect to pure PDMS.

In comparison with pure PDMS, the PDMS-10%PMN-PT allows an increase of more than 60% in the energy per unit volume harvested by the generator, while PDMS-1%PZT shows a minor improvement in the range of 23.5-37.4% [3].

Acknowledgements:
EB and MG acknowledge support from the EU FP7 project PIAP-GA-2011-286110-INTERCER2 and RS acknowledges support from EU FP7 project PIRSES-GA-2013-610547-TAMER.

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P3

A multibody model for planetary ball-milling

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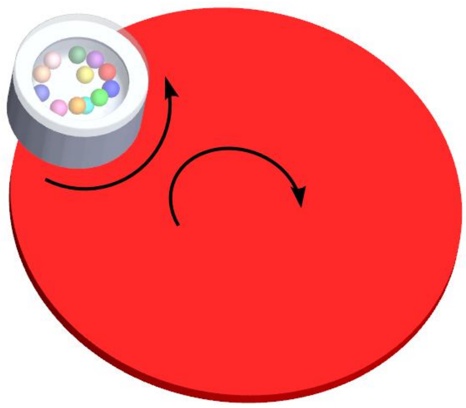
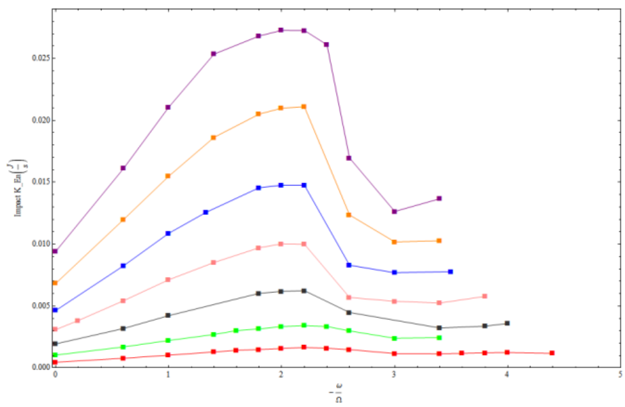
High-energy ball milling is a widely used technique for particle size reduction down to nanometer scale [1,2]. Different kind of materials can be ground, chiefly including metals [3] and ceramics [4], but organic and pharmaceutical compounds in particular can also be treated [5].

Grinding occurs by impact between milling media and powder particles inside a jar and therefore the investigation of energy transfer is crucial to understand the resulting grain size as well as possible induced deformations, defects and/or phase transformation. To assess the dependency of energy exchange on milling parameters, i.e., number and size of balls, jar size and geometry, velocity of revolving parts, quality and quantity of materials, etc., a dynamic mechanical model of a planetary ball-mill has been developed by using the multibody dynamics software MSC Adams [6]. Being the model based on numerical parameters, some experiments have been performed in order to determine their value. Results of the simulations point out relations between velocity of plate and jar, motion of grinding media and energy regimes of the process. In particular, there is a critical ratio of velocities corresponding to the maximum energy transfer: below this value ball motion is chaotic, whereas above, balls tend to stick to the jar wall.

Computer simulation outcomes are compared i) indirectly, with experimental data obtained by X-ray diffraction on a ceramic (fluorite), a metal alloy (Fe1.5%Mo) and a pharmaceutical compound used in the HIV-AIDS terapy (Efavirenz); ii) directly, with camera images and sound measurements recorded during the milling. Part ii) is in progress. As a further improvement, based on data from the above-mentioned model, a detailed analysis of defect and fracture behaviour is also being carried out.





Acknowledgement. The present work is supported by Fondazione Caritro, project "bando 2013 per progetti di ricerca scientifica nel settore delle scienze biomediche con il coinvolgimento di giovani ricercatori", project "Mechanically activated Active Pharmaceutical Ingredients: microstructural effects on drug dissolution and bioavailability". The authors are especially grateful to Dr D. Catelani (MSC software) and Dr Ing Mirco D'Incau for precious collaboration and support to the research work.

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P4

Analysis of dynamical effects in the formation of compaction bands

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The occurrence of compaction bands (CBs), strain localisation phenomena typically taking place under compressive stress regimes (and without shear straining evidence), causes significant anisotropy alteration of the permeability tensor. Thus, understanding the formation pattern of CBs is important in many geomechanical applications, especially when fluid extraction/injection from/into the ground is involved.

CBs have been both observed on site and reproduced in the lab, in geomaterials ranging from uncemented sands to soft sandstone and mudstone. While most of the available models to understand CB formation are focused on interpreting the onset of a single CB, e.g. within the framework of bifurcation theory [1], not many extensive studies have been dedicated to understand the documented periodicity of CBs.

In this work, dynamical effects induced by the formation of CBs are analysed by means of FEM modelling with a finite strain formulation [2], with reference to a horizontal layer of sandy, water-saturated material.

The propagation of longitudinal elastic waves caused by the sudden occurrence of a first CB is associated with a decrease of both total stress and pore pressure (Fig. 1). On the other hand, the abrupt volumetric collapse caused by the CB formation results in a dramatic pore pressure increase within the CB, locally vanishing the effective stress.

Furthermore, elastic waves that are reflected at any interface (a) with a softer material or (b) with a just formed CB carry a local increase of effective stress. This might bring about (depending on the considered geometry, at locations where such reflected waves collide) the formation of further CBs in a cascade fashion, according to a uniform spacing that is a function of the first CB position. The process of successive formation of CBs stops after some time, which is a function of the geometry of the layer and of the material's permeability [3].

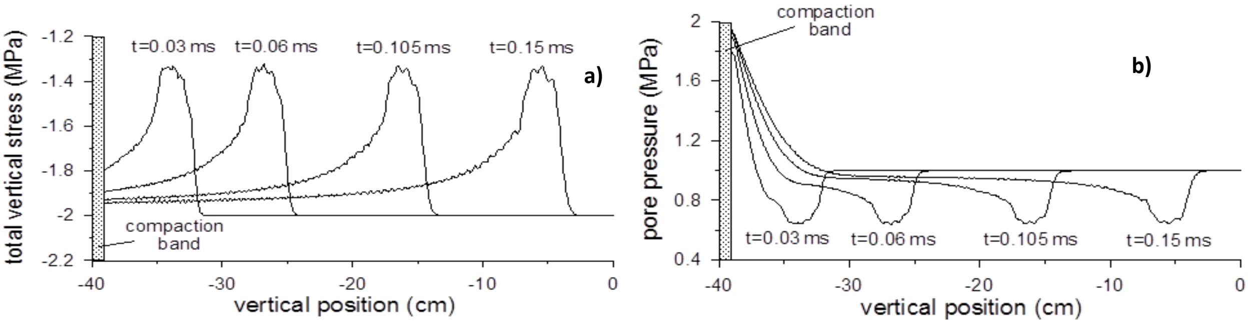

Fig.1. Elastic wave propagation in terms of (a) total stress and
(b) pore pressure induced by the formation of a 2-cm thick compaction band.

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P5

Ultrasonic tests on green bodies: forming pressure and evolution of the elastic characteristics

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Mechanical properties of green bodies, fundamental quantities to improve the design of ceramics, have been detected as a function of the forming pressure.

By means of both pressure and shear ultrasonic waves, several tests have been carried out on circular-shaped ceramic tablets made up of both alumina ALMATIS (grain size 0.5 μm) powders and alumina MARTODIX KM-96 ALBEMARLE (grain size 170 μm) powders.

This study shows that at higher compaction pressure correspond higher stiffness in terms of elastic and shear moduli. The obtained results open new prospective in design of ceramic materials.

Fig. 1. MARTODIX KM-96 ALBEMARLE green bodies surface formed at 4 MPa.

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P6

Cracks propagation in ceramic materials: a singular integral formulation

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The problem of a crack at the interface between two dissimilar ceramic materials, loaded by a general asymmetrical system of forces distributed along the crack faces is investigated. The proposed original formulation is based on integral transforms and two fundamental notions of linear elasticity: the Betti reciprocal theorem and the weight function approach. The Betti identity has been extensively used in the perturbation analysis of two and three-dimensional cracks [4]. In linear fracture mechanics, the concept of weight function, defined as singular non-trivial solutions of the homogeneous boundary value problem for a solid with a crack, was introduced by Bueckner [1]. Recently, symmetric and skew-symmetric weight function matrices have been derived for interfacial cracks in both isotropic and anisotropic materials [2, 3, 4]. Using these matrices together with the fundamental reciprocal identity (Betti formula), the elastic fracture problem is formulated terms of singular integral equations relating the applied loading and the resulting crack opening.

The derived compact formulation can be used to solve many problems in linear elastic fracture mechanics (for example various classic crack problems in homogeneous and heterogeneous anisotropic media, as piezoceramics or composite materials). This formulation is also fundamental in many multifield theories, where the elastic problem is coupled with other concurrent physical phenomena.

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Stress magnification and Notch Stress Intensity Factors for composite materials containing polygonal inclusions

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The rigid inclusion model predicting a singular stress field in an elastic plate (Fig. 1), is validated for the first time via photoelastic experiments under mode I [1]. Results show that the stress concentrations near corners of stiff inclusions can reach very high values leading to catastrophic failure of structural components. In particular, for the case of rhombohedral rigid inclusion, it is experimentally observed a stress magnifaction factor 5.3.

Notch stress intensity factors are derived for matrix containing small void and rigid polygonal inclusions subjected to remote self-equilibrated anti-plane shear load (mode III) described by a polynomial of generic order, which is found to be dependent on two constants for each order. By means of Schwarz-Christoffel map in a differential closed-form expression [2], it is shown that (i) a complex potential governing the out-of-plane problem is given by a closed-form formula and (ii) the notch stress intensity factors is strictly related to the unperturbed stress state at the singular point ($\tau^{\infty}_{yz}(a,0)$ for void and $\tau^{\infty}_{xz}(a,0)$ for rigid) and depend on a geometrical factor defined at varying the inclusion shape.

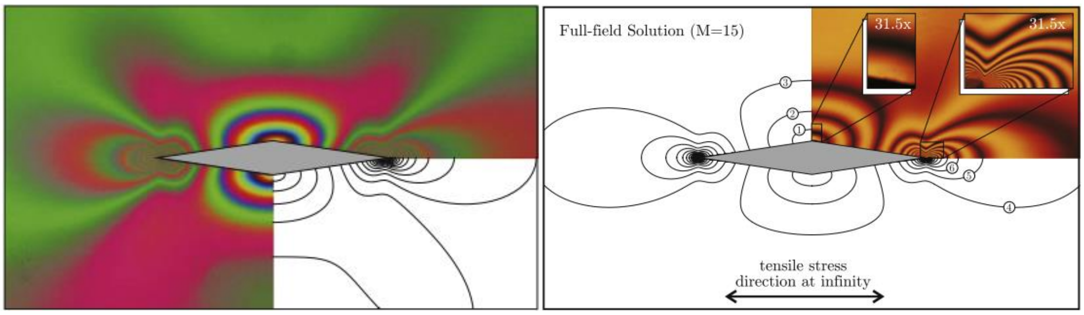

Fig. 1. White (left) Monochromatic (right) photoelastic fringes revealing an excellent description of the in-plane principal stress difference field near stiff rhombohedral rigid inclusion with Lx=15 and Ly=2.

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Mechanical models for instabilities induced by dry friction

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The experimental evidence of instabilities in elastic structures under follower forces has been recently shown in the work of Bigoni and Noselli [1]. The load provided to the structure has been realized exploiting the Coulomb friction.

The follower load in the Ziegler's column (a discrete structure) is induced by a frictional force acting on a wheel mounted at the end of the structure (Fig. 1). Possible instabilities for the system shown in Fig. 1 are flutter (blowing-up oscillations) or divergence (exponentially growing motion).

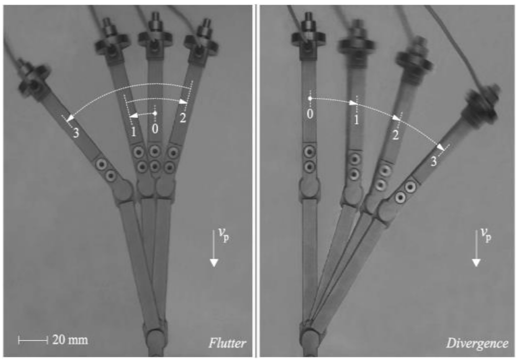

Fig. 1: Instabilities in Ziegler column.

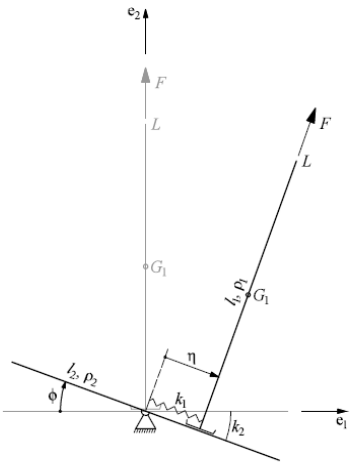

Fig. 2: System showing flutter under a tensile follower load.

Flutter instability can also affect continuous systems, as the Beck's column, while the divergence does not occur. These types of instabilities can arise even if the elastic structure is subject to a tensile follower force (Fig. 2).

All the experiments have been performed with a conveyor belt modified for research purposes (Fig. 3).

Fig. 3 Testing machine.

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Critical issues in the coaxial double ring test for ceramics and glass

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For the experimental measurement of the strength of glass and ceramics, the *panacea* would be to induce an almost constant and equibiaxial state of stress in a central portion of the tested specimen, sufficiently far from its borders. In fact, since the mechanical strength is mainly governed by the opening of surface cracks in mode I, the test should detect the size of the dominant crack far from the edges, where defectiveness is certainly higher than in the core due to the cutting process. In the coaxial double ring test, the circular portion of the specimen within the internal ring approximately achieves this ideal configuration, provided the ratio diameter/thickness is small enough to limit second order effects. The recommendations of ASTM C1499 (09) [1] are directed towards this goal, since they prescribe a variable geometry according to the thickness of the tested material. For what glass is concerned, it is commonly believed that the Coaxial Double Ring (CDR) test, and in particular the configuration with an additional overpressure suggested by the EN1288-2 standard [2], albeit complex, achieves the ideal equibiaxial configuration.

Here, a critical review of the Coaxial Double Ring (CDR) test is presented through an analytical theoretical approach, with particular attention to the effects of non-linearities. Assuming a Weibull statistical distribution of the defects, for the configuration with no overpressure we obtain expressions in closed form of the effective area [3]. This is a parameter that permits to re-scale the experimental data [4] according to a criterion of equal failure probability in a reference state, i.e., an equibiaxial state of stress acting on a unitary area. It is then possibile to conceive a new testing procedure, where the measured data are re-arranged in order to recover the ideal equibiaxial conditions.

Indeed, the procedure proposed by ASTM may involve very small ring diameters, and therefore the test may be very sensitive to localized defects or stress concentrations. On the other hand, the method with overpressure proposed by EN1288-2 [2] is unnecessarily complicated and inconsistent, because the induced state of stress is found to be far from being uniform and equibiaxial. As the EN1288-2 standard was used to define the reference strength of glass in product standards, we wonder if a supplementary experimental campaign must be considered for a more appropriate definition the material properties.

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