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# RÝCHLOSTNÁ KONŠTANTA PROPAGÁCIE STYRÉNSULFONÁTU SODNÉHO URČENÁ PLP-SEC TECHNIKOU

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Táto práca je zameraná na štúdium kinetiky propagačného kroku polymerizácie styrénsulfonátu sodného vo vodnom systéme, pričom doposiaľ o tom neexistujú žiadne štúdie, čo nás viedlo k preskúmaniu danej problematiky. Pulzná laserová polymerizácia (PLP), spojená s analýzou výsledného polyméru gélovou permeačnou chromatografiou (SEC), bola použitá na meranie rýchlostnej konštanty propagácie,  $k_p$ , SSNa vo vodnom rozpúšťadle, pri rôznych podmienkach polymerizácie, v koncentračnom rozmedzí monoméru od 5 do 20 hm. % a v intervale teplôt od 5 do 60 °C. Hodnoty rýchlostných konštánt propagácie SSNa vo vode priamoúmerne narastali so zvyšujúcou sa teplotou. V tejto práci bol použitý ako fotoiniciátor lítna soľ monoacylfosfinoxidu (Li-TPO). Hodnoty  $k_p$  vodných roztokov SSNa najprv narastali od koncentrácie 5 do 10 hm.% a od 10 do 20 hm.% dochádzalo k poklesu týchto hodnôt. Skúmaný bol taktiež vplyv prídavku soli na  $k_p$  polymerizovaného SSNa, pri ktorom boli použité soli alkalických kovov LiCl, NaCl, KCl, CsCl a LiBr, pričom hodnoty  $k_p$  rástli so zvyšujúcou sa koncentráciou soli v polymerizovanom roztoku. Aktivačné energie pre roztoky SSNa boli približne rovnaké a preexponenciálne faktory mierne klesali, avšak nebol viditeľný žiaden trend. Podobné výsledky Arrheniových parametrov boli pozorované u roztokov SSNa so soľou. Finálnym výsledkom tejto práce sú hodnoty  $k_p$  ako funkcia iónovej sily pre polymerizácie vodných roztokov SSNa a taktiež pre polymerizácie SSNa s prídavkom soli. Iónová sila narastala so zvyšujúcou sa koncentráciou SSNa. Podobný výsledok bol pozorovaný aj pre polymerizované vodné roztoky SSNa s prídavkom soli. Porovnaním výsledkov SSNa vo vodnom rozpúšťadle a styrénu v organickom rozpúšťadle sme zistili podstatné zvýšenie  $k_p$  pre polymerizácie SSNa vo vode, za čo sú zodpovedné vodíkové väzby prítomné vo vodných roztokoch. Týmito experimentálne zistenými údajmi sme prispeli k danej problematike určovania hodnôt  $k_p$  pre polymerizácie vo vodných systémoch a zároveň sme ju podrobne preštudovali. Táto práca vedie k novým otázkam ohľadom mechanizmu propagačného kroku, keďže výsledky nie sú úplne v súlade s teoretickým predpokladom rastúceho  $k_p$  so stúpajúcou koncentráciou úplne ionizovaných monomérov.

# INFLUENCE OF THE DYE SURFACE CONCENTRATION ON THE ENERGY TRANSFER EFFICIENCY IN SMECTITE COLLOIDS

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Hybrid colloidal dispersions were prepared from a synthetic layered silicate of saponite type (Sap) and cationic laser dyes, rhodamine 6G (R6G) and oxazine 4 (Ox4). The adsorption of dye molecules was confirmed by the changes in fluorescence spectra. Förster resonance energy transfer (FRET) was investigated using steady-state and time-resolved fluorescence (TRF) spectroscopies. The energy transfer occurred from R6G to Ox4 cations, playing the role of energy donor and energy acceptor respectively. The FRET efficiency increased with the concentration of the adsorbed dye molecules. Poisson probability density function was applied to model the characteristics of the dye molecules distribution on Sap particles. Using this model the expected values of FRET efficiencies were calculated. The theoretical and experimental results were in very good agreement. The theoretical model provides good tool to predict photophysical properties of the hybrid systems based on organic dyes and inorganic nanoparticles.

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# BILANČNÝ MODEL VÝROBY ČISTÝCH HOREČNATÝCH SOLÍ Z MAGNEZITU

Zuzana Fürdősová

Magnezit vo forme žiaruvzdorných materiálov, kovového horčíka, čistých horečnatých zlúčenín a kaustickej kalcinovanej magnézie, ktoré majú rozdielne chemické a fyzikálne vlastnosti, má svoje nezastupiteľné miesto vo svetovom aj slovenskom priemysle. Výroba kaustickej kalcinovanej magnézie a horečnatých zlúčenín je celosvetovo žiadaná, čo ovplyvnilo aj smerovanie mojej diplomovej práce. V práci som sa zamerala na prípravu čistých horečnatých solí, ktorá by bola založená na lúhovaní magnezitových surovín kyselinou chlorovodíkovou alebo octovou, na zostavenie bilančného modelu lúhovania a rafinácie výluhu a na štúdium vplyvu procesných faktorov na kinetiku lúhovania. Vychádzala som z prípravných pokusov, ktoré ovplyvnili voľbu vhodných podmienok, umožnili vypočítať spotrebu lúhovacích činidiel a vstupných surovín. Práca má poukázať na vplyv rozdielnych lúhovacích činidiel a na ekonomickú stránku procesu získavania horečnatých solí z magnezitu, najperspektívnejšej suroviny na našom území.

## MECHANICAL AND TRIBOLOGICAL PROPERTIES OF $Al_2O_3$ -MWCNTs COMPOSITES

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Alumina – multi-wall carbon nanotubes composites were prepared by new approach. This process comprises functionalization MWCNTs by acid treatment, stabilization of alumina-MWCNT dispersion with subsequent freezing has been used, which resulted in formation of granulated powder with homogeneous distribution of MWCNTs. This freeze granulation process makes it possible to retain the homogeneity of the aqueous suspension in granulated powders and make easy next processing. The ceramic composites were prepared by rapid hot pressing at 1550°C using these granulated powders. Uniform dispersion of carbon nanotubes in alumina matrix and full densification of composites are crucial requirements for improvement of electrical conductivity. However for improvement of mechanical and tribological properties is also important interfacial bonding between alumina and carbon nanotubes. In this work we investigated effect of content of homogeneously distributed MWCNTs on mechanical strength, fracture toughness and wear behaviour in rapid hot-pressed materials.

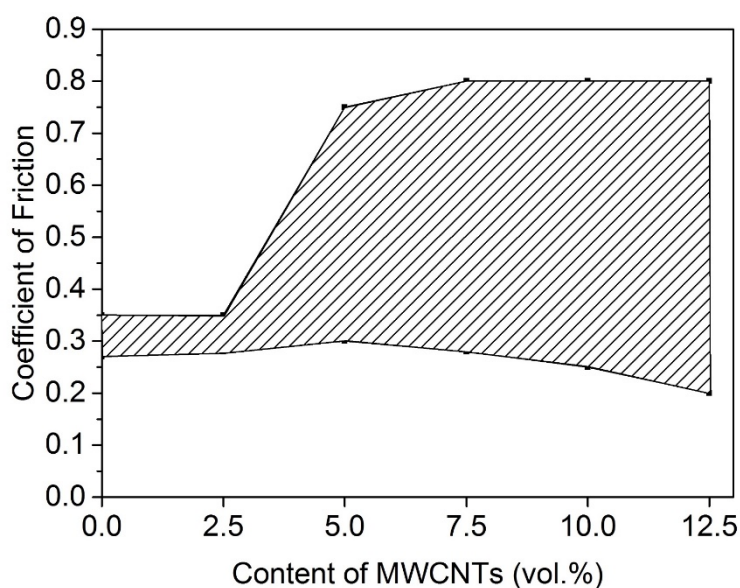


Fig.1: Coefficient of friction of Alumina-MWCNTs composites

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## BIOACTIVE SINTERING ADDITIVES OF SILICON NITRIDE

Michal Hičák

In this work we deal with preparation of dense silicon nitride based materials with bioactive properties. Pure silicon nitride is bioinert and we want to modify its properties to make it bioactive. Our tools are sintering additives and oxyacetylene torch. With combination of both we achieve a bioactive layer on the surface of silicon nitride ceramics.

## A CORROSION RESISTANCE OF TITANIUM DIBORIDE IN $\text{KF}-\text{AlF}_3-\text{Al}_2\text{O}_3$ MELT

Martin Kontrík

One of the major limiting factors in industrial applications of any structural material is its corrosion behaviour. The largest industrial application of molten fluoride salts is, by far, aluminium electrolysis (Hall-Heroult process). A newly proposed, eco-economic way, for aluminium production, based on the inert electrode system (for both, wettable cathode and inert anode) is expected to change current production process and make energy savings by a large margin at the zero emissions of  $\text{CO}_2$ . The Gibbs free energies calculations predestinate titanium diboride ( $\text{TiB}_2$ ) to be the candidate material for such a wettable inert cathode system.  $\text{TiB}_2$  is regarded as ideal for cathode material because of its excellent properties like its low electrical resistivity, wettability with molten aluminium and low solubility in aluminium. The scientific objectives of this work are therefore focused on the investigation of corrosion of a  $\text{TiB}_2$  ceramic in  $\text{KF}-\text{AlF}_3-\text{Al}_2\text{O}_3$  -based low-melting electrolytes. Before the corrosion testing the samples characterized in the terms of microstructure, density and porosity. The measured density agreed with the values provided by manufacturer and the  $\text{TiB}_2$  showed the overall porosity of about 6.7 %. A visual evaluation, after corrosion in  $\text{KF}-\text{AlF}_3-\text{Al}_2\text{O}_3$  (54.77–42.13–3.11 mole %) melt, at 680 °C, revealed only a few slight signs of corrosion. The corrosion attack was occasional and no time dependence has been detected. A pitting corrosion was found on the part of the samples, immersed in the melt. An average weight gain of about 4% was observed in all samples at all applied exposure times. This was caused due to a melt penetration into the open pores in the surface of ceramic material. The interaction between the material and the melt resulted into surface degradation, gradual dissolution of Ni-containing grain boundary phase, which eventually resulted in the dislodging of  $\text{TiB}_2$  grains and their gradual drift into the melt. The oxygen from the melt reacts with  $\text{TiB}_2$  to form  $\text{TiO}_2$  in orthorhombic „brookite“ form as the main corrosion product. Several unknown phases were observed in the melt. The MAS NMR spectroscopy confirmed that they contain aluminum in coordination 4, 5 and 6. Boron bonded in  $\text{BO}_3$  and  $\text{BO}_4$  was identified in the melt. It is expected the presence of aluminium oxoborate compounds as further corrosion products. The same result was observed by short-time experiment with a mixture of the same composition and addition 5 wt. %  $\text{TiB}_2$  of powder. The evolution of  $\text{BF}_3$  and its volatilisation form in the system was not confirmed.



# CHARACTERIZATION OF BENTONITE IN CONTACT WITH METALLIC ELEMENTS AFTER 18 YEARS OF IN SITU EXPERIMENT FEBEX

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The Deep Geological Repository (DGR) is currently the most accepted management option for the long-term isolation of High-Level Radioactive Wastes (HLRW). Based on a multi-barrier system (Engineered barrier system, EBS) in order to achieve the safety requirements for limiting the eventual release of radionuclides to the biosphere. This study aims to identify the geochemical and alteration processes induced in the bentonite by the corrosion of metal at the interface between bentonite and the metal barrier, present in the DGR gallery. The samples of bentonite come from the dismantling of the *in situ* Full-scale Engineered Barrier Experiment (FEBEX) in Grimsel (Switzerland). The samples cover different positions of the bentonite barrier to check the effect of saturation, heat and hydration on the observed geochemical processes (Fig.1). The XRD, TXRF, FTIR, SEM-EDS, ICP-OES, HPLC methods were used to examine the samples (CEC, solubility of ions, ability of exchange cations, iron absorption), and physical properties (e.g. BET and porosity).

The analysis of results revealed that the corrosion of the metallic elements has not generated significant changes in the properties of the bentonite, although, temperature and hydration seems to have a significant effect on the geochemical evolution of the interface and his alteration.

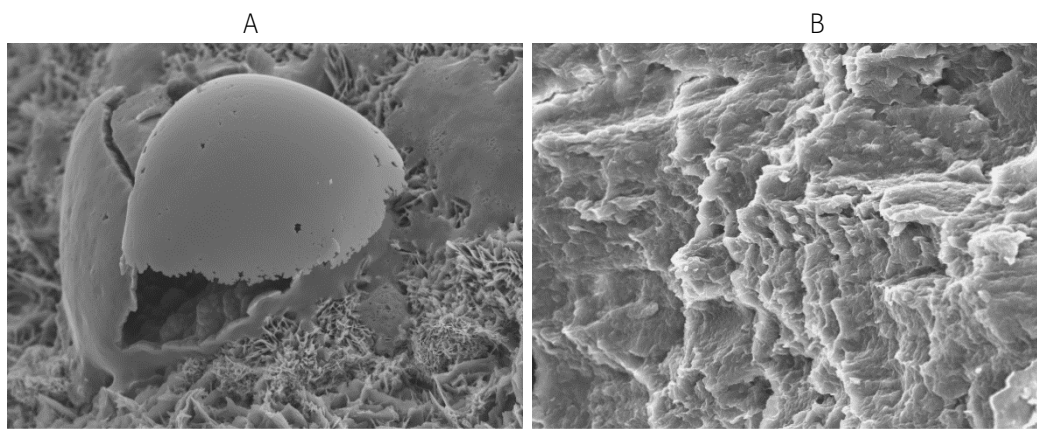


Fig.1. SEM-EDS images; A: Sample very close to the heater is showing the alteration in the interphase due to some ions (e.g. chlorine). B: Sample close to the granite barrier in the wettest part of the gallery is showing almost no corrosion, but indicating the probability of dissolution of the bentonite

## CORROSION OF ZIRCONIA – BASED DENTAL CERAMICS

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Excellent mechanical properties of zirconia-based materials combined with their superior aesthetics and biocompatibility characteristics have encouraged their application as bioceramics, particularly in the dental field. Ceramics made of zirconium oxide polycrystals stabilized in their tetragonal form by the addition of 3 mol% of yttrium oxide (denoted as 3Y-TZP) is a material of choice in advanced dental applications and dental implantology. However, past research on hip joints made from yttria doped zirconia ceramics revealed that this material was vulnerable to low temperature hydrothermal degradation (LTD), a phenomenon in which, due to the presence of water, the tetragonal – monoclinic phase transformation is triggered at the ceramic surface. This study investigated the effect of corrosion in acidic media and low temperature degradation (LTD) on yttria - stabilized zirconia (Y-TZP) commercial dental ceramics IVOCLAR, DOCERAM and a Ce-TZP based nano-composite material - LONGLIFE and its effect on ion leaching, phase composition and mechanical properties. Long – term exposure of commercial yttria-stabilized zirconia dental materials to acidic medium resulted in corrosion associated with leaching of yttrium from zirconia ceramics, partial destabilization of tetragonal zirconia and measurable increase of the content of monoclinic phase at the surface. This, in turn, increased susceptibility of the ceramics to low temperature degradation. Commercial dental ceramics IVOCLAR was the material least resistant to LTD. Based on these results a hypothesis has been formulated that corrosive attack of acidic media from regularly consumed beverages and food combined with poor mouth hygiene, or some health issues associated with excessive production of gastric acid may increase vulnerability of Y-TZP dental ceramics to LTD. However, to draw unambiguous conclusion, longer corrosion experiments are in progress.

**Keywords:** corrosion, low temperature degradation, dental implants, acetic acid, accelerated aging test.

## PREPARATION AND CHARACTERIZATION OF PRECURSOR DERIVED CERAMIC COATINGS WITH GLASS FILLER PARTICLES ON STEEL SUBSTRATE

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A novel environmental barrier coating system for steel consisting of a perhydropolysilazane (PHPS) bond coat and a polysilazane-based glass/ceramic composite top coat has been developed. Glass powders were added as filler materials in order to densify and seal the coatings at the temperatures of their application, to increase the coating thickness and to improve its adhesion to substrate. The slurry preparation as well as processing route, and microstructure of the coating system were optimised. After stabilizing the coating slurries, double layers consisting of a bond coat applied by dip coating and a top coat deposited by spray coating were prepared on stainless steel (AISI 441) substrates. The thermal treatment was performed in air at temperatures up to 900 °C. SEM investigation revealed the composite coatings composed of yttria-stabilized zirconia (YSZ), commercial barium silicate (G018-311, G018-385) and borosilicate (G8470) filler glass particles embedded in polymer derived ceramic matrix exhibited significant fraction of large closed pores with a diameter up to 40 µm, formed due to release of gases generated in the course of pyrolysis of the polysilazane. To reduce the porosity and the pore size of the coatings, powder precursor for the preparation of glass microspheres or glass microspheres prepared by flame synthesis were added as passive fillers. These formed a rigid skeletal structure in the coating, thus facilitating escape of gases during pyrolytic conversion of the organosilicon precursor. The optimized composite top coatings were prepared from the ceramic matrix forming polysilazane HTT1800 precursor (10 wt.%), filled with YSZ (41 wt.%) and a powder precursor ( $\text{Al}_2\text{O}_3\text{-Y}_2\text{O}_3\text{-ZrO}_2$ , 24 wt.%) as passive fillers. Commercial glasses G018-385 (12.5 wt.%) and G018-311 (12.5 wt.%) were added as sealing agents. After thermal treatment in air at 800°C, uniform and crack-free composite coatings on stainless steel with a thickness up to 100µm were prepared.

# THE INFLUENCE OF TEMPERATURE AND HEAD-GROUP STRUCTURE ON THE CONFORMATION OF THE SURFACTANTS INTERCALATED IN MONTMORILLONITE

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Keywords: near-infrared spectroscopy, organoclays, conformation, alkyl chain structure

Infrared (IR) spectroscopy became one of the main used techniques for characterization of organoclays. Their behavior and properties strongly depend on the structure and arrangement of the intercalated surfactants, most often alkylammonium cations, within clay mineral interlayers. The objective of this paper was to follow the effect of temperature and head-group structure on the ordering of surfactants with different alkyl-chain length. The samples were prepared from Na-montmorillonite (Mt) separated from the bentonite Jelšový Potok (JP, Slovakia) and alkylammonium ( $C_n-NH_3$ ) and trimethylalkylammonium ( $C_n-TMA$ ) cations. NIR spectroscopy in combination with a special diffuse reflectance cell allowing the *in-situ* measurement in the 25–400°C range was used for organo-montmorillonites (O-Mts) characterization. The NIR spectra of O-Mts showed the complex band in the 6100–5600  $cm^{-1}$  region related to the first overtone ( $2\nu_{CH}$ ) of the stretching vibrations of the  $CH_3$  and  $CH_2$  groups. The position of the  $2\nu_{as}CH_2$  component, observed in the 5820–5780  $cm^{-1}$  interval, reflected the ratio of disordered *gauche* and ordered *trans* conformers of the intercalated surfactants. To follow the effect of temperature on the alkyl chains ordering the C18-TMA, C18- $NH_3$ , C10-TMA, and C10- $NH_3$  samples were chosen. The O-Mts were heated up to 180°C to avoid deintercalation of the surfactants. Heating of the C18-TMA, C18- $NH_3$ , C10-TMA evoked an upward shift of the  $2\nu_{as}CH_2$  band position by 4, 3 and 3  $cm^{-1}$ , respectively, indicating the increased amount of disorder *gauche* conformers. In contrast, no change in the  $2\nu_{as}CH_2$  band position was observed for C10- $NH_3$ . Higher degree of disorder was found for all samples with  $-NH_3$  head-group compared to their counterparts with  $-TMA$  head-group.

# THEORETICAL STUDY OF SUBSTITUENT EFFECT ON THE HOMOLYTIC SE-H / TE-H BOND DISSOCIATION ENTHALPY (BDE) OF *para*-SUBSTITUTED BENZENESELENOLS AND BENZENETELLUROLS.

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**Keywords:** benzeneselenols, benzenetellurols, energetical state,  $\sigma$ -state,  $n$ -state, BDE

This work is focused on the theoretical investigation of two energetical states of phenoxy selenium and phenoxy tellurium radicals, namely  $\sigma$ -state ( ${}^2A'$ ) and the  $n$ -state ( ${}^2A''$ ). In this ongoing theoretical work, we also study BDE of *para*-substituted benzeneselenols and benzenetellurols in the gas phase. Calculated bond dissociation enthalpies are analyzed to shed light on the effect of the substituent located in the *para* position to selenium/tellurium atom.

The reactivity of organic radicals is of great interest because of the important role that these species play as reaction intermediates for example in organic synthesis and in the action of some powerful antitumor drugs. Benzeneselenol is among the most efficient radical traps known and plays a central role in radical reactions rate measurements. Selenium and tellurium compounds represent an important group of organic substances. They are a significant essential trace elements in the human body and also in organisms of other animals.

In this contribution we decided to study the BDEs of *para*-substituted benzeneselenols and benzenetellurols. Corresponding radicals were calculated for two lower-lying electronic states. First is  $\sigma$ -state ( ${}^2A'$ ), where the unpaired electron is almost fully localized on selenium/tellurium atom. In the second one, the  $n$ -state ( ${}^2A''$ ), is the unpaired electron partly delocalized into the benzene ring.

For calculations, we used Gaussian 09 program package. The geometries of all studied molecules and radicals were optimized using DFT/B3LYP/aug-cc-pVTZ approach with pseudopotential.

It turns out that the  ${}^2A''$   $n$ -state is the lowest-lying electronic state of both types of radicals. It is about 23 kJ mol<sup>-1</sup> more stable than the  $\sigma$ -state  ${}^2A'$  for benzeneselenol and 15 kJ mol<sup>-1</sup> for benzenetellurol. The first BDE of the benzeneselenol which corresponds to the lowest-lying state  ${}^2A''$  is calculated at 307 kJ mol<sup>-1</sup> with ROB3LYP/aug-cc-pVTZ approach. The second BDE (Se-H) value of  ${}^2A'$ , amounts to 330 kJ mol<sup>-1</sup> at the same level. For benzenetellurol, we have obtained BDE (Te-H) value of  ${}^2A''$  state 281 kJ mol<sup>-1</sup> and for  ${}^2A'$  state 296 kJ mol<sup>-1</sup> with ROB3LYP/aug-cc-pVTZ method. The electron donating (ED) groups such as OCH<sub>3</sub>, NH<sub>2</sub>, N(CH<sub>3</sub>)<sub>2</sub> in the *para* position tend to reduce the BDE (Se-H) values by 10–19 kJ mol<sup>-1</sup> for benzeneselenols and about 5–9 kJ mol<sup>-1</sup> for benzenetellurols. Electron withdrawing (EW) groups such as CN, CF<sub>3</sub>, NO<sub>2</sub> and MeSO<sub>2</sub> actually increase the BDE (Se-H) values by 6–10 kJ mol<sup>-1</sup> and the BDE (Te-H) values about 3–7 kJ mol<sup>-1</sup>.