Workshop program and Book of Abstracts



Manufacturing technologies, properties and applications of advanced structural ceramic materials

April 7, 2017

Institute of Power Engineering, Ceramic Department CEREL

Description

The workshop will be a scientific forum where international experts from both academia and industry can discuss about research and development in the field of ceramic science. The aims of the workshop are: (i) to present the actual manufacturing technologies used in industrial processes, (ii) to introduce the properties and propose applications of advanced structural ceramic materials and (iii) to disseminate recent discoveries in the modelling of ceramics.

Venue

The workshop will take place on April 7, 2017 at Grand Hotel Boutique Sp. z o.o. in Rzeszów, Poland. The Grand Hotel is located at 1a Dymnickiego street, just in the city centre. Traveling from Rzeszów Airport, one should take a bus indicated by letter "L" to the central train station of Rzeszów and then go on foot - the walking distance from Rzeszów central train station to the Grand Hotel is about 15 minute.

Organizer

The workshop is organized by Institute of Power Engineering, Ceramic Department CEREL, Research Institute situated in Boguchwała near Rzeszów in Poland.

Supporters







Manufacturing technologies, properties and applications

of advanced structural ceramic materials

PROGRAM

Friday, April 7, 2017

8.55 - 9.00 Opening

9.00 - 11.00 Plenary Session (Chairman: M. Krauz)

9.00 - 10.00 **Alan Wilmański, <u>Mirosław M. Bućko,</u>** Composites in the aluminum oxynitride – some 3d metal nitrides systems prepared from SHS-derived powders

10.00 – 11.00 <u>Zbigniew Pędzich</u>, Grzegorz Grabowski, Kamil Wojteczko, Agnieszka Wojteczko, Optimization of useful properties of alumina/zirconia composites for selected applications

11.00 - 11.30 Coffee break

11.30 - 13.00 Session I (Chairman: M. Gromada)

11.30 – 12.00 **Marek Grabowy**, Zirconia solid solutions as an brilliant example of engineering and functional materials – CEREL's R&D and production competences

12.00 – 12.20 Michał Kawalec, Ryszard Kluczowski, Mariusz Krauz, Overview of Fuel Cells

12.20 – 12.40 **Ryszard Kluczowski, Michał Kawalec, Mariusz Krauz,** Technology of Anode Supported Solid Oxide Fuel Cells in IEn OC CEREL

12.40 – 13.00 <u>Mariusz Krauz</u>, Ryszard Kluczowski, Michał Kawalec, Metal Supported Solid Oxide Fuel Cells – third generation of SOFC

13.00 - 14.00 Lunch

14.00 - 16.00 Session II (Chairman: R. Kluczowski)

14.00 – 14.20 <u>Magdalena Gromada</u>, Janusz Trawczyński, Michał Wierzbicki, Perovskite membranes for clean oxygen separation from air

14.20 – 14.40 **Vladimir Buljak**, **Milorad Milovančević**, Towards modeling of thermal cyclic of the elastic properties in porous ceramics

14.40 – 15.00 **Shwetank Pandey**, **Vladimir Buljak**, Parameter identification for Drucker-Prager Cap model through inverse analysis using only compaction curves 15.00 – 15.20 **Domenico Tallarico**, Natalia V. Movchan, Alexander B. Movchan, Michele **Camposaragna**, On the dynamic response of superlattices made of piezoelectric ceramics

15.20 – 15.40 **Philippe Godin, Séverine Romero Baivier,** Thermo-mechanical modelling of refractory ceramic behavior in use

15.40 – 16.00 <u>Achraf Kallel</u>, Severine Romero Baivier, Finite Element Analysis of the Compaction Behavior of Refractory Powders

16.00 - 16.30 Coffee break

16.30 - 18.30 Session III (Chairman: V. Buljak)

16.30 – 16.50 **Daniel Kempen**, Andrea Piccolroaz, Thermomechanical modeling and simulation of the sintering process of ceramics

16.50 – 17.10 **Nikolai Gorbushin, Gennady Mishuris,** Model of crack movement in bi-material

17.10 – 17.30 <u>Gennaro Vitucci</u>, Nikolai Gorbushin, Gennady Mishuris, History-dependent crack propagation in discrete chains

17.30 – 17.50 <u>Anastasiya Vinakurava</u>, Andrzej Skrzat, Feliks Stachowicz, Analysis of stressstrain state of the femur after resection using developed application based on micropolar theory

17.50 – 18.10 <u>Mojtaba Biglar</u>, Feliks Stachowicz, Tomasz Trzepieciński, Magdalena Gromada, The influence of metallic interface on micro-mechanical fracture and electrical behaviour of multilayer piezoelectric actuator

18.10 – 18.30 <u>Monika Perkowska</u>, Gennady Mishuris, Andrea Piccolroaz, Michał Wróbel, Hydraulic fracturing in ceramics

18.30 Dinner

Abstracts of Invited Lectures

Composites in the aluminum oxynitride – some *3d* metal nitrides systems prepared from SHS-derived powders

Alan Wilmański, Mirosław M. Bućko

AGH University of Science and Technology, Faculty of Materials Science and Ceramics al. Mickiewicza 30, 30-059 Krakow, Poland

e-mail: bucko@agh.edu.pl

Aluminium oxynitride, γ-alon, is a spinel-type structure solid solution of Al₂O₃ and AlN. Due to its good mechanical and chemical properties γ-alon has a great potential application in high-performance structural ceramics. Much attention has been focused on developing alon-based composites to improve its properties and performance. Additions of different types of hard ceramic phases such as Al₂O₃, AlN, SiC, ZrN, TiN and TiC have been investigated. Formation of such composites enhanced aluminum oxynitride hardness, flexural strength, toughness and especially wear resistance. The aim of the present work is to present a new idea of producing CMC composed of aluminium oxynitride matrix and tantalum nitrides nitride particle reinforcement. The precursor powders were formed in a single step process using the SHS synthesis.

Starting powder mixtures were composed of aluminium oxide, aluminium and some 3d metals (titanium, tantalum or niobium). Al₂O₃ and Al powders remained a ratio of 4:1 when adding other metals powder. The powder mixture were subjected to self-propagating high-temperature synthesis (SHS) in nitrogen atmosphere under a pressure of 3 MPa. The SHS-derived powders were ground and hot-pressed at 1750-1850°C for 1h under 25 MPa. The dense samples were composed of γ -alon, small amount of aluminum nitride and respective nitrides: MeN and Me₂N. Increase of the nitrides content in the composites improved significantly their mechanical properties. The samples prepared from the powder containing formally 30 mol% of the metals show Vicker's hardness over 16 GPa, fracture toughness about 7 MPa·m^{0.5} and especially wear resistance three order of magnitude better than dense corundum material.

Optimization of useful properties of alumina/zirconia composites for selected applications

Zbigniew Pędzich, Grzegorz Grabowski, Kamil Wojteczko, Agnieszka Wojteczko

AGH University of Science and Technology, Faculty of Materials Science and Ceramics, Department of Ceramics and Refractory Materials, Mickiewicza 30, 30-059 Kraków, Poland

e-mail: pedzich@agh.edu.pl

Work of many (not only mechanically loaded) devices consist in movement of their parts subjected to different types of friction and wear. It can cause serious damages which could decrease parameters of work;

Intensive wear rate even in small areas could causes in destroying of a large or/and complicated parts. Application of composites could be a solution in such cases;

Because the work conditions of these parts are very different, it is difficult to predict of optimal composition using basic mechanical characteristic (HV, K_{Ic} , σ , E, ...);

The goal of presented work is to pay attention on such aspects optimisation of composite microstructure which can not be described by mechanical parameters.



Fig. 1. The examples of real microstructures of composites in alumina/zirconia system: 35 vol.% $Al_2O_3/65$ vol.% ZrO_2 ; 15 vol.% $Al_2O_3/85$ vol.% ZrO_2 ; 85 vol.% $Al_2O_3/15$ vol.% ZrO_2 .



Fig. 1. Real examples of crack paths in 15 vol.% Al₂O₃/85 vol.% ZrO₂; 85 vol.% Al₂O₃/15 vol.% ZrO₂ composites.

Acknowledgements: The work was partly financially supported by the statutory funds of the Faculty of Materials Science and Ceramics under grant no. 11.11.160.617.

Abstracts of Lectures

The influence of metallic interface on micro-mechanical fracture and electrical behaviour of multilayer piezoelectric actuator

Mojtaba Biglar¹, Feliks Stachowicz¹, Tomasz Trzepieciński¹, Magdalena Gromada²

¹Rzeszow University of Technology, Department of Materials Forming and Processing, Al. Powstancow Warszawy 8, 35-959 Rzeszów, Poland
²Institute of Power Engineering, Ceramic Department CEREL, ul. Techniczna 1, 36-040 Boguchwała, Poland

e-mail: m_biglar@prz.edu.pl

This paper deals with micro-mechanical and electrical behaviour of multilayer piezoelectric actuator. The grain boundary formulation generated via assuming displacement compatibility equation and traction equilibrium equation, however, these equations are validated only in undamaged part of representative volume element (Fig. 1). A mixed mode cohesive law is presented and applied to model crack initiation and evaluation between grains. The boundary element method is found as a suitable method for implementation of these assumptions. The type of metallic interface is investigated on mechanical and electrical behaviour of multilayer actuator. The results indicate that the metallic interface plays a significant role in electrical output and mechanical micro-crack pattern of actuator.





Fig. 1. The final model chosen from SEM machine and (b) output of image processing algorithm

Acknowledgements: The research leading to these results has received funding from the People Programme (Marie Curie Actions) of the European Union's Seventh Framework Programme FP7/2007-2013/ under REA grant agreement No. PITN-GA-2013- 606878.

Towards modeling of thermal cyclic of the elastic properties in porous ceramics

Vladimir Buljak, Milorad Milovančević

Faculty of Mechanical Engineering, University of Belgrade, Serbia

e-mail: vbuljak@mas.bg.ac.rs

Within polycrystalline porous ceramics it is evidenced that during cooling from firing temperature, due to the pronounced thermal anisotropy of grains, micro cracks are gradually formed with decreasing temperature. Such cracking causes the drop in elastic properties of bulk material which, depending on the level of porosity, can be decrease even by 50% with respect to the value at high temperature. It is further observed that upon subsequent heating these cracks are closing and even totally healing at very high temperatures, bringing the elastic properties to its original value upon one thermal cycle [1]. This type of behavior is observed in a various ceramic materials and often represents an advantageous and tailored material property [2]. Despite its evident practical application, still there is no constitutive description of this phenomenon, capable of predicting the evolution of Young's modulus as a function of temperature history. In order to numerically model this behavior, clearly it is required to take into account fracture. Since during cooling only inter-crystalline fracture is observed, an appropriate approach could be the use of cohesive elements, as the crack patterns are a priori known. Major limitation of this approach is that the cohesive elements already implemented within commercial codes cannot take into account crack healing upon subsequent heating. In this study a novel cohesive element is developed and implemented within ABAQUS commercial finite element code which is capable of modeling both crack opening, closing and healing. This way a numerical framework is developed which can be further used to design a phenomenological model for thermal elastic hysteresis. In a subsequent phase, an inverse analysis based calibration procedure is developed, in which macroscopic properties are used to calibrate parameters entering into micro-crack model. The approach is centered on a minimization of a discrepancy function designed to quantify the difference between experimentally measured quantities and their computed counterpart. The obtained fracture properties of material can be used to predict general stress-strain response of bulk porous ceramic materials at diverse temperatures. This response is generally more difficult to measure within porous ceramics.

Acknowledgements: This study is related to a research project on new ceramic technologies and novel multifunctional ceramic devices and structures, within European Union's Seventh Framework Programme FP7/2007-2013/ under REA grant agreement number PITN-GA-2013-606878-CERMAT2, and the authors are gratefully acknowledging the financial support from it.

References:

- [1] Efemerov A M, Bruno G.: Modeling the impact of microcracking on the thermoelasticity of porous and microcracked ceramics, Philosophical Magazine, Vol. 93, pp. 691-717, 2013.
- [2] Joliff Y, Absi J., Glandus C, Huger M and Tassier-Doyen N.: Experimental and numerical study of the thermomechanical behaviour of refractory model materials. Journal of European Ceramic Society, Vol. 27, pp. 1513-1520, 2007.

Thermo-mechanical modelling of refractory ceramic behavior in use

Philippe Godin, Séverine Romero Baivier

Enabling Technology Department, VESUVIUS SA, Ghlin, BELGIUM

e-mail: philippe.godin@vesuvius.com

Modelling is a tool more and more used in the industry for the development of new products. This technology allows a better understanding of the behavior of the product in its conditions of use. Thus the modelling allows to optimize the product as well as its shape and materials to be used.

The Submerged Entry Nozzle (SEN) is the part which delivers molten steel from a tundish into a continuous-casting mold. The SEN is made of different refractories, and must be preheated properly to prevent problems such as cracks from thermal shock during initial filling. On this subject, a study performed on (SEN) is at present realized to highlight the behavior of the product during its use. An Accurate simulations of the use of SEN are highly useful to optimize the process as well as in the shapes of the materials.

In order to optimize this state of stress on the product, a numerical model was calibrated and validated thanks to laboratory trials. This simulation uses criteria of plasticity and failure with temperature, based on the Bigoni-Piccolraz yield function [1] (UMAT).



Fig. 1. Submerged entry nozzle in continuous casting



Fig. 2. Predicted stress distribution with UMAT inside tube

Acknowledgements:

We gratefully acknowledge financial support from European Union FP7 programme under project reference PITN-GA-2013-606878-CERMAT2 and the partners for the synergistic collaboration.

References:

[1] Bigoni, D. and Piccolroaz, A., (2003), A new yield function for geomaterials, Constitutive modelling and analysis of boundary value problems in geotechnical engineering, Napoli.

Model of crack movement in bi-material

Nikolai Gorbushin, Gennady Mishuris

Department of Mathematics, IMPACS, Aberystwyth University, Wales, UK

e-mail: nig15@aber.ac.uk

The treatment of cracks at microlevel is a progressive topic in dynamic fracture mechanics nowadays. This scope is aimed in the better understanding of fracture processes that happen right at the crack tip in solid materials. The mathematical study of such problems is able to make some predictions and draw some explanations for physical phenomena.

In this particular work we are concerned with a problem of an interfacial crack propagation in a brittle bi-material. The fracture process is supposed to be brittle and the model itself may be applied for the consideration of failure of bi-material ceramics.

We present the solution of the problem, derive the relation between the loading parameters and crack speeds. We show the peculiarities that are detected due to the microlevel and additionally due to the material parameters mismatch.

Acknowledgements: This work was supported by FP7 Marie Curie ITN transfer of knowledge programme under project PITN-GA-2013-606878-CERMAT2.

Zirconia solid solutions as an brilliant example of engineering and functional materials – CEREL's R&D and production competences

Marek Grabowy

Institute of Power Engineering, Ceramic Department CEREL Research Institute, 1 Techniczna St., 36-040 Boguchwała, Poland

e-mail: grabowy@cerel.pl

Zirconium dioxide usually as a dense polycrystalline ceramic is an extraordinary material amongst other oxides. It's traditional applications contain refractory materials, foundry moulds, glaze and paint pigments, abrasive materials. Specific mechanical properties of zirconia (being more exact - solid solutions on it's base) are a reason of ZrO₂ ceramic usage, in structural applications, grows all the time. High modulus of rapture and elasticity, very good wear resistance and very high (in comparison to other ceramics) fracture toughness gives zirconia ceramic the advantage over metals when it is used for: pomp plungers, pistons, guides, rollers, moulds and many other machine parts and elements. High refractoriness (melting point over 2700°C), very good chemical resistance, low wear in high temperature and low thermal conductivity, makes zirconia ideal material for special refractory applications like steel and alloys flow control systems (metering nozzles, slide gate plates, atomizing nozzles) or crucibles. High temperature oxygen ion conductivity phenomena, which takes place in some zirconia solid solutions, makes possibility to use zirconia as a solid state electrolyte working in fuel cells, oxygen sensors or oxygen pumps. It can not be also forgotten that unique combination of very good mechanical properties and biocompatibility makes zirconia one of the most important material in medical implants business.

The base of such a spectacular and still growing success of ZrO_2 as structural and functional material is the bond character and specific polymorphism. In room temperature pure zirconium dioxide has monoclinic symmetry. Temperature rise effects in transformation to tetragonal and further to regular phase. The change from monoclinic to tetragonal is accompanied with a few percent volume change, which practically makes the use of pure ZrO_2 in structural applications impossible. Alloying the ZrO_2 structure with some cations makes the tetragonal and regular phase stable in room temperature. Controlling the phase composition by the amount of doped cation and modifying the microstructure, it is possible to influence, within the wide range, properties like mechanical strength, fracture toughness or thermal shock resistance. This correlations has allowed to develop a series of zirconia based solid solutions which has found it's use in so many various applications.

Zirconium dioxide containing Y_2O_3 in solid solution (Y-TZP) has an important use as a material for machine parts and elements. In a specific application it is faced with thermal shock, abrasive wear and mechanical impacts. The aim of this work was to find the correlation between the preparation method of Y-TZP, phase composition, microstructure and properties, specifically it's fracture toughness. It is shown that, by the choice of yttria precursor, chemical composition, sintering and aging conditions it is possible to modify phase composition and microstructure and by that the mechanical properties and thermal shock resistance of the material. New very high fracture toughness (13 MPam^{1/2}) and high bending strength (1100 MPa) material has been developed.

Perovskite membranes for clean oxygen separation from air

Magdalena Gromada¹, Janusz Trawczyński², Michał Wierzbicki³

¹Institute of Power Engineering, Ceramic Department CEREL, Research Institute, 1 Techniczna St., 36-040 Boguchwała, Poland ²Wroclaw University of Technology, Division of Chemistry and Technology of Fuels, 27 Wybrzeże Wyspiańskiego St., 50-370 Wrocław, Poland ³Institute of Power Engineering, Research Institute, Thermal Processes Department, 36 Augustówka St., 02-981 Warszawa, Poland e-mail: gromada@cerel.pl

According to the present state of the art, the cryogenic air separation is the best available technology when realizing large-scale oxyfuel power plants. However, the Air Separation Unit (ASU) based on the perovskite oxygen membranes is suggested as the promising alternative for cryogenic method [1]. The oxyfuel power plant integrated with ASU, where the oxygen membrane module is used was proposed by Hashim et al. and Stadler et al. [2, 3]. The essential requirement for the commercial application of the oxygen membranes for oxy-combustion purposes is to increase the oxygen permeation flux through membrane and develop the effective technology of dense tubular oxygen membranes manufacturing. The effectiveness of membrane described by the oxygen flow permeating through it depends, among others, on the chemical composition of perovskite material, the technology of membrane forming (extrusion, isostatic pressing), the membrane thickness (range controlled by diffusion or surface processes), its microstructure and the operating temperature as well as the gradient of oxygen partial pressures at both side of membrane [4].

The membranes manufactured from perovskite-type oxide prepared by the solid state method showed the low resistance of oxygen transport on grain boundaries, and therefore they reveal greater effectiveness. The additional advantage of this method is its greater efficiency in comparison with other ones, which will have huge importance on membranes manufacturing cost at commercial scale. Additionally, the high values of the oxygen permeation flux have been obtained for the dense planar BSCF membranes as well as the long-lasting test (two thousand hours) confirmed their durability [5]. Tubular membranes that are more useful in industrial practice due to their greater effective surface, mechanical stability and easiness of application, were manufactured as the dense thin-walled tubes made by isostatic pressing and extrusion. The measurements of the oxygen permeation flux than the membrane made by isostatic pressing [6].

Acknowledgements: This scientific work was supported by the National Centre for Research and Development, within the confines of Research and Development Strategic Program "Advanced Technologies for Energy Generation" project no. 2 "Oxy-combustion technology for PC and FBC boilers with CO2 capture". Agreement no. SP/E/2/66420/10. The support is gratefully acknowledged.

References:

[1] I. Pfaff, A. Kather, Energ. Procedia 1 (2009) 495-502.

[2] S. S. Hashim, A. R. Mohamed, S. Bhatia, Renew. Sust. Energ. Rev. 15 (2011) 1284-1293.

[3] H. Stadler, F. Beggel, M. Habermehl, B. Persigehl, R. Kneer, M. Modigell, P. Jeschke, Int. J. Greenh. Gas Con. 5 (2011) 7-15.

[4] H. Lu, Y. Cong, WS Yang, Solid State Ion 177, 595 (2006).

[5] M. Gromada, J. Świder, J. Trawczyński, M. Stępień, M. Wierzbicki, Bull. Mater. Sci. 38 (1) (2015) 23–28.

[6] M. Gromada, J. Trawczyński, M. Wierzbicki, M. Zawadzki, Ceramics International 43 (2017) 256-261.

Finite Element Analysis of the Compaction Behavior of Refractory Powders

Achraf Kallel, Severine Romero Baivier

Vesuvius Group, Enabling Technologies Department, Ghlin, Belgium

e-mail: Achraf.kallel@vesuvius.com

Powder compaction modelling have been widely studied during the last decades. However, it remains a complex work since the material changes from the loose state to the bulk compacted state. Regarding the literature survey, powder densification could be divided in two main approaches: microscale contact models [1] and continuum macroscopic models [2]. Constitutive models based on the second approach are generally implemented into finite element softwares. Thus, they offer the possibility of modelling the compaction at the part scale for near net shape purposes.

In this work we report on the assessment of the Drucker-Prager - CAP model for the simulation of the manufacturing of refractory products [3]. The model parameters are defined as functions of the relative density and the temperature. Building on the simulation predictions, the final shape and the process settings are tuned to optimize the compaction sequences and the tooling shape (Figure 1a). Then, the stress field in the obtained geometry is computed in respect with the the density distribution after the compaction step (Figure 1b).



Fig. 1. a) density distribution in a stopper at the end of the compaction b) Stress field in the nose of the stopper during the casting step.

Acknowledgements: We gratefully acknowledge financial support from European Union FP7 programme under project reference PITN-GA-2013-606878-CERMAT2 and the partners for the synergistic collaboration.

References:

[1] P. Pizette, C.L. Martin, G. Delette, P. Sornay, F. Sans, Powder Technology 198 (2010) pp240–250.

[2] H.G. Kim, O. Gillia, P. Doremus, D. Bouvard, Int. J. Mech. Sci. 44 (2002) pp2523-2539.

[3]L.H. Han, J.A. Elliott, A.C. Bentham, A. Mills, G.E. Amidon, B.C. Hancock, Int J Solids Struct. 45 (2008) pp3088–3106.

Overview of Fuel Cells

Michał Kawalec, Ryszard Kluczowski, Mariusz Krauz

Institute of Power Engineering Ceramic Department CEREL, 1 Techniczna St., 36-040 Boguchwała, Poland

e-mail: kawalec@cerel.pl

Fuel cells are electrochemical devices that allows for direct conversion between electrochemical potential of fuel and oxidizer to usable electronic current in the process sometimes called "flameless combustion". In most general terms, fuel cell consist of anode and cathode (electrodes) with electrolyte that separate them. At anode side, fuel is oxidized (burned) and at the cathode side oxidizer is reduced. Main function of electrolyte is to ensure electrical separation between electrodes, disallowing direct electron current and at the same time allowing ion transport, to propagate reaction on electrodes. Difference of potentials between electrodes are harvested by means of current collectors applied to electrodes, giving electrons alternative route to follow. Depending on electrolyte type, fuel cells (FC) are usually divided into Polymer Electrolyte Membrane FC or Polymer Exchange Membrane (PEMFC), Alkaline FC (AFC), Phosphoric Acid FC (PAFC), Molten Carbonate FC (MCFC) and Solid Oxide FC (SOFC). Nowadays, most research and development is dedicated to PEMFC, low temperature (below 100 °C), hydrogen fuelled FC with polymer electrolyte conducting protons and SOFC, high temperature (above 700 °C), hydrogen or natural gas fuelled FC with solid oxide as oxygen ion conducting electrolyte. As single FC usually cannot yield enough power for most application, FCs are usually connected together into stacks. PEMFC stacks are already commercially available and SOFC stacks are in field tests.



Fig. 1. SOFC working principle diagram



Fig. 2. Commercially available PEMFC stack from Horizon, Singapur

Thermomechanical modeling and simulation of the sintering process of ceramics

Daniel Kempen, Andrea Piccolroaz

University of Trento, Trento, Italy

e-mail: Daniel.Kempen@unitn.it

For engineers it is useful to know in advance the amount of shrink during the sintering process, so that the ready-sintered parts are as close as possible to the desired shape. The current standard models of sintering have laid the focus on isothermal conditions during the firing. Our aim is to extend the current theory of sintering to account for non-isothermal conditions. A key feature of the model is the Bigoni-Piccolroaz yield function that has successfully been used to simulate plastic behavior during powder pressing [1]. The model of the thermomechanical coupling is based on the development of Simo and Miehe [2].

We have developed a material model and have implemented it into a Finite Element code. Currently we are running experimental tests to be able to calibrate the model over the full range of densities and temperatures. Specimen were partially sintered at different temperatures to reach final densities that lie between green body and fully sintered. First results show a steep increase of strength, while the relative density increases very slightly. Therefore, the density increase alone cannot be taken as the only material parameter governing the strength increase during sintering.



Fig. 1. Stress-Strain diagram of the pilot study's partially sintered specimen under uniaxial compression

Acknowledgements: The authors acknowledge financial support from the European Union's Seventh Framework Programme PITN-GA-2013-606878-CERMAT2.

References:

[1] Bigoni, D., and Piccolroaz, A. Yield criteria for quasibrittle and frictional materials. International Journal of Solids and Structures 41, 11-12 (2004), 2855–2878.

[2] Simo, J. C., and Miehe, C. Associative coupled thermoplasticity at finite strains: Formulation, numerical analysis and implementation. Computer Methods in Applied Mechanics and Engineering 98, 1 (1992), 41–104.

Technology of Anode Supported Solid Oxide Fuel Cells in IEn OC CEREL

Ryszard Kluczowski, Michał Kawalec, Mariusz Krauz

Institute of Power Engineering Ceramic Department CEREL, 1 Techniczna St., 36-040 Boguchwała, Poland

e-mail: kluczowski@cerel.pl

Anode Supported Solid Oxide Fuel Cells (AS-SOFC) belong to intermediate temperature kind of fuel cells with operating temperature range between 550 and 800°C and fuelled by hydrogen or natural gas. Institute of Power Engieneering Ceramic Department CEREL (IEn OC CEREL) produces complete fuel cells of various sizes and shapes (Fig. 1) which are composed of four main layers as follows in sequence: anode support, electrolyte layer, barrier layer and cathode layer (Fig. 2) [1]. The main part which is responsible for mechanical strength of whole cell is porous anode support with thickness ranging from 0,5 to 1,0 mm. Anode support consists of powdery composite of ittria stabilized zirconia (YSZ) and nickel [2] working as ionic and electronic conductor respectively. The second layer consists of gadolinium doped ceria. Last layer is porous cathode layer with thickness of 30 microns made of perovskite material characterized by mixed ionic-electron conductivity. In IEn OC CEREL anode supports for AS-SOFC are currently produced by novel high-pressure injection moulding method [1, 2]. Electrolyte, barrier and cathode layers are applied with screen printing method. Production technology elaborated in IEn OC CEREL allowes production of fuel cells in semi-technical scale with very good electrical parameters. Maximum tested power density of OC CEREL AS-SOFC at 800°C is 1,25 W/cm² [1].



Fig. 1. Anode Supported Solid Oxide Fuel Cells AS-SOFC



Fig. 2. Cross section of AS-SOFC (CEREL) (SEM-BSE 2000x)

References:

[1] R. Kluczowski, M. Krauz, M. Kawalec, J.P. Ouweltjes *"Near net shape manufacturing of planar anode supported solid oxide fuel cells by using ceramic injection molding and screen printing"* Journal of Power Sources 268 (2014) 752-757.

[2] M. Kawalec, R. Kluczowski, M. Krauz, *"Manufacturing technology of AS-SOFC prepared with different commercially available precursors"* E3S Web of Conferences 10, 00033 (2016).

Metal Supported Solid Oxide Fuel Cells – third generation of SOFC

Mariusz Krauz, Ryszard Kluczowski, Michał Kawalec

Institute of Power Engineering Ceramic Department CEREL, 1 Techniczna St., 36-040 Boguchwała, Poland

e-mail: krauz@cerel.pl

Solid oxide fuel cells (SOFCs) have been object of continuous interest for the last few decades due to their efficient direct conversion of chemical energy into electricity, fuel flexibility and environmental benefits. The operating temperature of SOFCs at a level of 800-1000°C introduces limitations in SOFCs stacks fabrication and operation. The lower operating temperature permits the use of less expensive stainless steel as supports and interconnectors. A metal substrate with a thickness of a few hundreds of micrometers is advantageous for SOFCs since it provides good electrical conduction, high mechanical strength, favourable thermal distribution due to the high thermal conduction and rapid start-up times [1]. Metal supported SOFCs would also enable conventional metal joining techniques to be used in the stack assembly.

Two conventional powder metallurgy methods were utilized for preparation of porous structures – Tape Casting and High Pressure Injection Molding. Circular shapes were produced by laser cutting from both TC and HPIM green tapes. The sintering of as prepared green samples was carried out in a tube vacuum furnace equipped with rotary and oil diffusion pumps. The solvents and the binders were removed in situ during the sintering cycle. The deposition process of the electrolyte on selected porous supports was done by DCIJP (Fig. 1) and PVD (Fig. 2). Anode and cathode layers were deposited by screen printing method.



Fig. 1. Electrolyte deposited by DCIJP method [1].



Fig. 2. Electrolyte deposited by PVD method

References:

[1] R. I. Tomov, M. Krauz, A. Tłuczek, R. Kluczowski, Venkatesan V. Krishnan, K. Balasubramanian, R. V. Kumar, B. A. Glowacki, "Vacuum-sintered stainless steel porous supports for inkjet printing of functional SOFC coatings", Mater Renew Sustain Energy (2015) 4, 14.

Hydraulic fracturing in ceramics

Monika Perkowska¹, Gennady Mishuris², Andrea Piccolroaz³, Michal Wróbel²

¹Enginsoft, Trento, Italy ²Aberystwyth University, Aberystwyth, United Kingdom ³University of Trento, Trento, Italy

e-mail: monikaperkowska@hotmail.com

Ceramic materials are widely used not only in everyday life, but also in many engineering areas. Nowadays ceramic components are utilized in various technologies, being exposed to heavy and complex mechanical loadings including the hydromechanical interactions or tribological wear. Under certain operating conditions the ceramic components may be subjected to creation of hydraulic fractures. This mechanism of damage can appear e.g. in ceramic sliding bearings or high pressure ceramic filters. Thus, credible modelling and control of the underlying physical phenomenon is crucial for many technological applications, especially as not much attention has been paid to this problem so far.

An accurate prediction of the crack initiation and propagation is one of the most important problems in fracture mechanics. In most real-life applications the crack often propagates under mixed mode loading. Therefore not only the criterion for the fracture extension, but also the respective conditions for its directional orientation are of importance. The situation becomes even more complicated when one considers the fracture induced by injection of viscous fluid and resulting non-standard conditions of crack surface loading combined with possible infiltration of the porous material by fracturing fluid.

Recently, a new propagation criterion for the hydraulic fracture, accounting for Mode I and hydraulically induced shear stress, has been introduced in [1]. It has been proved that the standard linear elastic fracture mechanics criterion is not appropriate for hydrofracturing. Following this finding, we propose an extension of the methodology and results to Mode II and Mode III. A comprehensive analysis of the direction of the crack propagation is conducted. An impact of the hydraulically induced tangential traction on the fracture extension process is examined. The new fracture propagation criteria based on the energy release rate condition are proposed. A comparative analysis of respective criteria is provided.

Acknowledgements: The authors acknowledge financial support from the European Union's Seventh Framework Programme PITN-GA-2013-606878-CERMAT2.

References:

[1] Wrobel M., Mishuris G., Piccolroaz A. (2016) Energy release rate in hydraulic fracture: Can we neglect an impact of the hydraulically induced shear stress? *International Journal of Engineering Science*, 111: 28-51.

Parameter identification for Drucker-Prager Cap model through inverse analysis using only compaction curves

Shwetank Pandey, Vladimir Buljak

Faculty of Mechanical Engineering, University of Belgrade, Serbia

e-mail: shwetank.1991@gmail.com

Cold compaction of ceramic powders is a phase in production of ceramic components that preceeds high temperature sintering. Different techniques are used to model this phase, based, either on granular material considerations, or on continuum mechanics approaches. Difficulty related to such modelling is mostly connected to the fact that initial granular material has fairly different mechanical behavior than the finally formed dense one which is called "green body". An additional complication comes from significant changes in elastic properties of the green body with increasing compaction pressure. Many researchers are using constitutive models employed in soil mechanics, like Drucker-Prager Cap (DPC) model, to describe compaction process. In order to address the above mentioned features, some authors have introduced, and numerically implemented, the field dependency of constitutive parameters from the original DPC model. By this adjustment the elasto-plastic coupling observed during compaction can be taken into account, but the number of sought parameters increases making the identification more complex. This leads from the fact that the parameters need to be identified at different densities to predict the evolution of parameters over the whole compaction process. The state of the art techniques rely on destructive tests like Brazilian tests, crush tests etc. Thus, identifying these parameters as a function of relative density (that is related to compaction pressure) significantly increases the required number of experiments on compacted bodies making the characterization highly tedious and expensive [1-2]. In the current research, we propose an alternate, and hopefully advantageous, solution for constitutive parameter identification through Inverse Analysis (IA) methodlogy. IA synergically combines the experiments with numerical simulations and mathematical programming for minimization of discrepancy between experimentally measured quantities and their computed counterpart. This method promises to eliminate the need to perform destructive tests, as the compaction curve itself is enough for calibration of the model. IA relies on sensitivity of sought parameters with respect to the experimentally measured quantities and in order to achieve this, the molds for compaction with different geometries, which are easy to produce, will be employed. The results are presented as a comparison of parameters with experimentally obtained values from destructive tests.

Acknowledgements: This study is related to a research project on new ceramic technologies and novel multifunctional ceramic devices and structures, within European Union's Seventh Framework Programme FP7/2007-2013/ under REA grant agreement number PITN-GA-2013-606878-CERMAT2, and the authors are gratefully acknowledging the financial support from it.

References:

- [1] Han, L.H., Elliot, J.A., Bentham A.C., Mills, A., Amidon, G.E. and Hancock, B.C.: A modified Drucker-Prager Cap model for die compaction simulation of pharmaceutical powders, International Journal of Solids and Structures, Vol. 45, pp. 3088-3106, 2008.
- [2] Cunningham, J.C., Sinka, I.C. and Zavaliangos, A.: Analysis of Tablet Compaction. I. Characterization of Mechanical Behavior of Powder and Powder/Tooling Friction, Journal of Pharmaceutical Sciences, Vol. 93, pp. 2022-2039, 2004.

On the dynamic response of superlattices made of piezoelectric ceramics

Domenico Tallarico¹, Natalia V. Movchan¹, Alexander B. Movchan¹, Michele Camposaragna²

¹Deparment of Mathematical Sciences, University of Liverpool, Liverpool (UK) ²Thermo-mechanical Competence Centre, Enginsoft SPA, Bergamo (IT)

e-mail: dtalla@liverpool.ac.uk

Experimetal and theoretical challenges in the modelling and testing of devices containing piezoelectric ceramics are briefly reviewed. Special attention is given to composite materials containing more then one piezoelectric ceramic in their building blocks.

We construct the Bloch-Floquet dispersion diagrams for the coupled elastic (EL) and electromagnetic (EM) waves propagating through a 1D layered piezoelectric superlattice [1, 2]. In addition, we present a mathematical method based on the multiple scattering technique. This method allows us to quantify the scattering spectrum for EL and EM waves by a finite number of piezoelectric layers. Specifically, we present possible energy conversion mechanisms associated with internal resonances of the piezoelectric stack [2].

A 2D periodic piezoelectric structure is introduced. The unit cell of this structure coincides with the one of an infinite checkerboard-like structure, where the "white" and "black" rectangles are different piezoelectric materials. Compared to the 1D case, the dispersion surfaces are constructed numerically. Special attention is given to the dynamic anisotropy and to localisation phenomena [2], interpreted via the analysis of dispersion surfaces within the first Brillouin zone.

Acknowledgements: DT gratefully acknowledges the People Programme (Marie Curie Actions) of the European Union's Seventh Framework Programme FP7/2007-2013/ under REA grant agreement n. PITN-GA-2013-606878.

References:

[1] Sabina, F.J., and Movchan, A.B. Interfacial effects in electromagnetic coupling within piezoelectric phononic crystals. Acta Mech Sin **25**: 95. <u>doi:10.1007/s10409-008-0201-y</u>.

[2] Tallarico, D., Movchan, N., Movchan, A., and Camposaragna, M. (2016) Propagation and filtering of elastic and electromagnetic waves in piezoelectric composite structures. Math. Meth. Appl. Sci., doi: <u>10.1002/mma.3893</u>.

Analysis of stress-strain state of the femur after resection using developed application based on micropolar theory

Anastasiya Vinakurava, Andrzej Skrzat, Feliks Stachowicz

Rzeszow University of Technology, Department of Materials Forming and Processing, Al. Powstancow Warszawy 8, 35-959 Rzeszów, Poland

e-mail: vinakurava@prz.edu.pl

The aim of this study is provide analysis of stress-strain state of the femur after resection using developed application based on micropolar theory. Surgery is the main method of treatment both benign and malignant tumors in the bone tissue of limbs. As a result of sectoral resection strength of bone is getting lower and lead to risk of fractures and cracks appearing, which drastically reduces the functionality of the limb and the quality of patient life [1].

To investigate the stress-strain state of the bones before and after resection with regard to micropolar theory custom application has been developed and validated in several benchmark tests including stress concentration problem and contact problem (Fig 1). Therefore, developed application based on micropolar theory work with 8-node hexahedral elements so some preporation of the femur bone model for futher investigation has been provided.

Calculations were carried out for the β -TCP implant located in a proximal part of the femur bone. The comparative analysis of the stress-strain state of an intact bone and femur with ceramic implant showed that the contact between implant and bone tissue significantly affects distribution of stresses near the area of post resection defect (Fig 2).





Fig. 1. Example of couple stresses results obtained for contact problem (benchmark test)

Fig. 2. Distribution of von-Mises stresses in bone tissue after sectoral resection

Acknowledgements: The research leading to these results has received funding from the People Program (Marie Curie ITN transfer) of the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement No PITN-GA-2013-606878 - CERMAT2

References:

[1] Lee, T.: Predicting failure load of the femur with simulated osteolytic defects using noninvasive imagining technique in a simplified load case, Ann Biomed Eng., 35 (2007), 642-650.

History-dependent crack propagation in discrete chains

Gennaro Vitucci, Nikolai Gorbushin, Gennady Mishuris

Department of Mathematics, IMPACS, Aberystwyth University, Wales, UK

e-mail: gev4@aber.ac.uk

Discrete models find numerous applications in material modeling. They have been used for various investigations, among which fracture in crystals, fiber-reinforced composites, solid foams.



infinity.

We are here interested in dynamic crack propagation in the simplest case of infinite discrete chains of oscillators and the admissible steady-state regimes of the fracture wave. In the last five decades the problem has been tackled by different authors and the solutions have allowed to identify the structure behavior by calculating the way dynamic phenomena influence the so-called lattice trapping. In other words, how much energy is invested in the crack progression and how much is carried away by waves originating at the crack tip increasing the toughness with respect to static fracture.

We add to well-known solutions the influence of non-instantaneous fracture criteria for the linear elastic bonds. One assumes that the stress for failure must be averaged during the incubation time, the other that an integral measure of the overstretch must be taken in account.

Such treatment can widen the application of the discrete approach to real materials and modifies the regimes of admissibility for the fracture wave other than the force-velocity relations.

Acknowledgements: The research was supported by FP7 Marie Curie ITN transfer of knowledge programme under project PITN-GA-2013-606878-CERMAT2.