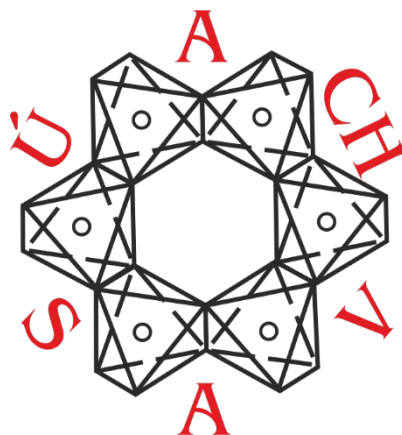


Súťaž mladých pracovníkov do 35 rokov
na ÚACH SAV Bratislava

Program



Bratislava, 19. 10. 2022

Program Súťaže mladých pracovníkov do 35 rokov

Ústav anorganickej chémie SAV v Bratislave, miestnosť č. 107

09:00 Zahájenie

09:05

Daniel Moreno – Halloysite interacting with two herbicides

09:25 Sanam Bashir – DFT-D3 study of the structural stability of montmorillonite clay with different polymers

09:45 Ramu Ambati – Corrosion of partially submerged samples in molten FLiNaK salt

10:05 Alper Güneren – Enhancing the electrochemical performance of silicon-graphite anodes for Li-ion batteries

Prestávka (10:25 – 10:35)

10:35 Dhiya Krishnan – The electrical conductivity of the molten systems $(\text{LiF}-\text{CaF}_2)_{\text{eut.}}-\text{NdF}_3$ and $(\text{LiF}-\text{NaF})_{\text{eut.}}-\text{NdF}_3$ as electrolytes for the neodymium electrowinning

10:55 Jakub Michalík – Preparation and characterization of Er^{3+} and Yb^{3+} doped YAlO_3 precursor powders and glass microspheres with optical properties

11:15 Mokhtar Mahmoud – Innovative Dye Sorbent Based on 3D Printing Technique

11:35 Florian Lemken – Long-Range Indirect ^{13}C - ^{31}P Coupling in Isostructural Nickel, Palladium, and Platinum Complexes

Prestávka (11:55 – 12:35)

12:35 Viktória Planetová – Aggregation induced changes in absorption and fluorescence spectra of cyanine dyes

12:55 Guido De La Torre – Study the use of diverse sintering additives in silicon nitride to improve their bioactivity

13:15 Naser Hosseini – Joining of silicon carbide ceramics for extreme environments

13:35 Akrity Anand – Copper-magnesium co-substituted mesoporous bioactive glass for bone tissue engineering

13:55 Bruno Wolfrum - Red emission enhancement of $\text{YAG}:\text{Eu}^{3+}$, $\text{YAG}:\text{Mn}^{4+}$ nanocrystals in YAG aggregates

14:30 Vyhlásenie výsledkov

Členovia komisie:

Ing. Blanka Kubíková, PhD. – predseda komisie

Mgr. Monika Tatarková, PhD. – člen komisie

doc. Ing. Mária Chromčíková, PhD. – člen komisie

Mgr. Stanislav Komorovský, PhD. – člen komisie

Mgr. Marián Matejdes, PhD. – člen komisie

Halloysite interacting with two herbicides

Daniel Moreno-Rodríguez*, Eleni Gianni, Ľuboš Jankovič, Eva Scholtzová and
Miroslav Pospíšil

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Abstract

The spiral tubular morphology of the halloysite mineral presents a large specific surface area, porosity, and high adsorption capacity on both surfaces. Thus, the halloysite can interact with pollutants like herbicides, e.g., the atrazine and diuron molecules that negatively affect the environment and animals. Therefore, the main aim was to study the immobilisation of the atrazine and diuron molecules by the halloysite tubular structure and the possible interactions on the different surfaces of this clay.

Force field methods were applied for the geometry optimisation and molecular dynamics using the COMPASS force field [1] on the atrazine-halloysite and diuron-halloysite models. Different herbicide loading ratios on the inner and outer parts of the halloysite structure were selected to find the preferable adsorption surface.

The simulations showed that the inner surface of the halloysite presented stronger interactions with both herbicides, especially with diuron (e.g., binding energies per atrazine and diuron molecules were 115 ± 2 and 130 ± 3 kJ.mol⁻¹, respectively) than on the outer surface. Besides, the herbicide's arrangement on both halloysite surfaces depended on the concentration and mutual interactions. Finally, increasing herbicide concentration on the inner surface was limited by free space and the adsorption capacity became gradually saturated for both atrazine and diuron.

Acknowledgements

Author is grateful to the Scientific Grant Agency VEGA (Grant 2/0021/19) and the Slovak Research and Development Agency (Grants APVV-18-0075 and APVV-19-0487).

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DFT-D3 STUDY OF THE STRUCTURAL STABILITY OF MONTMORILLONITE CLAY WITH DIFFERENT POLYMERS

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Abstract

In the last decade, advanced hybrid materials based on the clay minerals and polymers have been widely studied due to their unique properties. Clay-polymer hybrids gained considerable attention from researchers since the pioneering research of the Toyota research team on montmorillonite-filled Nylon 6 in 1980s¹. Polymer materials have some limitations, such as low mechanical strength, high solvent sensitivity, and low heat resistance. Clay minerals are used to overcome these limitations and enhance the performance of polymers². Clay-polymer hybrids provide remarkably improved mechanical, thermal, and gas barrier properties. Moreover, the use of clay-polymer hybrids in industrial and environmental applications are increasing due to their intrinsic properties³.

Montmorillonite (Mt) is the most usable clay from the smectite group as well as the beidellite, hectorite and saponite. The layered structures of smectites consist of two tetrahedral (T) and one octahedral (O) sheets connected through apical oxygens. The possible isomorphous substitution in the tetrahedral sheets by trivalent ions (e.g., Al³⁺/Si⁴⁺) and/or divalent ions in octahedral sheets (e.g., Fe²⁺, Mg²⁺/Al³⁺) generates a negative layered charge. It is compensated by the exchangeable interlayer cations, e.g., Ca²⁺, Na⁺, Li⁺, mostly hydrated⁴. The exchangeability of the interlayer cations, low cost, and abundance of the smectites are some of the advantages which makes them usable for clay-polymer hybrids⁵.

In the presented work, a detailed study of the structural stability of proposed models *via* intercalation energies and hydrogen bond interactions between montmorillonite and polymers were performed by the DFT-D3 method. The Perdew, Burke, and Ernzerhof (PBE) functional based on the generalized gradient approximation (GGA) theory was used for the description of the exchange-correlation energy⁵. The structural models of the hybrid structures of montmorillonite and pentamers units of polyethylenimine, Mt-PEI (Figure 1a), and Mt with poly(2-methyl-2-oxazoline), Mt-PMOx (Figure 1b), respectively, were examined. The DFT-D3 studies showed that both polymers are anchored onto the basal surface of Mt through moderate to weak bonds C_p-H...O_b hydrogen bonds. The experimental results of physicochemical characteristics of both composite materials are in good agreement with the theoretical results⁶.

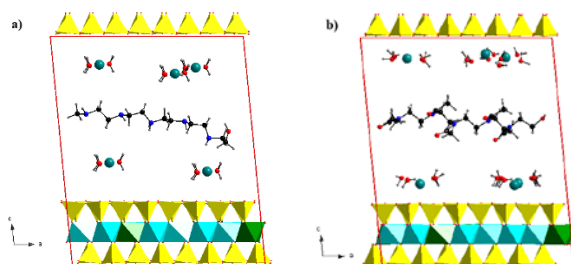


Figure 1. Initial structural models of a)Mt-PEI b)Mt-PMOx.

Acknowledgments:

This work was supported by grants from Scientific Grant Agency (project No. VEGA 02/0021/19) and Slovak Research and Development Agency (projects No. APVV-18-0075, APVV-19-0487)

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CORROSION OF PARTIALLY SUBMERGED SAMPLES IN MOLTEN FLiNaK SALT

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Abstract

This research, discusses the finding of corrosion phenomenon of SS316L, Incoloy-800H and Hastelloy-G35 in a partially immersed environment of molten FLiNaK salt, for a period of 100Hrs at 700°C. Both SS316 and Incoloy-800H alloy are recognised and certificated for high temperature application reactors. Therefore, it is essential to understand the corrosion resistance of these material in the molten FLiNaK salt environment. The results of the experiment the weight loss caused by the corrosion process followed by the progressive diffusion of F, K and Na into the sample metal and a progressive diffusion of alloying elements outward. The corrosion of the of the alloy shows the different mechanism in the corrosion process. Finally, the X-rd analysis of the salt show the different compound formed from the corrosion process.

ENHANCING THE ELECTROCHEMICAL PERFORMANCE OF SILICON-GRAPHITE ANODES FOR LI-ION BATTERIES

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Abstract

Increasing the lifetime along with the capacity of Si-based anodes have been challenging for researchers because of huge expansion problem of silicon up to 300% and various inputs of the system. The main aim of this study was to optimize the parameter for silicon-graphite anode and adaptation of newly synthesized alginate-based binders in order to enhance the electrochemical performance. In the first step, 20:80 wt% Si/Graphite powders which produced at different milling conditions was used to investigate the effect of powder properties on electrode behavior. It was found that powder with smaller crystallite size provides higher capacity due to more inner porosity. In second step, Dopamine alginate and sulfonated alginate were produced to assess the binder influence on capacity retention. FTIR was carried out to detect the new functional groups. The well investigated PVDF and CMC/SBR binder combination was used for a comparison. The weight ratio of active material, carbon black, and binder was 80:10:10. Anodes were prepared by coating N-Methyl pyrrolidone based (PVDF) and DI water based (other binders) slurries on Cu foil. The coated Cu foil was dried at 100°C under 150mBar in vacuum furnace, punched in circular electrodes of 18mm radius and assembled in Argon filled glove box. Tests were carried out between 0.01 and 1,5V vs. Li/Li⁺ potential window. 0.2C and 0.2/0.5/1/2/0.2C-rate was applied respectively for galvanostatic charging-discharging and rate capability test. It discovered that sulfonated alginate can stand with the expansion of Si, prevents the electrical contact loss and improves the discharging capacity around 600 mAh/g after 30 cycles.

The electrical conductivity of the molten systems $(\text{LiF}-\text{CaF}_2)_{\text{eut.}}-\text{NdF}_3$ and $(\text{LiF}-\text{NaF})_{\text{eut.}}-\text{NdF}_3$ as electrolytes for the neodymium electrowinning

Michal Korenko, Dhiya Krishnan, František Šimko, Priščák Jozef

ABSTRACT

The electrical conductivity of the systems $(\text{LiF}-\text{CaF}_2)_{\text{eut.}}-\text{NdF}_3$ and $(\text{LiF}-\text{NaF})_{\text{eut.}}-\text{NdF}_3$ has been investigated based on the principle of impedance phase shift measurements. The study deals with varying NdF_3 molar content (0%-20%) in molten $(\text{LiF}-\text{CaF}_2)_{\text{eut}}$ and $(\text{LiF}-\text{NaF})_{\text{eut}}$ mixtures. The conductivity of both measured systems increases with the temperature and decreases with the increasing content of NdF_3 . In addition, it was observed that the $(\text{LiF}-\text{CaF}_2)_{\text{eut.}}-\text{NdF}_3$ system exhibits lower resistivity when compared to the $(\text{LiF}-\text{NaF})_{\text{eut.}}-\text{NdF}_3$ system. The X-ray diffraction of the solidified samples were analysed after the conductivity measurements. This study establishes a more complete database for $(\text{LiF}-\text{CaF}_2)_{\text{eut}}-\text{NdF}_3$ and $(\text{LiF}-\text{NaF})_{\text{eut.}}-\text{NdF}_3$ systems and facilitates commercialisation of the investigated results within industries where high-temperature electrochemical applications find use. This investigation also expects to find useful information for the electrometallurgical applications for the possible electrowinning of the related rare earth elements (like Nd, Gd and Sm).

Preparation and characterization of Er³⁺ and Yb³⁺ doped YAlO₃ precursor powders and glass microspheres with optical properties

J. Michalík, B. Pecušová, J. Valúchová, M. Parchovianský, A. Prnová, R. Klement, D. Galusek

Keywords: erbium, ytterbium, yttrium aluminum garnet, SEM, sol-gel Pechini method, XRD

Yttrium aluminum garnet (Y₃Al₅O₁₂ – YAG) and yttrium aluminate perovskite (YAlO₃-YAP) doped with rare earth elements such as Er, Ce and Nd is quite often used to produce solid phase lasers. One of the major applications is Er doped YAG and YAP, which could obtain laser emission around 1500 nm though the ⁴I₁₃ → ⁴I₁₅ transition. However, this system has a drawback, that is the erbium shows a low absorption cross section that limits the pump efficiency. This is solved by co-doping the system with ytterbium ions since these ions shows a high absorption cross section and the absorption band is broader than the shown by erbium ions. Most of YAG and YAP materials are used in monocrystalline form. For this purpose, single crystals are grown for long periods at high temperatures (Czochralski method, Vernuli synthesis). Recently, polycrystalline materials prepared by sintering of precursor powder with different quality (level of homogeneity, particle size and uniformity), which depends on the preparation method (solid-state, precipitation, sol-gel) are also popular. However, even these procedures are technologically and financially demanding. As a solution the preparation of yttrium aluminate glasses by flame synthesis in the form of amorphous, glassy microspheres and subsequent HP sintering is offered.

In the present work, we describe the preparation of precursor powders with YAlO₃ composition, doped with different amounts of Yb³⁺ and Er³⁺ ions (Tab. 1). These powders were prepared by sol-gel Pechini method, and their quality was assessed by XRD, IR and Raman analysis. The amorphous nature of the prepared precursor powders was observed by XRD and IR spectroscopy after heat treatment at 550 °C. Partial crystallization of the prepared precursor powders was observed after heat treatment at 1000 °C. XRD analysis of partially crystalline samples show presence mainly YAG, YbAG and ErAG as majority phases. Samples contained also traces of crystalline Yb₂O₃, YAP and YbAP. In IR and Raman spectra of partially crystalline powders were observed typical metal-oxygen vibration in YAG, YbAG and ErAG. The powder precursors were further processed by flame synthesis into the form of glass microspheres. The optical properties of the prepared glass microspheres were monitored. The glass microspheres showed emission bands characteristic of erbium ions.

Tab.1 The list of prepared samples

Sample name	(Al ₂ O ₃) [mol.%]	(Y ₂ O ₃) [mol.%]	(Yb ₂ O ₃) [mol.%]	(Er ₂ O ₃) [mol.%]
YAPYbEr1	49,87	24,94	24,94	0,25
YAPYbEr2	49,95	24,97	24,97	0,10
YAPYbEr3	49,87	9,97	39,90	0,25
YAPYbEr4	49,95	9,99	39,96	0,10
YAPYbEr5	49,87	19,95	29,92	0,25
YAPYbEr6	49,95	19,98	29,97	0,10

Acknowledgment:



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Innovative Dye Sorbent Based on 3D Printing Technique

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ABSTRACT

Synthetic dyes are released in wastewater from different industrial outlets, such as paper, cosmetics, leather, printing, textile industries etc. Most of these industries utilize large quantities of dyes and release these dye contaminants into the environment as wastewater effluents. The objective of our work is to fabricate an efficient material for treating wastewater. Additive manufacturing (3D Printing) technologies enable the fabrication of objects with complex geometries in much simpler ways than conventional shaping methods. In the current study, we have applied stereolithography (SLA), which belongs to a family of additive manufacturing known as vat-polymerizations. All these machines are built around the same principle, using a light source, a laser or a projector to solidify a photosensitive resin into a hardened material. Pharmaceutical glass waste was milled and sieved below 40 μm . Fine glass waste was suspended in the photocurable resin with a solid loading weight of 55 wt%. Gyroid structures were printed with a layer thickness of 50 μm . After debinding, and sintering, the printed gyroids were immersed in 2.5 molars of sodium hydroxide for initiating alkali activation for 1 hour. The printed activated and non-activated gyroids were examined to adsorb methylene blue dye, and the adsorption efficiency of the printed glass gyroids was compared to other recent printed materials including titania, carbon, and ceramic filters.

Keywords: additive manufacturing; dye sorbents; glass waste; stereolithography; water treatment.

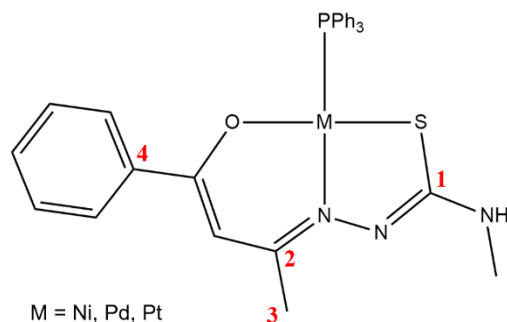
Long-Range Indirect ^{13}C – ^{31}P Coupling in Isostructural Nickel, Palladium, and Platinum Complexes

Florian Lemken, Victor M. Miranda, Olga L. Malkina

Abstract for Young Scientists Competition 2022

^{13}C – ^{31}P J -coupling is an important factor in the interpretation of ^{13}C -NMR spectra of phosphorus containing organic molecules. The high spin-polarisability of the phosphorus atom allows for intensive coupling with carbon atoms separated by several formal bonds (long-range coupling). This provides significant complications for correspondence schemes commonly used in the interpretation of ^{13}C -NMR spectra. Further, long-range couplings often transfer through a molecule along various paths not limited to coupling covalent bonds (“through-bond”), but also including “through-space” coupling in which electrons transfer magnetisation in absence of any formal bond (e.g. via lone-pairs). Theoretical analyses of coupling pathways [1] have aided several studies of long-range J -coupling (e.g. ref. [2]).

Three isostructural complexes of valence isoelectronic metals (cf. fig. 1) containing PPh_3 ligands were synthesised, and their ^{13}C -NMR spectra were measured. Therein, three long-range C-P-couplings were observed for the Ni & Pt system. The Pd system however featured one additional coupling. Given that the complexes are valence isoelectronic it is counterintuitive to observe one coupling only in one system, especially considering that this system is featuring the centre of middle size making relativistic effects an unlikely explanation. Furthermore, $^4J(\text{C3-P}) > ^3J(\text{C2-P})$ was found for all systems despite the clear expectation that the coupling intensity for vicinal carbon atoms would be lower for the atom further away from the common coupling partner.



Carbon	J_{CP} values (Hz)		
	Complex 1	Complex 2	Complex 3
1	$^3J = 18.2$	$^3J = 11.7$	$^3J = 10.2$
2	$^3J = 1.7$	$^3J = 3.3$	$^3J = 3.3$
3	$^4J = 3.3$	$^4J = 4.8$	$^4J = 4.2$
4	–	$^4J = 1.4$	–

Figure 1: 5-hydroxy-N,3-dimethyl-5-phenyl-4,5-dihydro-1H-pyrazole-1-carbothioamide triphenyl phosphine complexes and J -coupling constants / Hz between P atom and designated C atoms.

To explain both counter intuitive observations a theoretical analysis was performed in our group. This analysis started from visualising coupling pathways for observed C-P-couplings to identify the most essential structural elements for the transfer of magnetisation in the molecules, respectively. We investigated the effect of solvation implicitly and explicitly as well as the effect of internal dynamics at those structural elements with respect to J -coupling constants using highly accurate relativistic DFT methods. Our analysis indicates that the propagation includes intermediate “through space” coupling within an otherwise “through-bond” coupling path, which was never reported in the literature.

Acknowledgments:

We acknowledge VEGA (2/0135/21), APVV (SK-FR-19-0001 & APVV-19-0516), PHC Stefanik project SCALP, CRBFC's CHIMENE project, CNRS, PIA excellence ISITE-BFC program's COSMICS project, FEDER.

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AGGREGATION INDUCED CHANGES IN ABSORPTION AND FLUORESCENCE SPECTRA OF CYANINE DYES

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Keywords: Aggregation, TD-DFT, Cyanine dyes, spectral properties.

The aggregation of molecules and its effect on absorption and emission spectra has become a focus of research interest in recent years (Bujdák, 2018). The aim of this work was to elucidate the thermodynamics and optical properties of the studied systems using computational chemistry methods. Our research focused on aggregation, its mechanism, and its influence on absorption and emission spectra.

Two different cationic cyanine dyes; pseudoisocyanine (PIC), which several scientific groups have reviewed in the past (Würthner et al., 2011; Shindy, 2017), and oxocyanine dye (OxCy) have been studied. Using computational chemistry methods, we simulated the geometries and spectra of the monomers and two kinds of dimers: J and H dimers. We worked with the methods of TD-DFT (M062X, CAM-B3LYP, MN15, wB97XD) and ab initio (SCS-MP2). The results were then compared with experimentally measured spectra. The effect of aggregation on the absorption and emission spectra has been investigated.

We found that the vibration of the molecules was responsible for the presence of two bands in the absorption spectra of the monomer molecules of PIC and OxCy. We proved this statement by simulating the vibrationally resolved absorption spectra. In addition, we also focused on elucidating the mechanism of aggregation and investigating the various factors that influence this process (e.g., temperature and solvent). The effects of thermodynamics (enthalpy and entropy) on the formation of molecular aggregates have been investigated. We used the interaction or Gibbs energy as an indicator of the solution's stability and the percentage of each dimer. Simple approximate models, such as the monomer-dimer model, were used for thermodynamic calculations, as well as more sophisticated quantum-chemical DFT methods, with which we were able to individually analyse the Gibbs energy contributions and, based on this, to better understand the aggregation mechanism.

Gained knowledge helped to explain the unique photophysical properties of PIC and OxCy dyes adsorbed on the surface of layered silicate (Boháč and Bujdák, 2018).

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STUDY THE USE OF DIVERSE SINTERING ADDITIVES IN SILICON NITRIDE TO IMPROVE THEIR BIOACTIVITY.

Guido De la Torre Olvera

ABSTRACT

This work aims to enhance the bioactivity of inert surface of silicon nitride by using diverse sintering additives and applying two surface modification methods plasma etching and oxyacetylene flame treatment. Different kinds of sintering additives such as calcium silicate (CaSiO_3), calcium silicate and yttria ($\text{CaSiO}_3\text{-Y}_2\text{O}_3$), silicates as forsterite (Mg_2SiO_4), arkemanite $\text{Ca}_2\text{Mg}(\text{Si}_2\text{O}_7)$, and cerium oxide ($\text{CeO}_2\text{-CaSiO}_3$) were used to improve bioactivity properties of silicon nitride. Samples were sintered at temperature ranging from $1600\text{ }^\circ\text{C}$ to $1750\text{ }^\circ\text{C}$ using spark plasma sintering (SPS). The properties such as relative density, young modulus, hardness, fracture toughness and strength were measured to find out material with most promising mechanical properties. The surface of the samples were then treated with an oxyacetylene flame to develop a bioactive layer on the outer surfaces or, plasma etching were applied. In addition, other parameters which influence the formation of bioactive layer including nozzle distance, temperature, and flame time to evaluated. In vitro testing of Human pulmonary fibroblast cells, MRC5 was used to test potential cytotoxicity and cell viability for two weeks. As a result, methods used for surface modification was successful due to that proliferation of the fibroblast cells.

Joining of silicon carbide ceramics for extreme environments

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ABSTRACT

In this work, the joining of SiC ceramics with ZrSi₂ alloy and ZrSi₂-C powder mixture filler was investigated. The alloy was applied on the joining surfaces of the materials in the form of slurry, then the pressure-assisted joining was performed using Field Assisted Sintering Technology at different temperatures. The joints with pure ZrSi₂ showed a non-homologous interlayer, consisting of both ZrC and remaining ZrSi₂. In addition, a significant reaction with SiC substrate was observed, leading to a dissolution of SiC and infiltration of the filler into the base materials. When ZrSi₂-C filler was used, the uniform ZrC-SiC interlayer was formed by in-situ reactions between ZrSi₂ and C. The interfacial bonding between SiC materials and the strength of the joints was significantly improved with the increasing joining temperature.

Keywords: Joining, CVD-SiC, high-temperature ceramics, ZrSi₂

COPPER-MAGNESIUM CO-SUBSTITUTED MESOPOROUS BIOACTIVE GLASS FOR BONE TISSUE ENGINEERING

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ABSTRACT

Mesoporous bioactive glasses (MBG) are vastly investigated materials to repair, restore and regenerate osseous tissues owing to its bioactivity, nontoxic, biodegradability properties. The biological activities of MBG can be customized by adding therapeutics ions such as copper (Cu) and magnesium (Mg). The addition of therapeutics in MBG can provide more functionalities such as angiogenesis, osteogenesis and antibacterial characteristics. In this contribution Cu and Mg co-doped (1:1 ratio) MBG with nominal glass composition of $80\text{SiO}_2-(15-2x)\text{CaO}-5\text{P}_2\text{O}_5-x\text{CuO}-x\text{MgO}$ ($x=0.5, 1$ and 2 mol%), was prepared by sol-gel based evaporation induced self-assembly technique (EISA).

The compositional analysis of co-doped system characterized by ICP-OES techniques which confirmed the presence of dopant ions in requisite amount, although the amount of P_2O_5 was lower (<0.5 mol. %) for all the prepared glasses in respect of nominal compositions. XRD confirms the amorphous phase of glass while BET confirms the formation of high surface area for co-doped powders (~ 319 m^2/g) in contrast to control glass (~ 253 m^2/g).

All the MBGs powder showed apatite formation when immersed in simulated body fluid (SBF). XRD results confirms the formation of hydroxyapatite (HAp) layer on the surfaces of MBG after 7 days, while SEM images showed initiation of the formation of apatite after 1 day of soaking. The ionic extract of co-doped powders were cultured with MC3T3-E1 preosteoblast cells and normal human dermal fibroblast cells (NHDF). Both cells showed viability above 50% at MBG extract concentrations of 1 wt./vol.% or lower. Alkaline phosphatase (ALP) activity was performed using normal osteogenic medium and osteogenic medium supplemented with differentiation medium (such as ascorbic acid, beta glycerophosphate and dexamethasone). All co-doped system has enhanced in vitro differentiation and mineralization activity when supplemented with differentiation medium. For antibacterial result with sequential increase in Cu concentration the zone of inhibition for the bacteria is more prominent.

In conclusion, the co-doping of MBG powder (up to 2mol.%) showed improved bioactivity, biocompatibility and antibacterial effect and could be considered as promising materials for bone tissue regeneration applications.

Keywords: bioactive glass, hydroxyapatite, osteoblast cells

Red emission enhancement of YAG:Eu³⁺, YAG:Mn⁴⁺ nanocrystals in YAG aggregates

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ABSTRACT

The widespread substitution of fluorescent lighting by solid-state lighting in the last decade enabled important energy savings, going from 60 lm·W⁻¹ for a mercury vapour lamp to light-emitting diode (LED) lamps released last year achieving 210 lm·W⁻¹[1]. These new light sources generally lack in the orange–red part of the spectrum. Red radiation in common light fixtures demands harsh conditions for the synthesis of the emitting species, generally doped fluorides or nitrides. In addition, to improve the colour uniformity cast by the lamps, visible–light diffusers are blended in the resin containing the phosphors. Herein is proposed a combination of safer to synthesise phosphors and inclusion of the diffusers in the phosphor matrix, as an attempt to improve the optical properties. A blend of SiO₂ nanospheres acting as light scatterers and Y₃Al₅O₁₂ garnet (YAG) doped with Ce³⁺ ions is compared to an inclusion of such scatterers in the same matrix. Then, YAG:Eu³⁺ and YAG:Mn⁴⁺ powders are synthesised to study their viability as red emitters.

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