

Keynote Forum February 25, 2019

Material Science 2019



2nd International Conference on

Materials Science and Engineering February 25-26, 2019 | Paris, France



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Volodymyr Chernenko

Ikerbasque - Basque Foundation for Science, Spain

Magnetic shape memory materials: Scientific background and practical horizons

New multifunctional materials, called magnetic shape memoryalloys (MSMAs), comprise those off-stoichiometric Heusler-type X2YZ compounds (where X and Y are transition metals and Z belongs to the III-V group in the periodic table of elements), which exhibit martensitic transformation (MT) accompanied by a complex magnetic reordering. Due to strong interactions between structural and magnetic degrees of freedom in the vicinity of MT, they exhibiting giant properties, such as magnetic field induced strain, magnetoresistance, inverse magnetocaloric effect alongside conventional shape memory and superelasticity effects. These properties can be easily tuned by the composition variation, doping or heat treatments. MSMAs are cost-effective, rare-earth-element free and nontoxic. They can be conventionally divided into two major groups: ferromagnetic shape memory alloys (FSMAs), such as prototype Ni-Mn-Ga, especially suitable for actuation, and the metamagnetic shape memory alloys (MetaMSMAs), such as Mn-rich Ni-Mn-X (X=In, Sn, Sb), particularly important for magnetocaloric applications. Both types of materials are

capable to efficiently transduce the thermal, mechanical and magnetic energies into each other under conjugating fields producing cross-linked effects on both macro- and micro-(nano)scale. In this talk, we introduce the underlying physical mechanisms responsible for such energy conversions and the origin of the related performances of these materials. A broad range of the possible applications, such as actuation, sensing, energy harvesting and ferroic cooling will be reviewed

Speaker Biography

Volodymyr Chernenko has completed his PhD at the age of 26 years from Moscow State University, Russia. He is the Ikerbasque research professor at BCMaterials & University of Basque Country. He has 38 years of research experience in centres in Ukraine, Germany, Japan, Italy, United States, France, Switzerland, Australia, Spain, Hong Kong and Russia. He is the author and co-author of 14 patents and 315 original papers in ISI scientific journals and 5 book chapters with more than 8400 citations and h-index equal to 46 (Google Scholar). He is an International fellow awardee of the Helmholtz Association (Germany) since 2014. He is world-wide known as one of the founders of the new research area "Ferromagnetic shape memory alloys" being organizer and/or invited speaker of many International conferences.

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Van Kerckhove Gunther

OCSiAl Europe Sarl, Luxembourg

Tuball[™] single wall carbon nanotubes: Health, safety & environmental issues

The company OCSiAl is been founded in 2009 and is also the first SWCNT manufacturer who has completed his EU-REACH registration for a tonnage band of up to 10T/a and is planning to receive approval for a tonnage band up to 100T/y by the end of Q3/2019. At the end of the 2017 we achieved our signed consent order with the EPA that allows us to import up to 25T/y.

Because Tuball[™] is used and also tested in various applications on an ongoing basis, also receiving a lot of interests worldwide. That is why it is obvious that the company OCSiAl is establishing the necessary regulatory and quality standards worldwide.

The first part of this presentation will aim at providing a short introduction of our Tuball[™] substance and his product line, a second part of the presentation will be about the morphology vs Health & Safety status, the third part is an overview about the status and plans of the ongoing registrations compliance. The fourth and last part of the presentation will focus on the health, safety and environmental aspects of our Tuball[™] substance and the different applications. As SWCNT manufacturer, OCSiAl is doing continues investments in improving our understanding of our different (new) Tuball products themselves and potential hazards through their (entire) life cycle. We are involved in generating additional test data and collaborating with industry associations and networks.

This presentation will describe the steps being taken by the company's H&S Lead manager, Van Kerckhove Gunther to successfully introduce our carbon nanotubes (SWCNT's) regulatory status and outline our (future) plans for numerous of studies and qualifying our TubalI[™] substance including the different kind of compositions

Speaker Biography

Van Kerckhove Gunther holds an engineer diploma in chemistry and plastic technology and Bachelor in Safety advisor (2005). With over 10 years of invaluable experience in SHEQ managing projects and resources in an effective and efficient manner. Highly focused with a comprehensive knowledge and understanding of various industries and sectors such as plastic engineering, automotive, trailer building, composite engineering/ development, chemical industry, logistics, Operational services and consulting. As a true professional he is always willing to challenge the status quo and improve on existing standards. Since June 2016 he joined the company OCSiAl as an H&S manager, responsible for the regulatory affairs worldwide.

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Raafat El-Hacha

University of Calgary, Canada

Strengthening concrete structures using shape memory alloy

Chape Memory Alloy (SMA) has been attracting the researchers **J**from different fields due to their superior properties. SMA is categorized as smart material with unique class of alloy for its ability to undergo large deformation as well as energy dissipation capacities while maintaining a superelastic response and returning to its original shape through stress removal (Super Elasticity) used for new construction or through heating (Shape Memory Effect "SME") used for strengthening applications. This presentation focuses on the use of SMA with the SME characteristics. The SME represents the ability of the SMA to recover its original shape after being deformed beyond the elastic limits through heating. The strain recovered in this transformation process can be utilized for prestressing applications. Therefore, by having the pre-strained SMA reinforcement (bars or strips) attached to the Reinforced Concrete (RC) members and then applying heat above the activation temperature the SMA will recover the inelastic strain and thus a presressing force will be developed in the RC member. In other words, the pre-strained SMA itself can be used as the supplementing prestressed reinforcement in flexural strengthening of RC beams/slabs by eliminating the use of specialized equipment such as hydraulic jacks. Another strengthening application is confining RC columns using SMA wires. This confinement technique relies on the recovery stress generated as the SMA wire transforms to its recovery (undeformed) state. The confinement methodology simply involves wrapping a pre-strained SMA wire along the perimeter of the column. Then, heating the wire using an electrical current above a predefined transformation temperature would trigger the SME of the SMA that allows the wire to return to its original state while a reactive force is created by the wires producing an active confinement pressure. Findings from many researchers added a valuable knowledge to the field of strengthening RC structures and widened the potential applications of the SMA in the structural engineering field.

Speaker Biography

Raafat El-Hacha is a Professor of Structural Engineering at the University of Calgary in the Department of Civil Engineering. His pioneer research has been recognized as pushing the boundary of knowledge in using innovative and smart advanced materials for strengthening existing structures and for new construction, such as fibre reinforced polymers (FRP), shape memory alloy, and ultra-high performance concrete for hybrid structural systems in bridge applications and other structures. He published over 220 journal and conference papers, co-authored 3 refereed design guidelines. Supervised and graduated 42 PhD and MSc students. Served as guest editor for 3 journals and edited/co-edited 8 conference proceedings. He is a Fellow of the International Institute for FRP in Construction (IIFC) and the Canadian Society of Civil Engineers (CSCE). He is the recipient of several awards and fellowships including the CSCE Casimir Gzowski Gold Medal, CSCE Excellence in Innovation in Civil Engineering Award, IIFC President's Award, Killam Professorship Award, Erasmus Mundus International Fellowship (twice) and many others for his outstanding academic and professional achievements.

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Marc BRUNEL

Rouen Normandy University, France Interferometric imaging for the characterization of ice particles and droplets in the atmosphere

The characterization of water droplets or ice particles in the atmosphere is important for aircraft safety and meteorology. Interferometric out-of-focus imaging offers an interesting solution: The technique allows indeed size measurements of both kinds of particles, leading to a possible estimation of Ice Water Content and Liquid Water Content. In this technique, liquid droplets generate two-wave interference patterns whose frequency gives the droplet's diameter. Ice crystal characterization is based on the analysis of speckle patterns. Prototypes based on interferometric particle imaging have thus been developed and tested in flight. In this lecture, the instrumentation developed to perform accurate size measurements will be described. The presentation will address:

(i) the principle of the analysis of speckle patterns for ice crystal sizing, (ii) the development of laboratory instrumentation around a freezing chamber, (iv) their combination to ice crystal growth simulation using phase field modelling, (v) the generation of programmable pseudo-particles using a Digital Micromirrors Device and (vi) design considerations for the realization of an airborne instrument.

Speaker Biography

Marc BRUNEL has completed his PhD in 1996 from Paris-Sud University, France. He is a Professor in Rouen Normandy University. He has published over 120 articles in International periodic journals. His domains of research in laboratory CORIA are interferometric imaging of particles, digital holography, laser / particle interaction, and laser metrology.

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Chang C Guo N and Yam KM

National University of Singapore, Singapore

Graphene based solid-state catalysis: From computational understanding to applications

raphene has attracted enormous interests due to its Jpotential applications in solid-state physics. Recently, it has been shown that graphene can also be used as excellent solid-state catalysts for various of chemical reactions, therefore opening new opportunities for graphene applications in solidstate chemistry. The pristine graphene itself is chemically quite inert. Consequently, the central issue in graphene catalysis is to activate graphene using practical physical or chemical ways. Many ways have been proposed to enhance reactivity of graphene such as doping graphene with metal impurity atoms, applying a modest mechanical strain in graphene, creating vacancy defects, and decorating graphene with functional groups. However, the real applications of graphene solidstate catalysts (GSSC) are still rather limited so far mainly due to the fact that all those proposed methods require the direct treatment of graphene, which is very difficult for large-scale fabrication in a controllable manner. In this talk, we proposed

a promising new way of activating graphene: To activate graphene by doping the underlying metal substrate with single atom impurities or vacancies. In this way, the direct treatment of graphene is no longer needed, therefore the large-scale industry applications become possible. More interestingly, the proposed method implies an unusual type of singleatom catalysts. We expect the results presented to stimulate new experiments and open new avenue for future design and applications of graphene-based single-atom catalysts.

Speaker Biography

Zhang C earned his PhD in Computational Physics in University of Florida, USA. Now, he is an Associate Professor for the department of physics and chemistry in National University of Singapore. He has published 80+ papers on reputable journals that have been cited over 4500 times, and his publication H-index is 28. Currently, he is the guest editor of Catalyst for the special issue "graphene based catalysis" and an editorial board member of scientific reports.

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Stasse M and Héroguez V

CNRS University of Bordeaux, France

Elaboration of double emulsion based polymeric capsules for fragrance

We aim at encapsulating fragrances made of a variety of lipophilic species to slow down their diffusion. Our strategy is to develop capsules by polymerizing the water intermediate phase of an oil-in-water-in-oil double emulsion. In other terms, our system consists in a direct emulsion of fragrance (O1) in a water phase (W) containing monomer, initiator and crosslinker. To obtain the double emulsion, this direct emulsion, stabilized by a hydrophilic surfactant, is itself dispersed in an external lipophilic solvent used in perfumery (O2) and stabilized by a lipophilic surfactant. Polymerization of the intermediate water phase aim at obtaining a 3D network. This strategy exhibits the following advantages over other nowadays proposed capsules: polymerization only takes place in the water phase owing to the solubility of the monomer and the obtained 3D network is supposed to play the role of an effective barrier limiting the diffusion of the inner lipophilic species towards either the external solvent or air.

Such a strategy implies combining formulation for the elaboration of the double emulsion using two antagonistic surfactants, a hydrophilic and a lipophilic one and polymerization of the intermediate phase. Insertion of the polymerizable

species in the double emulsion shall not destabilize it. Some monomers exhibiting interfacial affinity and interfering with the formulation of the double emulsion have to be avoided. By varying the nature of the monomers, the initiator to monomer ratio and the crossliknker to monomer ratio, capsules with high encapsulation efficiencies and with various mechanical properties have been obtained.

Speaker Biography

Schmitt V is a senior researcher. After a Ph-D in Strasbourg, she moved to Lund in Sweden for a post-doctoral position before getting hired at CNRS in Nancy with a permanent position. Since 1998, she is working at Centre de Recherche Paul Pascal in Bordeaux, France. Her research focuses on the elaboration and characterization of dispersed model systems like suspensions, emulsions and foams in view of addressing the link between structure and properties. She has a special interest on emulsions and foams stabilized by particles and on double emulsions. This presentation is part of a collaboration she continues with Héroguez V, a CNRS senior researcher too, specialized in the synthesis of nanoparticles (NPs) by Radical and Metathesis Polymerizations in dispersed media (suspension, dispersion, mini- microemulsions). She has high level expertise in Macromolecular Engineering. She has developed specific methods for producing polymeric NPs exhibiting controlled architecture, shape, and chemical composition. In particular, pH and thermosensitive NPs have been designed in order to allow release of active molecules with spatiotemporal control.

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Raafat El-Hacha

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Flexural strengthening of concrete structures using prestressed fibre reinforced polymers

ibre reinforced polymers (FRP) reinforcement has been used for flexural strengthening either as an externally bonded (EB) system in the form of FRP laminate (sheets, plates or strips) applied to the soffit tension side of the reinforced concrete (RC) members or as a near-surface mounted (NSM) system in the form of FRP strips or bars embedded inside a pre-cut groove into the concrete cover at the tension side of the RC member filled with epoxy adhesive. Although flexural strengthening using non-prestressed FRP reinforcement can remarkably increase the ultimate strength of a member, it does not significantly change the behaviour of the member under service loads or substantially increase the stiffness of the member. It should be noted that in non-prestressed FRP strengthening application only a portion of the strength of the FRP reinforcement is effective and the system is a passive strengthening technique that remains inactive until additional loads are applied. To achieve an increase in the stiffness of the member, the strengthening system must be active rather than passive. Thus, to improve the efficiency of the system, the FRP reinforcement should be prestressed before being bonded to the concrete. Therefore, by prestressing the FRP, the material is used more efficiently because a greater portion of its tensile capacity is employed, and it contributes to the load-bearing capacity under both service and ultimate conditions. Prestressing the EB and NSM FRP reinforcement requires a special anchorage system that should be practical in implementation. In general, prestressing is used to enhance the flexural behaviour of reinforced concrete members under service loads especially in bridges and (or) beams that have large spans and there is a limitation on the



deflection and serviceability conditions. Because of their high tensile strength properties, FRP materials have great advantages for use in prestressing and post-tensioning strengthening applications. The specialized application of prestressing the FRP reinforcement for flexural strengthening of structures combines the noncorrosive and lightweight benefits of the FRP reinforcement with the advantages associated with external prestressing. However, the challenging part of the active FRP strengthening system is the application of the prestressing force to the FRP material using appropriate practical anchorage and prestressing system. A comprehensive review on the techniques and anchorage systems developed to prestress the EB and NSM FRP with the focus on the practicality of the prestressing systems where the FRP is prestressed against the member itself, and the performance of members strengthened using prestressed FRP reinforcement are discussed in this presentation.

Speaker Biography

Raafat El-Hacha is a Professor of Structural Engineering at the University of Calgary in the Department of Civil Engineering. His pioneer research has been recognized as pushing the boundary of knowledge in using innovative and smart advanced materials for strengthening existing structures and for new construction, such as fibre reinforced polymers (FRP), shape memory alloy, and ultra-high performance concrete for hybrid structural systems in bridge applications and other structures. He published over 220 journal and conference papers, co-authored 3 refereed design guidelines. Supervised and graduated 42 PhD and MSc students. Served as guest editor for 3 journals and edited/co-edited 8 conference proceedings. He is a Fellow of the International Institute for FRP in Construction (IIFC) and the Canadian Society of Civil Engineers (CSCE). He is the recipient of several awards and fellowships including the CSCE Casimir Gzowski Gold Medal, CSCE Excellence in Innovation in Civil Engineering Award, IIFC President's Award, Killam Professorship Award, Erasmus Mundus International Fellowship (twice) and many others for his outstanding academic and professional achievements.

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Qi Zhang Biaolin Peng

Cranfield University, UK

Thermal strain induced large electrocaloric effect of relaxor thin film on LaNiO₃/ Pt composite electrode with the coexistence of nanoscale antiferroelectric and ferroelectric phases in a broad temperature range

Ferroelectric/antiferroelectric thin/thick films with large electrocaloric (EC) effect in a broad operational temperature range are very attractive in solid-state cooling devices. We demonstrated that a large positive electrocaloric (EC) effect (maximum $\Delta T \sim 20.7$ K) in a broad temperature range (~110 K) was realized in Pb_{0.97}La_{0.02}(Zr_{0.65}Sn_{0.3}Ti_{0.05})O₃ (PLZST) relaxor antiferroelectric (AFE) thin film prepared using a sol-gel method. The large positive EC effect may be ascribed to the in-plane residual thermal tensile stress during the layer-by-layer annealing process, and the high-quality film structure owing to the utilization of the LaNiO₃ /Pt composite bottom electrode. The broad EC temperature range may be ascribed to the great dielectric relaxor dispersion around the dielectric peak because of the coexistence of nanoscale multiple FE and AFE phases. Moreover, a large pyroelectric energy density (6.10 Jcm⁻³) was harvested by using

an Olsen cycle, which is much larger than those (usually less than 10⁻⁴Jcm⁻³) obtained by using direct thermal-electrical, Stirling and Carnot cycles, etc. These breakthroughs enable the PLZST thin film an attractive multifunctional material for applications in modern solid-state cooling and energy harvesting.

Speaker Biography

Qi Zhang is an academic staff at Cranfield University and a visiting professor at Wuhan University of Technology. He joined Cranfield University as a research fellow in 1996 following the completion of a PhD at Monash University in Australia. He is a fellow in IOM3 and has sat on the EPSRC Peer Review College since 2006. He became a Senior Research Fellow in 1998 and then Senior Lecturer in 2007. He is currently supervising PhD students from the UK, EU, China, Iraq and Thailand. He has a strong background in ferroelectric thin and thick films and their applications in ferroelectric memory, pyroelectric and electrocaloric effect in the synthesis of nanofunctional materials and their applications in ink-jet printing, surface modifications and nanomaterials for energy storage, etc.

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Andrei N Salak

University of Aveiro, Portugal

Multifunctional layered double hydroxides

ayered Double Hydroxides (LDHs) are composed of the alternating positively-charged mixed metal (typically, MII-MIII) hydroxide layers and the interlayers occupied by anions and water molecules. The metal cations in the layers are coordinated by O-H units forming 2D structures in which the oxygen octahedra are edge-linked. LDHs find a wide use in catalysis and as anion exchangers and adsorbents. Magnetic, luminescent and others) cations in the hydroxide layer due to their individual or cooperative phenomena can induce new effects and novel functionalities in these materials. The characteristic feature of such modified LDHs is that their physical and chemical properties are tuned by means of continuous variation of the anion content in the interlayer. Moreover, provided that at least one of MII and MIII is magnetic, a MII-MIII cation ordering can result in formation of various magnetic frameworks. In this respect, LDHs are convenient and unique objects for the experimental modelling of the 2D quantum magnets and other cooperative effects. Because of the layered nature, the LDH

crystallites are very anisotropic. Therefore, such objects are suitable for formation of arranged nanostructures. An ability of LDHs to intercalate anion-molecular complexes offers also the opportunity for a 2D arrangement of the species which are the independent functional units such as magnets, ferroelectrics, photovoltaics. Ordered arrangement of the functional units in interlayer are expected to result in enhancement of the respective effects and even to induce new effects.

Speaker Biography

Andrei N Salak completed his PhD in 1994 at the Institute of Solid State and Semiconductor Physics (Minsk, Belarus). In 2002, he received a post-doctoral position in CICECO - Centre for Research in Ceramics and Composite Materials at the University of Aveiro (Aveiro, Portugal). At present, he is an Invited Researcher at CICECO. He specializes in crystal structure determination and characterization dielectric and magnetic properties of inorganic solids, particularly perovskite-like materials and layered ion exchangers. He is a co-author of more than 100 papers in international peer-reviewed journals with over 1200 citations.

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Cefe López

Institute of Materials Science of Madrid, Spain Self assembled materials for photonic applications

Self-assembly comprises the bottom up techniques whereby mostly small objects (from atoms to microparticles) organize into larger architectures. Among those colloidal techniques are optimal for the fabrication of optical functionality structures like photonic crystals and photonic glasses. Complemented with templating, these techniques show immense potential since, further to the possibilities in morphologies reachable; they expand through the materials available.

One of the most relevant features of these systems, directly related with their photonic functionality is order. Order is a crucial ingredient for complexity, which turns a crucial ingredient for functionality.

In this presentation, some of the most relevant aspects of selfassembly and templating techniques paying special attention to the role of order; how to combat, create or control it and how to put it to use to obtain photonic functionalities have been reviewed.

Speaker Biography

Cefe López completed his PhD at the Universidad Autónoma de Madrid, Spain. Currently he heads a group (luxrerum.org) in the Materials Science Institute in Madrid that accumulates more than twenty years' experience in photonic materials. His work covers materials synthesis and optical properties with special emphasis in order and disorder and its impact in photonic properties of materials. His 150 publications have been cited over eight thousand times and has been serving as an editorial board member of reputed journals.

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Printability of polymers in additive manufacturing: The example of copolyester

he printability conditions of copolyester are investigated using different instrumental techniques such as infrared camera observations, Differential Scanning Calorimetry, Scanning Electron Microscopy, X-ray micro-tomography, and mechanical testing. The Fused Deposition Modelling (FDM) technique is used to fabricate various types of specimens for the purpose of assessing both the thermal and mechanical properties of copolyester. The optimal conditions for 3D printing of copolyester are determined based on the influence of dimensional scaling, printing temperature, and type of layups. Thermal behavior is determined by looking at the thermal cycling on both prints and rafts as a function of the process conditions. Tensile properties are measured for both the raw and printed copolyester and the loss in mechanical performance including stiffness, plasticity and failure is quantified with respect to the printing temperature. In addition, the microstructural arrangement is investigated using X-ray micro-tomography to reveal the nature, the extent, and the 3D arrangement of defects. Analysis of ruptured samples is performed using SEM analysis. The results reveal a significant non-linear effect of the printing temperature on the performance of copolyester. A complex microstructural arrangement of defects is revealed including a regular network of porous structure. The failure of printed copolyester is explained through SEM analysis by the combination of three different damage mechanisms. These results suggest a strong correlation between the observed thermal cycling and the mechanical performance of copolyester.

Speaker Biography

Guessasma S is a mechanical engineering scientist, a by-fellow of the Churchill College, University of Cambridge, UK. He is presently a senior scientist at INRA (France) conducting a research activity in the field of additive manufacturing of biosourced materials. He has a key interest on hot topics in mechanical engineering, processing and materials science. He has several contributions related to the microstructural interpretation of material performance, mechanical modelling, image analysis, and in-situ experiments. He has published over 100 papers in different research fields.

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