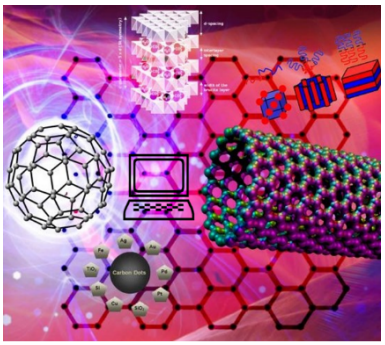
Bulgarian Academy of Sciences

Institute of Chemical Engineering

2ND SEMINAR

ON

INVESTIGATIONS, MODELING AND OPTIMIZATION OF NANOCOMPOSITES STRUCTURES



Book of Abstracts

2 APRIL, 2025

Institute of Chemical Engineering

Acad. G. Bontchev Str, Bl. 103, Sofia, Bulgaria

BULGARIAN SCIENCE FUND

The Organizing committee appreciates the financial support of Bulgarian National Science Fund, Contract № КП-06-Н57/3/15.11.2021 under the project: "Optimal safety loads and geometry for layered nanocomposites under thermo-mechanical loading"

Organised by

Institute of Chemical Engineering – Bulgarian Academy of Sciences, Sofia, Bulgaria

2nd Seminar on Investigations And Modeling of Nanocomposites Structures
Book of Abstracts
Sofia, 2025

Compiled by RaykaVladova,
Edited by Rayka Vladova, Tatyana Petrova

ORGANISING COMMITTEE

Prof. Dr. T. Petrova	Institute of Chemical Engineering
Assoc. prof. Elisaveta Kirilova	Institute of Chemical Engineering
Assoc. prof. Rayka Vladova	Institute of Chemical Engineering
Assist. Apostol Apostolov	Institute of Chemical Engineering
Alexander Moravski	Faculty of mathematics and informatics, Sofia University "St. Kliment Ohridski"

Chairman of the Organizing Committee

Assoc. prof. Rayka Vladova	Institute of Chemical Engineering

VENUE

Bulgarian Academy of Sciences,
Hotel of Bulgarian Academy of Science
50 "Shipchenski prohod" blvd
1113 Sofia, Bulgaria

FOR CONTACTS:

E-mail: r.vladova@iche.bas.bg
Phone: (+359-2) 979 34 81

SCIENTIFIC COMMITTEE

Prof. Dr T. Petrova	IChE-BAS
Assoc. Prof. Dr E. Kirilova	IChE-BAS
Prof. DSc K. Petrov	IChE-BAS
Prof. DSc V. Beshkov	IChE-BAS
Prof Dr.-Ing. W. Becker	TU-Darmstadt, Germany
Prof. DSc J. Ivanova	EPU, Pernik
Prof. Dr. P. Dineva-Vladikova	IM-BAS
Assoc. Prof. Dr. S. Parvanova	UACG
Assoc. Prof. Dr. S. Zheleva	Univ. A. Zlatarov-Burgas
Assoc. Prof. Dr. A. Georgieva	Univ. A. Zlatarov-Burgas
Assoc. Prof. Dr. P. Popova-Krumova	IChE-BAS

Scientific Secretary

Assoc. Prof. Dr. E. Kirilova	IChE-BAS

PLENARY LECTURES

Plenary Lectures PL-01

SH wave scattering by a nanocrack in a graded piezoelectric half-plane with nanorelief

Tsviatko Rangelov[1,*], Petia Dineva[2]

[1]Institute of Mathematics and Informatics, Bulgarian Academy of Sciences

[2]Institute of Mechanics, Bulgarian Academy of Sciences

e-mail: rangelov@math.bas.bg

Abstract

The presentation focuses on an exponentially graded piezoelectric (PEM) half-plane featuring a nanorelief along its surface boundary, which also includes a blunt nanocrack. The system is subjected to anti-plane time-harmonic elastic SH waves propagating at an incident angle in the nano half-plane. The model integrates the continuum mechanics approach with the Gurtin-Murdoch surface elasticity model, accounting for the surface elasticity properties of nanoobjects. An efficient, non-hypersingular traction boundary integral equation method (BIEM) is developed, verified, and applied in simulation studies. This method is based on an analytically derived Green`s function for a graded PEM half-plane. A parametric study illustrates the significant influence of factors such as material gradient magnitude, surface elasticity, nanocanyon and nanocrack characteristics, coupled electromechanical fields, and applied dynamic load properties on the amplitude of generalized stress concentration factors (GSCFs) near the nanocrack.

Keywords: PEM graded half-plane, nanorelief, nanocrack, Gurtin-Murdoch model, BIEM, dynamic GSCFF.

Acknowledgments

This work is partially supported by the Bulgarian National Science Fund, contract No КП-06-Н57/3/15.11.2021.

Plenary Lectures PL-02

Closed-form analysis of debonding initiation in multi-layered systems

Debora Linn, Wilfried Becker *

TU Darmstadt, Institute of Applied Dynamics, Darmstadt, Germany

e-mail: becker@fsm.tu-darmstadt.de

Abstract

In mechanical engineering, aerospace engineering and civil engineering, but also in nano-structures and nano-material design there are many situations where multilayer configurations occur. This can, for instance, be the case in the local overlap region of nano-structures and nano-materials where distributed nano-reinforcement particles are applied. Under given mechanical or thermal loading due to the dissimilar material properties typically stress concentrations will arise at the ends of the involved layers which might lead to the onset of debonding cracks and a subsequent debonding failure.

In order to assess such situations in the framework of linear elasticity theory a closed-form analytical approach is suggested based on layerwise displacement representations that take into account singular stress concentrations. From this by means of the principle of minimum potential energy an approximate closed-form description of the resultant deformation and stress distribution can be derived and validated by accompanying finite element calculations.

In order to assess potential failure in the framework of finite fracture mechanics debonding cracks of finite length are introduced and the corresponding incremental energy release is identified. Using the hybrid failure criterion suggested by Leguillon [1] then it can be clearly concluded whether such debonding failure will happen in reality or not. By a corresponding optimization problem also the minimal critical loading leading to failure can be determined. This is of high significance for the practical application.

Keywords:

Debonding initiation, closed-form analysis, finite fracture mechanics, hybrid failure criterion

References:

[1] Dominique Leguillon: Strength or toughness? A criterion for crack onset at a notch. European Journal of Mechanics – A/Solids 21 (2002) 61-72**.**

KEY LECTURES

Key Lectures KL-01

Optimal safety intervals for geometry and loads in polymer nanocomposites by multi-parameter optimization

Tatyana Petrova[1,*], Elisaveta Kirilova[1], Alexander Moravski[2],

Rayka Vladova[1], Apostol Apostolov[1]

[1]Institute of Chemical Engineering, Bulgarian Academy of Sciences,Acad. G. Bonchev Str., Bl.103, 1113 Sofia, Bulgaria

[2]Faculty of Mathematics and Informatics, Sofia University "St. Kliment Ohridski",5 James Bourchier Blvd., 1164 Sofia, Bulgaria

e-mail: tancho66@yahoo.com, t.petrova@iche.bas.bg

Abstract

The optimization problem for finding the optimal design (geometrical dimensions) and the optimal loading (mechanical and thermo-mechanical) for layered nanocomposite structures (NC) without delamination in them, is defined and solved. The optimization problem is multi-parametric (MOP) with single objective function; the nanocomposite geometry (length and layers' thicknesses) and the magnitude of static loading (mechanical or/and thermal difference) are considered as parameters and through MOP they vary in preliminary fixed technological limits; the NC material properties remain fixed constants. As an objective function (OF) in the MOP the analytical model criterion for "no delamination" in the NC is used. The OF is a function of the NC materials' properties and of the abovementioned parameters. The implementation of MOP is done by authors' developed programs, using metaheuristic Genetic Algorithm in Mathcad and in some cases, by alternative deterministic algorithm in Mathematica. The developed MOPs are applied successfully on distinct NC - graphene/SU-8/PMMA, graphene/MoS_2/PET, WS_2/SU-8/PMMA, Mxene/PMMA, and hBN/PMMA. The applied optimal values (or intervals of values) for the parameters are obtained for all considered case studies. It was checked that at these optimal values, the model interfacial shear stress (ISS) maximal value does not exceed the ultimate shear stress (USS) in the interfacial layer. The obtained results were also compared with the available literature data for the optimal values for some of the parameters in the considered case studies.

Keywords: multi-parametric optimization; nanocomposites; optimal loads; optimal design

Acknowledgements

The authors thanks for the financial support of the Bulgarian National Science Fund by contract No. КП-06-Н57/3/15.11.2021 under the project "Optimal safety loads and geometry for layered nanocomposites under thermo-mechanical loading".

Key Lectures KL-02

Producing and characterization of PtCoP alloy coatings on powdered carbon support

Jenia Georgieva[1], Angeliki Banti[2], Sotiris Sotiropoulos[2], Rositsa Mechkova[1]

[1]Rostislaw Kaischew Institute of Physical Chemistry, Bulgarian Academy of Sciences,

Sofia 1113, Bulgaria

[2]Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece

e-mail: jenia@ipc.bas.bg

Abstract

The development of effective catalysts for oxygen reduction reactions (ORR) is crucial for improving the performance of fuel cells electrocatalysts. Highly active carbon-supported PtCo/C nanocatalysts were successfully prepared by electroless deposition of a CoP coating with subsequent spontaneous galvanic replacement of $Co(OH)_2$ by more noble Pt. Pt metal is generally used as electrocatalyst in polymer electrolyte fuel cells (PEFC).The received active particles are uniformly dispersed on Vulcan XC-72 support with a narrow particle size distribution centered around 2-4 nm. The composition and surface morphology of the samples were characterized by scanning electron microscopy and energy-dispersive X-ray spectroscopy (SEM/EDS) and transmission electron microscopy (TEM). The electrochemical behavior of the PtCo/C composits was evaluated by cyclic voltammetry (CV). Linear sweep voltammetry (LSV) experiments were used to assess the catalytic activity towards the ORR. The Pt mass-specific ORR current density of the PtCo/C electrode is 28 mA mg^{-1} at an overpotential of η=380 mV, which is higher than that of both a commercial Pt/C catalyst (6.4 mA mg^{-1}) and a similarly produced PtCu/C electrode (7.6 mA mg^{-1}) [1], indicating the beneficial effect of even a small (<1% w/w) quantity of Co in the catalyst on Pt ORR activity.

References:

[1] Bart Geboes, Ioanna Mintsouli, Benny Wouters, Jenia Georgieva, Alexandros Kakaroglou, Sotiris Sotiropoulos, Eugenia Valova, Stephan Armyanov, Annick Hubin, Tom Breugelmans, Applied Catalysis B: Environmental, 2014, 150– 151, 249– 256.

Key Lectures KL-03

Low temperature synthesis of corundum ceramics and study of the effect of specially introduced nanoadditives

Adriana Georgieva, Margarita Georgieva*, Irena Markovska

Prof. Dr. Assen Zlatarov University Burgas, Faculty of Technical Sciences, Department of Chemical Technology, 8000, Burgas, Bulgaria

e-mail: margaritageorgieva727@gmail.com

Abstract

The present paper reports for the synthesis of finely porous corundum ceramics by the method of diffusion dominated solid state sintering at temperature relatively low for corundum materials - 1300°C, 1450°C and 1500°C, using specially introduced additives as follows: 3 mass % TiO_2, graphene nanostructures - 2 mass% GnP or 20 mass% G3 and nanosized Al_2O_3. The initial powders and the ceramics synthesized from them were characterized mainly by the methods of Infrared spectroscopy, X-ray phase analysis, Scanning electron microscopy. The results obtained from the studies carried out showed that the introduction of additives of definite type and quantity has certain e on the sintering temperature and the recrystallization processes. The X-ray phase analysis proved that the main crystalline phase in the ceramics synthesized from blends G1, A1 and C0 was corundum. The main functional groups present in the compositions of the ceramic samples synthesized were determined by FT-IR. Using SEM, it was proved that the introduced nano-additives initiated the formation of fine-grain and fine-pore structure with corundum grain sizes ranging from 0,2 to 2 μm. The decreased ceramics synthesis temperature, in this case, was mainly due to the additive TiO_2 (3 mass%) included in the initial blends and the high dispersity of the initial materials. The additives specially introduced in the ceramics obtained (TiO_2, G3, GnP, nano Al_2O_3) lead to a decrease of the synthesis temperature by 15÷25%. The corundum-based samples containing additives were studied to determine the more important physicochemical properties, e.g. water absorption (WA, %), apparent density (Papp, g/cm3) and apparent porosity (Papp, %).

Keywords: Corundum ceramics, Low temperature synthesis, Nano-additives, Graphene nanostructures

Acknowledgements

The authors wish the express their gratitude to the Scientific research institute at the University "Prof. Dr. Assen Zlatarov"- Burgas (contract No University Scientific Research Project - 498/2024) for the assistance provided for the realization of the present study.

Key Lectures KL-04

Multi-parameter optimization of layered Ti_3C_2 Mxene/PMMA nanocomposite under mechanical loading

Alexander Moravski[1,*], Tatyana Petrova[2], Elisaveta Kirilova[2], Rayka Vladova[2], Apostol Apostolov[2]

[1]Faculty of mathematics and informatics, Sofia University "St. Kliment Ohridski", 5 James Bourchier Blvd., 1164 Sofia, Bulgaria

[2]Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., Bl. 103, 1113 Sofia, Bulgaria

e-mail: alexmoravski@protonmail.com

Abstract

In this study, a methodology for finding the optimal safe values for the geometry and the magnitude of the axially applied mechanical load for a Ti_2C_3Mxene Mxene/PMMA layered nanocomposite (NC) was presented. First, the analytic solutions for the interface shear stress (ISS) in the middle layer of NC are obtained by applying the previously developed 2D method of the stress function and the minimisation of the strain energy. The solutions corresponded to two cases of NC geometry, physically answering to thinner or thicker layers in NC (here, noted by RR and CR respectively). Afterwards, a delamination criterion based on the model ISS is formulated for the purposes of the optimization task - no debonding in the NC. A multi- parameter optimization problem is defined with this criterion and 5 parameters: the magnitude of axial load and 4 geometric parameters – length and layers' thicknesses of NC. Then, Mathematica is used to compute and find the distinct combinations of optimal values of 5 parameters, which ensure no debonding in the Ti_2C_3Mxene/PMMA NC.

The results from the optimization show, that for each of the cases (RR or CR), the intervals of optimal safety values for 5 parameters are different. For RR (thinner case of NC) h_1 vary as (0.567nm÷1nm); respectively, (0.35nm÷0.783 nm) for h_1 in CR (thicker case of NC). For h_2 the intervals are (0.66μm÷1μm) for RR and (0.66μm÷20μm) – for CR. For ha they are (1nm÷14 nm) for RR and (1nm÷34 nm) for CR. For maximal possible axial load, at RR it varies as (0.193 GPa÷0.417 GPa) and for CR - as (0.385 GPa÷4.22 GPa). The graphics of model ISSs for the each of the obtained optimal combinations of 5 parameters are also different, but at all cases the maximal values in ISS distributions do not exceed the critical ultimate shear stress in the middle layer in the NC. The latter confirms independently the obtained optimization results; so, the proposed methodology can be used for the appropriate design in similar nanostructures and devices to ensure their safe operation without failure.

Acknowledgements

This study is performed by the financial support under the contract No. КП-06-Н57/3/15.11.2021 with Bulgarian National Science Fund for the project „Optimal safe loads and geometry for layered nanocomposites under thermo-mechanical loading ".

POSTER SESSION

Nanocomposites – experimental

Poster session NE-01

Calcium carbonate nanoparticles as a filler for gelatin-based biofilms: preparation, characterization and properties

Dimitrina Kiryakova[1,*], Antoniya Ilieva[2], Ganka Kolchakova[1]

[1]Department of Materials Science, Assen Zlatarov University, Y. Yakimov Str. 1, Burgas 8010, Bulgaria,

[2]Department of Chemical Technologies, Assen Zlatarov University, Y. Yakimov Str. 1, Burgas 8010, Bulgaria

e-mail: dskiryakova@abv.bg

Abstract

Gelatin-based biofilms filled with calcium carbonate nanoparticles synthesized from Rapana Venosa shells were prepared by the solvent casting technique. The content of nanoparticles in films ranges from 0.5 to 5.0%. The water content, water absorption, solubility in water, tensile properties, and biodegradation were investigated and compared with those of the control gelatin film. Results showed that the addition of nanofiller reduces the solubility in water and water absorption of the films with 5.0% of nano calcium carbonate by 58% and 64%. In contrast to the initial gelatin film, the incorporation of $CaCO_3$ nanoparticles into the materials, regardless of the amount, increases the values of the elongation at break. The reinforcing effect of nanofiller on the gelatin samples was found when 5.0% nanoparticles were added. These materials have a maximum tensile strength and Young's modulus of 7.16 and 70.3 MPa, respectively. It has been proven that nanoparticles make films more resistant and less susceptible to degradation after exposure to the surface of a compost soil for a period of 6 months and could be used to extend the service life of biofilms.

Keywords: calcium carbonate nanoparticles, gelatin, biofilms, solution casting, properties

Poster session NE-02

Synthesis and properties of Cu -doped fine dispersed ceramic pigments

Fila Yovkova*, Mariela Minova, Adriana Georgieva, Irena Markovska

Prof. Dr. Assen Zlatarov University Burgas, Faculty of Technical Sciences, Department of Chemical Technology, 8000, Burgas, Bulgaria

e-mail: fila_03@abv.bg

Abstract

The presented work investigates the synthesis and properties of fine dispersed ceramic pigments from the Al_2O_3 - SiO_2 system. The synthesis of the pigments was carried out by the solid-phase sintering method. As initial materials, were used both pure materials and waste raw materials – waste rice husks. In the first case, Al_2O_3 and $SiO_2.nH_2O$ were used as a pure initial materials. The more active, amorphous form of $SiO_2.nH_2O$ was chosen, instead of the crystalline form of silica. Rice husk is a waste product containing about 20% SiO_2. By burning rice husk in an oxidizing environment, the amount of SiO_2 increases significantly. For the purposes of the experiment, rice husk ash (RHA) with a 94.47% SiO_2 content, was used. The synthesis was carried out at temperatures of 1350 ^{0}C and 1400 ^{0}C with a 1-hour isothermal period. In both starting compositions - from pure and from waste raw materials, the amount of chromophore is 5% Cu. The chromophore of copper was introduced in the form of CuO. Fine dispersed gray pigments were obtained. The synthesized pigments from the Al_2O_3 - SiO_2 system were investigated by a number of methods - SEM, X-ray diffraction, Infrared spectroscopy, Color characteristics, etc. The results of scanning microscopy show that clusters of particles are formed. The color of the pigments was determined spectrally with a tintometer from the company Lovibond Tintometer RT 100 Colour. The pigments with the best color characteristics are those obtained from pure raw materials (Al_2O_3 and $SiO_2.nH_2O$) at 1400 ^{0}C for 1 hour - resp. (a) = - 3.6 and (b) = 5.6.

Keywords: Fine dispersed ceramic pigments, Cu-chromophore, Rice husk, Solid-state sintering, SEM

Acknowledgements

The authors express their gratitude to the Scientific Research Fund, Contract No. KP-06-N87/14 for the assistance provided in the implementation of this study.

Poster session NE-03

Synthesis and properties of Ni-doped fine dispersed ceramic pigments

Mariela Minova*, Fila Yovkova, Irena Markovska, Adriana Georgieva

Prof. Dr. Assen Zlatarov University Burgas, Faculty of Technical Sciences, Department of Chemical Technology, 8000, Burgas, Bulgaria

e-mail: minova_m@abv.bg

Abstract

This work aims to synthesize fine dispersed ceramic pigments by the solid-phase synthesis method. Two series of pigments were obtained – from pure and waste raw materials. In the first case, pure raw materials - Al_2O_3 and SiO_2 were used. The initial SiO_2 was introduced into the mixtures as amorphous $SiO_2.nH_2O$. An amorphous form of silica -$SiO_2.nH_2O$ was chosen because it is significantly more reactive than ordinary quartz sand and has a degree of particle dispersion in the range of 2÷7μm. In the second case, Al_2O_3 and oxidized rice husk ash (RHA) were used, which contained 94.47% of silica. The synthesis was carried out at temperatures of 1350 ^{0}C and 1400 ^{0}C with 1 hour of the isothermal period in a Nabertherm oven. The chromophore used was Ni, introduced into the mixtures as NiO. The amount of the chromophore was 5%. Fine dispersed pigments with a blue-green color were obtained. The synthesized pigments were studied by a number of methods - X-ray diffraction, infrared spectroscopy, DTA, etc. Using the CIELab system, which gives a numerical expression of the visual sensation of color, the basic color characteristics of the pigments were determined - color, brightness, color hue. The pigments synthesized from pure raw materials at 1350 ^{0}C had the best indicators, respectively (a) = - 15.2 and (b) = - 4.9.

Keywords: Fine dispersed ceramic pigments, Ni-chromophore, Rice husk, Solid-state sintering, CIELab system

Acknowledgments

The authors express their gratitude to the Scientific Research Fund, Contract No. KP-06-N87/14 for the assistance provided in the implementation of this study.

Poster session NE-04

Electrically-induced bending of electrically-poled flexible PVDF films

Todor Vlakhov*, Yordan Marinov, Angel Dimitrov, Georgi Hadjichristov,

Georgi Nadjakov

Institute of Solid State Physics, Bulgarian Academy of Sciences,

72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria

e-mail: todor_vlakhov@issp.bas.bg , todor1987@abv.bg

Abstract

Polarized flexible thin films (30 – 70 μm thick) of the ferroelectric and piezoelectric polymer poly(vinylidene fluoride) (PVDF) were fabricated by solution casting technique simultaneously with the application of a high-voltage (3 kV) static electric field (transversally to the films). The structural properties and the complex electrical impedance of the prepared films having electrically-induced electric dipoles were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), and optical microscopy. They were compared to the properties of PVDF films prepared under the same conditions but without a high-voltage field. The reverse flexo-electrical effect, i.e., the small mechanical changes after the application of an electric field (both direct-current, DC, and alternating-current, AC, in the frequency range up to 1 kHz) in the films that possess electrically-induced electric dipoles, was experimentally studied. The results obtained for the investigated films showed a clear electrically-induced bending at a threshold voltage of about 6 V of the electric filed applied perpendicularly to the films, as well as an increasing strength of this effect as the magnitude of the applied electric field increases. The method of electrical poling is feasible for production of thin flexible polymeric films that can bend upon relatively small voltage, thus being useful for relevant applications.

Acknowledgments

This work was supported by the Ministry of Education and Science of Bulgaria, through the National Research Fund of Bulgaria (research project "Liquid crystal nanocomposites for applications in photonics, sensors and biomedicine", No. KP-06-N58/6/2021). T. Vlakhov gratefully acknowledges the support by Bulgarian Ministry of Education and Science under the National Research Programme "Young scientists and postdoctoral researchers-2", approved by DCM 206/07.04.2022 (for the year 2025).

Poster session NE-05

Preparation of epoxy/ organoclay composites. Structural characterization of composites and study of their mechanical properties

Verislav Angelov *, Rumen Krastev, Todor Batakliev

Institute of Mechanics, Bulgarian Academy of Sciences

Acad. G. Bonchev St., bl.4, 1113 Sofia, Bulgaria

e-mail: v.angelov@imbm.bas.bg

Abstract

The present research aims to obtain epoxy composites with organoclay filler and to investigate some of their mechanical properties.

Epoxy composites were obtained by the method of "in situ" polymerization in the Laboratory "OLEM" at Institute of Mechanics-BAS and the mechanical characteristics (hardness and Young's modulus) were tested on a TIRA TEST machine. Epoxy composites with fillers - Cl-20A, Cl-30B, 1.44 P, 1.28 E, 1.31 PS have worse mechanical properties than neat epoxy resin. Composites with organoclay 1.34 TCN show slightly better mechanical properties, compared to pure epoxy resin.

The X-ray diffraction (XRD) measurements were performed on the organo-clay epoxy composites. The X-ray diffractograms were obtained using Bruker D8 Advance diffractometer with Cu Kα radiation (λ = 0.15418 nm) and LynxEye detector. Using the peak position (2θ) in the XRD patterns, the inter layer space was calculated through the Bragg's law: $n\lambda = 2d \sin\theta$, where λ is the wavelength of the incident wave (λ = 0.15418 nm), d is the spacing between the layers of organo-clay in the composites.

***Keywords**:* preparation, epoxy resin, organoclays, XRD

Poster session NE-06

Synthesis, characterization and application aspects of barium titanate-based ceramic samples with graphene nanostructures introduced

Adriana Georgieva*, Fila Yovkova, Krasi Panayotova

Prof. Dr. Assen Zlatarov University Burgas, Faculty of Technical Sciences, Department of Chemical Technology, 8000, Burgas, Bulgaria

e-mail: adriana_georgieva79@yahoo.com

Abstract

The share of research work aimed at finding innovative approaches to the synthesis of new porous ceramic products to be applied as filters for purification of waste waters, as adsorbents, heat-insulation materials and other components with high thermal resistance, as well as biomedical and catalytic substrates has recently increased. The present paper reports for the preparation of barium titanate based ceramic samples containing up to 2 mass% graphene nanostructures (graphene nanoplatelets GnP), synthesized by the method of solid-state sintering. The methods of X-ray diffraction, Infrared spectroscopy, Scanning electron microscopy and Light microscopy were used for the characterization of the initial blends and the titanate ceramic samples obtained from them. The results obtained from the analyses showed that the introduced nano-additive initiated the formation of fine-grain porous structure with grain sizes from 0.5 to 1 μm. Some basic physic mechanical properties of the samples synthesized were determined, e.g. water absorption (WA, %), apparent density (P_{app}, g/cm^3) and apparent (open) porosity (P_{app}, %). It had apparent density, close to the theoretical one - 5.51 g/cm^3, certain open porosity - 2.04 % and minimal water absorption - 0.37 %. Some aspects of their application are proposed.

Keywords: Ceramic samples, Barium titanate, Graphene nanostructures, Porous ceramic materials, Physic mechanical properties

Acknowledgements

The authors wish the express their gratitude to the Scientific research institute at the University "Prof. Dr. Assen Zlatarov"- Burgas (contract No University Scientific Research Project - 498/2024) for the assistance provided for the realization of the present study.

Poster session NE-07

Adhesive bond between dentin and nanocomposite material crowntec

Mariana Dimova-Gabrovska[1,*], Yoana Brusarska[1], Elisaveta Kirilova[2], Spartak Yanakiev[3], Dobrinka Damyanova[4] , Stefan Rangelov[1]

[1]Department of Prosthetic Dental Medicine, Faculty of Dental Medicine, Medical University – Sofia, 1 Sv. Georgi Sofiyski St., Sofia 1431, Bulgaria

[2]Institute of Chemical Engineering, Bulgarian Academy of Sciences, Academician G. Bonchev, B1.103, Sofia 1113, Bulgaria

[3]Medical College "Yordanka Filaretova" – Sofia, Medical University – Sofia, 3 Yordanka Filaretova St., Sofia 1431, Bulgaria

[4]Department of Pediatric Dental Medicine, Faculty of Dental Medicine, Medical University "Prof. Dr. Paraskev Stoyanov" – Varna, 55 Marian Drinov St., Varna 9002, Bulgaria

e-mail: marianadimova@abv.bg

Abstract

Introduction. A strong adhesive bond between materials and dentin is essential for the durability and effectiveness of fixed permanent restorations.

Objective. The aim of this study is to investigate, in a laboratory setting, the adhesive bond of specimens made of the nanocomposite material CROWNTEC and dentin using the adhesive system RelyX Unicem.

Materials and Methods. The test specimens were grouped according to their orientation during printing. In Group A, the normal vector to the surface formed an angle of 0º with the printing platform, in Group B – 45º, and in Group C – 90º. The specimens were bonded to dentin blocks using a thin layer of composite cement. The tests were conducted using a MultiTest 2.5-i universal testing machine. The shear bond strength testing device consisted of two metal plates sliding against each other in a single plane – a "frame" with an opening and a "knife". The test specimens were fixed in the stationary frame, with the cement bond positioned at the interface between the "knife" and the "frame".

Results. In the shear bond strength testing of hybrid material specimens bonded to dentin blocks using RelyX Unicem composite cement (3M), we found that the highest shear strength was recorded in Group C, with a result of 3.0 MPa, followed by Group A with 2.4 MPa and Group B with 2.0 MPa. The lowest result was observed in a specimen from Group B – 0.2 MPa.

Conclusion. The group with the highest shear bond strength was Group C, while the lowest shear strength was recorded at an angle of 45º. Therefore, the strongest adhesive bond is expected in areas with horizontally oriented material layers for each crown.

Keywords: additive technologies; adhesive bond; shear strength

Acknowledgments

This study was funded by the Medical University of Sofia, Bulgaria, GRANT № 132/29.05.2024.

Poster session NE-08

Wear resistance of nanocomposite structures

Mariana Dimova-Gabrovska[1], Yoana Brusarska[1], Elisaveta Kirilova[2], Dobromira Shopova[3], Dobrinka Damyanova[4], Stefan Rangelov[1,*]

[1]Department of Prosthetic Dental Medicine, Faculty of Dental Medicine, Medical University – Sofia, 1 Sv. Georgi Sofiyski St., Sofia 1431, Bulgaria

[2]Institute of Chemical Engineering, Bulgarian Academy of Sciences, Academician G. Bonchev, B1.103, Sofia 1113, Bulgaria

[3]Department of Prosthetic Dental Medicine, Faculty of Dental Medicine, Medical University -Plovdiv, Hr. Botev Bulv. 3, 4000, Bulgaria

[4]Department of Pediatric Dental Medicine, Faculty of Dental Medicine, Medical University "Prof. Dr. Paraskev Stoyanov" – Varna, 55 Marian Drinov St., Varna 9002, Bulgaria

e-mail: marianadimova@abv.bg

Abstract

Introduction. Research in the field of three-dimensional printing confirms its application in prosthodontics. The mechanical properties of nanocomposite materials should be comparable to those of natural dental tissues.

Objective. The aim of this study is to investigate, in a laboratory setting, the wear resistance of experimental nanocomposite specimens additively manufactured from CROWNTEC.

Materials and Methods. The test specimens were divided into groups based on their spatial orientation during printing. In Group A, the normal vector to the surface formed an angle of 0º with the printing platform, in Group B – 30º, in Group C – 60º, and in Group D – 90º. The tests were conducted using a "Sofia" chewing simulator. Factory-made silicon nitride spheres were used as antagonists, and distilled water was used as the liquid medium. The specimens underwent 50,000 cycles of chewing simulation. An analytical balance Mettler Toledo ME303 was used to measure the results.

Results. The specimen with the greatest mass loss after testing was from Group B, where the measured wear mass was 0.048 g. In Group A, the highest weight loss was 0.019 g, in Group C – 0.015 g, and in Group D – 0.011 g. The lowest material loss was recorded in Group D, where the specimen's weight before testing was 6.489 g, and after 48 hours in distilled water and chewing simulation, it was 6.487 g.

Conclusion. The lowest material loss was observed in Group D. Therefore, it is recommended that the layers during the printing of structures be positioned parallel to the printing platform for optimal wear resistance.

Keywords: additive technologies; wear resistance; nanocomposite materials.

Acknowledgments

This study was funded by the Medical University of Sofia, Bulgaria, GRANT № 132/29.05.2024.

Poster session NE-09

Optimal safe loading and geometry of layered nanocomposites, used for preliminary fixed prosthodontic appliances

Mariana Dimova-Gabrovska[1,*], Radina Moskova[2], Stefan Rangelov[1]

[1]Department of Prosthetic Dental Medicine, Faculty of Dental Medicine, Medical University – Sofia, 1 Sv. Georgi Sofiyski St., Sofia 1431, Bulgaria

[2]Faculty of Dental Medicine, Medical University - Sofia, St. Georgi Sofiiski 1, 1431, Sofia, Bulgaria

e-mail: marianadimova@abv.bg

Abstract

Introduction. Nanocomposites, used for the making of temporary restorations are and existential part of contemporary dental materials.
Aim: The aim of this systematic review is to categorise the most frequently used nanocomposites, used for the fabrication of provisional restorations on the basis of representative results from tests for flexural strength, elastic modulus measurement, etc.
Materials and Methods. A survey was conducted in English based on keywords in different articles in the following databases: PubMed, Google Scholar, Science Direct, and Scopus. A rigorous selection of the information collected for the systematic review was performed by implementing the Preferred Reporting Items for Systematic reviews and Meta-Analyses (PRISMA). Out of 141 scientific research articles 63 meet the inclusion criteria and are included in this article.
Results. The conducted survey indicates that some of the most frequently used laboratory tests of optimal safe loading and geometry are the tests for flexural strength, elastic modulus, etc. With the limitations of this survey, it can be deducted that nanocomposites have better mechanical and aesthetic qualities compared to conventional polymethyl methacrylate (PMMA).
Conclusion. The resistance of the nanocomposites to mechanical loads is greater compared to the resistance of conventional materials. It depends on the concentration and the combinations of nanofillers. This ensures safer and long lasting use in the manufacturing and application of provisional fixed prostheses.

Keywords: nanocomposites, provisionals, safe load and geometry.

Poster session NE-10

Structural properties of ion-conducting polymer-nematic liquid-crystalline nanocomposites with single-walled carbon nanotube additives

Todor Vlakhov, Georgi Hadjichristov, Yordan Marinov, Angel Dimitrov

Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria

We investigated the structural properties of flexible films (thickness about 50 μm) of nematic nanocomposites produced from nematic liquid crystals pentylcyanobiphenyl (5CB), polymer polyethylene oxide (PEO) complexed with the salt sodium metaperiodate ($NaIO_4$) as an ion donor, and by inclusion of single-walled cabon nanotubes (SWCNTs). The composition of the films was: 5CB:PEO weight ratio 70:30 wt.%, $NaIO_4$ 5 wt.%, and the concentration of SWCNTs was varied from 0 to 0.25 wt.%. The diameter and the average length of SWCNTs were 1.5 nm and 7 μm, respectively. The modifications of the properties of PEO-5CB-$NaIO_4$-SWCNTs films due to addition of SWCNTs at various concentrations were inspected. The microstructure of the films was characterized by polarizing optical microscopy, XRD and SEM. It was found an improvement in the morphology of PEO-5CB-$NaIO_4$-SWCNTs sodium-ion-conductive films due to the addition of SWCNTs. Such nematic nanocomposites have a potential for dielectric applications.

Acknowledgements: Work supported by the Ministry of Education and Science of Bulgaria (MESB), through the National Research Fund of Bulgaria (research project „Liquid crystal nanocomposites for applications in photonics, sensors and biomedicine“, No. KP-06-N58/6/2021). T. Vlakhov gratefully acknowledges the financial support by the MESB under the National Research Programme „Young scientists and postdoctoral researchers–2“ approved by DCM 206/07.04.2022, for the year 2025.

POSTER SESSION

Nanocomposites – modeling

Poster session NM-01

Analytical and numerical modelling of the behaviour of a concrete nanocomposite with a central crack under monotonically increasing temperature

Gergana Nikolova*

Institute of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria

e-mail: gery@imbm.bas.bg

Abstract

The analytical and numerical modelling of the behaviour of a concrete nanocomposite under monotonically increasing temperature is presented. The research methodology includes analytical modelling based on Linear fracture mechanics (LEFM) to determine the thermal stresses and Stress intensity factors (SIF) in a concrete nanocomposite with a symmetrically located central crack, considering the influence of both crack length and the temperature. The numerical solutions are obtained by using the specialized software product Wolfram Mathematica, including the generation of special macros to automate the calculations of the thermal stresses and temperature distribution in uncracked and cracked concrete composites, with or without the addition of nanoparticles. The obtained results show that for small cracks the difference between the SIF values of the two materials (concrete composite without/with 2% nano-SiO_2) is minimal, while for larger cracks the SIF value of the nanocomposite is significantly higher, but not too large, which preserves the relative stability of the material. The ordinary concrete is more brittle and susceptible to cracking due to its lower strength and elastic modulus, while concrete with added nanoparticles is more resistant to thermal and mechanical loads. It can withstand higher loads without reaching its critical failure point, which makes it a better choice for long-lasting and thermally resistant structures. The developed detailed mathematical models provide a convenient tool for analytical and numerical analysis that can be applied in the design of sustainable building materials.

Keywords: Concrete nanocomposite; Nano-SiO_2; Central crack; SIF; LEFM; Numerical results; Thermal stresses

Poster session NM-02

The influence of the crack geometry - length and orientation angle, temperature and nano-SiO_2 content on the behaviour of a concrete nanocomposites with a central crack

Gergana Nikolova*

Institute of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria

e-mail: gery@imbm.bas.bg

Abstract

In this work, the influence of temperature and nano-SiO_2 content (1%, 1.5% and 2%) on the Energy release rate (ERR) values in a concrete nanocomposite with a central symmetrically located crack was analysed. The study additionally considered the influence of the orientation angle (0°, 30°, 45°) and the crack length on the ERR value. A mathematical model based on Linear elastic fracture mechanics (LEFM) was developed to calculate the thermal stresses and ERR and the numerical simulations were performed in a software Wolfram Mathematica. Macros were generated to automate the analysis and to quickly assess the influence of the elastic modulus, crack geometry and Stress intensity factor (SIF) on the ERR value. The obtained analytical and numerical results show that the concrete with 1.0% nano-SiO_2 has the best balance between thermal cracking resistance and mechanical stability. With increasing percentage of nano-SiO_2 (1.5% and 2%), ERR increases, but the increase becomes significant at larger crack lengths. At high temperatures and cracks lengths with an angle greater than 30°, the ERR value is the largest, and the crack becomes unstable. The recommended optimal content of nano-SiO_2 in concrete is 1.0%, since the ERR value is the lowest and this helps to achieve thermal resistance and limits the propagation of the initial crack. The developed mathematical model can be useful in the design and optimization of high-temperature resistant structures made of concrete nano-SiO_2 composite materials.

Keywords: Concrete nanocomposite; 1%, 1.5% and 2% nano-SiO_2; Central crack; LEFM; Numerical results; SIF and ERR

POSTER SESSION

Nanocomposites - Optimization

Poster session NO-01

Aplication of Me-pan nanocomposite membrane in two-stage ultrafiltration of industrial wastewater

Milena Miteva[1], Violeta Raykova[2,*]

[1]Burgas State University "Prof.Dr. Assen Zlatarov", Burgas, Bulgaria

[2]Technical University of Sofia - Faculty and College of Sliven, Sliven, Bulgaria

e-mail: rmkpetrovi@abv.bg

Abstract

Membrane technologies and processes are an adequate technological opportunity to overcome modern industrial and ecological challenges regarding water resources. With this aim, the application potential of polyacrylonitrile (PAN) membrane and modified by a surface-deposited Fe-Cr-Ni nano layer (Me)-PAN membrane were investigated in the ultrafiltration process. The membranes were used individually and in combination for the purification of industrial wastewater from hydrodistillation of oil-bearing roses, containing 15.80 $mgEm_{KMnO4}$/ml total organics. The transport and separation characteristics of the membranes were determined according to changes in pressure and the manifestation of the response by their structural morphology. The range of changes in their permeability values reaches up to 19 $l/m^2.h$ for the unmodified membrane and up to 3.7 $l/m^2.h$ for the metallized one. The process is optimized by a combined approach, with ultrafiltration being carried out sequentially and continuously, in the following two stages: 1. Ultrafiltration through a PAN membrane to obtain permeate (P1); 2. Ultrafiltration of P1 with the Me-PAN membrane to obtain permeate (P2). It has been established that in the two-stage ultrafiltration the permeability remains the same for the 1st stage, but for the 2nd it reaches 13 $l/m^2.h$ at 0.5 MPa. The content of total organics in P2 is reduced to 1.74 $mgEm_{KMnO4}$/ml with a rejection and purification of wastewater to 89%. Thus, in addition to the rehabilitation of the treated wastewater, an opportunity is also offered for subsequent targeted utilization of the separated unique and valuable bio-resources contained in the wastewater from the processing of oil-bearing roses.

Keywords: Ultrafiltration, Metal nano layer coating, Nanometalized polymer membrane, Nanocomposite membrane, Industrial wastewater treatment, Recovery of bio-resources

Poster session NO-02

Analysis of parameters influencing delamination in thermo-mechanically loaded graphene/polymer layered nanocomposites

Apostol Apostolov*, Tatyana Petrova, Elisaveta Kirilova, Rayka Vladova

Bulgarian Academy of Sciences, Institute of Chemical Engineering, Acad. G. Bonchev str., Bl.103, Sofia 1113, Bulgaria

e-mail: a_apostolov@iche.bas.bg

Abstract

BACKGROUND: The aim of this work is to predict analytically and determine the factors, influencing the interface delamination in layered graphene-polymer nanocomposite structures, subjected to external static thermo-mechanical loading. The considerable main factors are the geometry characteristics of the nanocomposite structure and the magnitude and type of external loading. The expected results will serve as a fast prognosis tool in the future experimental and model research on the graphene-polymer nanocomposite behaviour.

METHODOLOGY: Here, a 2D analytical modeling (stress-function variational method) of stresses and strain fields in 3-layered nanocomposites, subjected to thermo-mechanical loading, is used. In short, the applied method allows obtaining and solving analytically a differential equation of 4th order with constant coefficients, regarding the unknown axial stress function σ_1 in the first layer (nanolayer). Two types of analytical model solutions for the axial stress σ1 in the nanolayer are derived, with coefficients depending on the geometry of the three-layer nanocomposite, its material properties and external load. All other stresses, including interface shear stress (ISS) in the layers, are expressed by σ_1 and its derivatives. The criterion for the interface delamination in the structure is defined, where USS is the ultimate shear stress of interface (adhesive) layer. The parametric analysis of the factors, influencing interface delamination, has been performed and investigated for 3 numerical examples of combine loaded graphene-polymer nanocomposites: graphene/SU-8/PMMA, graphene/SU-8/PET, graphene/MoS_2/PET. The factors under consideration are: layers' thicknesses, layers' length, and magnitude of external load – mechanical and thermal one. All calculations of ISS and respective parametric analysis are done by authors developed Mathcad programs.

RESULTS: It has been found, that the factor with the strongest effect on delamination is the magnitude of the applied external mechanical load. The next influencing factor is the geometry of the nanocomposite structure and, in particular, the thicknesses of the layers comprising the considered nanocomposite structures. According to the degree of influence, they can be arranged in the following order – thickness of the polymer matrix, thickness of the graphene layer, thickness of the middle interface layer. The temperature has little effect on delamination. The least influence on the delamination has the length of the overlap zone. These results make possible to determine the significance of the factors, affecting the delamination in the investigated nanocomposite structures, given their wide and safety application as a part of various industrial devices, like smart electronics, sensors, etc.

Acknowledgment

This study has been carried out with the financial support of contract No. КП-06-Н57/3/15.11.2021 with Bulgarian National Science Fund.

POSTER SESSION

Nanocomposites synthesis, structure, properties and applications

Poster session NS-01

Degradation of synthetic dyes by the use of nanosized composite catalysts and microorganisms

Nadezhda Shukova[1,*], Nadia Armenova[1], Dzhamal Uzun[2], Adriana Gigova[2], Ognian Dimitrov[2], Mariela Dimtrova[2], Ljutzkan Ljutzkanov[1], Elena Razkazova-Velkova[1]

[1]Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 103, Sofia 1113, Bulgaria

[2]Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria

e-mail: nastemi1@abv.bg

Abstract

In recent decades, the pollution of water bodies by huge volumes of untreated industrial wastewater contaminated with organic dyes (e.g. paper, cosmetics, textiles, plastics, etc.) has been considered an ecological crisis with a dangerous impact. Wastewaters polluted with dyes are a major restriction for the sustainable development of many industries.

Azo dyes make up approximately 60 % of the total dye production per year. They are a class of synthetic chemical compounds characterized by their azo group (–N = N–) and complex aromatic structures.

A screening for an appropriate catalyst for azo dyes degradation was conducted among nanosized composite catalysts ZnO, TiO_2, ZrO_2 incorporated on a matrix of activated carbon and sole activated carbon. The TiO_2 is proved to be suitable for the process. The chosen catalyst is characterized by scanning electron microscopy, X-ray diffraction, EDS. Additionally the surface of the catalyst is detrmined by iodine adsorption. Experiments with different conditions with TiO_2 were carried on.

Methylene blue, Congo red, Methyl orange are used as model solution of dyes. The strain *Pseudomonas putida 1046* is used for bacterial degradation of the same dyes. This strain shows tolerance to the dyes up to concentrations of 250 mg/l. *P. putida* 1046 decolors Methylene blue and Congo red with concentration of 250 mg/l for 42 h up to 96% and 92% respectively. *P. putida* 1046 shows tolerance in the presents of TiO_2 so experiments for simultaneous microbial and catalytic degradation of Methylene blue were conducted. No synergetic effect was observed.

***Keywords*:** Nanosized composite catalyst ZnO-, TiO_2-, ZrO_2- catalysts, degradation of dyes, Methylene blue, Congo red, Methyl orange, Pseudomonas putida 1046

***Acknowledgments*:**

This research was funded by the Bulgarian National Science Fund, grant number KP-06-N67/6 from 12 December 2022.

Poster session NS-02

Nanosized ZrO_2 as a composite catalyst for oxidation processes

Nadezhda Shukova[1,*], Dzhamal Uzun[2], Adriana Gigova[2] , Ognian Dimitrov[2], Mariela Dimtrova[2], Ljutzkan Ljutzkanov[1], Elena Razkazova-Velkova[1], Konstantin Petrov[2]

[1]Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 103, Sofia 1113, Bulgaria

[2]Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria

e-mail: nastemi1@abv.bg

Abstract

Nanosized ZrO_2 composite catalyst is obtained on a biochar by a patented technology. It includes pyrolization with simultaneous activation of sunflower husks impregnated with the precursor of the catalysts. Additionally structured nanosized ZrO_2 composite catalyst is prepared on a carbon felt.
It is intended to use the catalysts for oxidation and electrooxidation processes mainly sulphide ions and synthetic dyes. The catalyst over sunflower husks is characterized by scanning electron microscopy, X-ray diffraction, XPS and BET. Additionally the surface of the catalyst is detrmined by iodine adsorption.
As electrocathalyst, electrodes are manufactured and investigated in model solutions with content 65 mg/l S^{2-} and 18 g/l NaCl by means of cyclic voltammetry, galvanostatic measurements and Tafel slopes. The electrodes are designed and optimized in terms of the amount of catalyst and binder (PTFE). The electrodes comprised of 40 mg/cm^2 of catalytic mass within the electrode exhibit a lower overpotential following the galvanostatic measurements.
Catalytical investigation with different conditions are carried on. The structured nanosized ZrO_2 composite catalyst is used for oxidation of sulfide ions and it is proved that it doesn't lose its catalytical properties after several cycles of experiments.

Keywords: Nanosized composite catalyst, structured composite catalyst, ZrO_2, oxidation processes

***Acknowledgments*:**
This research was funded by the Bulgarian National Science Fund, grant number KP-06-N67/6 from 12 December 2022.