



**Abstract Book
of the Central European Training School on
Neutron Techniques**



Budapest, 2021

Published by

Budapest Neutron Centre

ELKH Centre for Energy Research

URL: <https://www.bnc.hu/>
<https://www.ek-cer.hu/>

Abstract book of the Central European Training School on Neutron Techniques

<https://www.bnc.hu/cets/>

Edited by

Katalin Bajnok

Electronic edition

Budapest, 2021

ISBN: 978-615-01-3029-3



Table of contents

Oral presentations	1
O-01: Growth and In-field Behaviour of Rare-Earth Disilicates (<i>M. Islam</i>).....	2
O-02: Robustness of neutron guides (<i>P. Kárpáti</i>).....	3
O-03: Contributions to the study of different synthesis methods for biocompatible silver and gold nanoparticles (<i>L. Anda</i>).....	4
O-04: Characterization of pure and nickel doped manganese hexacyanoferrate cathode materials (<i>M. Maisuradze</i>).....	5
O-05: Structural investigations of 3D printed UV curable polymer-based sensors (<i>C. Mendes-Felipe</i>).....	6
O-06: Higher metal-insulator transition temperature and signature of second order magnetic phase transition in NdNiO ₃ nanoparticles (<i>S. Roy</i>).....	7
O-07: Monte Carlo modelling of the carbon-oxygen logging measurement (<i>J. G. Szűcs</i>).....	8
O-08: Aggregation of binary mixtures of sodium deoxycholate and sodium cholate in aqueous solutions with the addition of 6% propanol and 6% isopropanol (<i>V. Tepavčević</i>).....	9
O-09: Characterization of lanthanide environments in amorphous systems and investigation of chemical durability of conditioned radioactive waste (<i>I. Tolnai</i>).....	10
O-10: Neutron Bragg-edge tomography for phase transformation of metallic materials (<i>K. Van Tran</i>).....	11
O-11: Unveiling the Drug Delivery Systems using X-ray and neutron techniques (<i>F. Yokaichiya</i>).....	12
Poster presentations	13
P-01: Characterization of electronic waste with neutron and X-ray based techniques (<i>N. Buczkó</i>).....	14
P-02: Preliminary study of neutron spectra for “LvB” Compact Neutron Source (<i>H. Shuai</i>).....	15
P-03: Citrate coated superparamagnetic iron oxide nanoparticles for magnetically controlled immune therapy (<i>A. Nasser</i>).....	16
P-04: Etioplasts are more susceptible to salt stress than chloroplasts and etio-chloroplasts of wheat (<i>Triticum aestivum</i> L. cv. Mv Béres) (<i>R. Ounoki & R. Hembrom</i>).....	17
P-05: Investigation of the supramolecular organization of polyurethane-based multiblock copolymers using small-angle neutron and X-ray scattering (<i>A. A. Pavlova</i>).....	18
P-06: Monocomponent micelle formation of the cationic surfactant (1-tetradecyl)trimethylammonium bromide in the water solution containing Poloxamer 188 (<i>K. Popović</i>).....	19
P-07: E8 Spectra of Quasi-one-dimensional Antiferromagnet BaCo ₂ V ₂ O ₈ under transverse magnetic field (<i>K. Puzniak</i>).....	20
P-08: Study of protection and detection materials used in nuclear medicine: Case of ira-Therapy center, Gamma Camera and PET-Scan (<i>A. Radi</i>).....	21
P-09: Role of dopants on the phase stabilization and magnetism of Magnetic Shape Memory Alloys (<i>N. A. Río-López</i>).....	22
P-10: Quantitative detection of trace elements and heavy metals in coastal sediments using Neutron Activation analysis (preliminary results) (<i>P. K. Rouni</i>).....	23
P-11: Amino acid encoded Metal-Organic Framework Adsorbents for Heavy Metals (<i>A. Valverde</i>).....	24

4th October, 2021

Oral presentations

Growth and In-field Behaviour of Rare-Earth Disilicates

Manisha Islam^{1,}, M. Ciomaga Hatnean¹, G. Balakrishnan¹, P. Manuel², D. Khalyavin²,
F. Orlandi², J. Ollivier³, and O. Petrenko¹*

¹ Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom

² ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom

³ Institut Laue-Langevin, 71 avenue des Martyrs, F-38000 Grenoble, France

* manishaislam@gmail.com

The chemically complex rare-earth disilicates form seven different crystalline polymorphs and have been found to have luminescent and optical properties, giving potential for applications such as crystal scintillators and the detection of gamma and x-rays. Despite their interesting polymorphic properties, little is known of the magnetic properties of these compounds due to their complex structural phase diagram.

Here, both polycrystalline and D-type single crystals of the rare-earth disilicates have been synthesised via the floating zone technique [1], including D-type $\text{Er}_2\text{Si}_2\text{O}_7$. The D-type $\text{Er}_2\text{Si}_2\text{O}_7$ has a $P2_1/b$ space group, with the magnetic Er^{3+} ions located in a honeycomb-like distorted lattice. The most interesting behaviour is that the D-type $\text{Er}_2\text{Si}_2\text{O}_7$ orders magnetically below 1.8 K with a proposed four-sublattice antiferromagnetic arrangement of the magnetic moments [2]. In field, a significant increase of the magnetic unit cell was found with non-integer magnetic peaks indexed as $(0, k+1/2, l+1/2)$, $(0, k+1/3, l)$ and $(0, k+2/3, l)$, where k and l are integers. Further inelastic neutron scattering measurements on IN5 at the ILL agree with the previous zero field and in-field structure.

References

- [1] M. C. Hatnean, O. Petrenko, M. R. Lees, T. E. Orton, and G. Balakrishnan, *Cryst. Growth. Des.* 20, 6636-6648 (2020)
- [2] M. J. M. Leask, P. R. Tapster, and M. R. Wells, *J. Phys. C Solid State* 19, 1173 (1986)

Robustness of neutron guide systems

Péter Kárpáti^{1,2,}, Márton Markó¹*

¹ Neutron Spectroscopy Department, Centre for Energy Research

² Budapest University of Technology and Economics

* karpati.peter@ek-cer.hu

Neutron guide provides an effective tool for transporting neutrons over long distances as long as 150 meters. Neutron guides consist of typically 0.5 m pieces. In the reality the guide elements are not perfectly aligned. This misalignment has two effects. On the one hand, the surface normals have deviations from the optimal one (angular misalignment) as the neighbouring guide segments are tilted relative to each other. Moreover, the mismatch between the neighbouring guide elements causes a transport loss (positional misalignment). The impact of the angular misalignment is negligible compared to the positional misalignment. The influence of the imperfections on the brilliance transfer gets a progressively essential issue especially for long guides. The angular and positional misalignment results in loss in brilliance transfer. Previous studies have addressed this problem in order to estimate the magnitude of the misalignment but these treatments do not provide a general description or are mathematically unfounded. We propose a general, statistical, mathematically founded description of the geometrical imperfection of the guide structure based on theoretical considerations. Since the misalignment is given by the tolerance that the providers can accept, we assumed that the value of the misalignment has a top-hat distribution in between the positive and negative tolerance. Furthermore, since McStas simulation package cannot handle such effect like misalignment, the implementation of the misalignment into McStas is a crucial issue. A modified McStas component was created so that the different approximations of the misalignment can be compared to the result of the simulation and the impact of the misalignment on the guide performance can be determined for any shape guide system. We show the effect of the positional and angular misalignment in a few realistic guide systems by using a modified McStas component appropriate for modelling the guide misalignment.

Contributions to the study of different synthesis methods for biocompatible silver and gold nanoparticles

Anda Les^{1}, Daniela Pricop¹, Vasilica Tucureanu², Iuliana Motrescu³, Dorina Creanga¹*

¹ Alexandru Ioan Cuza University Physics Faculty, Iasi, Romania

² Grigore T. Popa University of Medicine and Pharmacy, Iasi, Romania

³ Ion Ionescu de la Brad University of Agricultural Sciences and Veterinary Medicine, Iasi, Romania

* les.anda@yahoo.com

In the last years, extensive research was done to develop innovative methods for synthesizing and functionalizing metal nanoparticles by employing bioactive compounds. Two great advantages were evidenced– the first one is related to the eco-friendly behavior of the synthesis by-products released into environment, while the second one is represented by the facilitated internalization of these nanoparticles if used as drug nano-carriers together with a lower nanotoxicity [1]. We approached: (i) the stabilization of colloidal gold nanoparticles (AuNPs) in lipid-chitosan coating by photoactivation; (ii) the stabilization of silver colloidal nanoparticles by using vegetal reducing-capping extracts.

(i) The functionalization of AuNPs, (synthesized by adapted Turkevich method), the organization of a lipid layer at the surface of the nanoparticles photoactivated in visible light followed by the addition of chitosan has determined the increase of their stability in colloidal suspension; thus, the blue shift of LSPR (localized Surface Plasmon Resonance) band suggests a size reducing as well as a decreasing in band intensity. The comparative analyses suggested a stronger binding of chitosan to the photoactivated nanoparticles compared to those that were not previously irradiated.

(ii) When biological reducing agents (green tea extract, lemon juice and mulberry extract) were applied in the synthesis of silver nanoparticles (AgNPs), the increase of the LSPR band intensity was recorded compared to citrate-based synthesis of similar silver nanoparticle [2]. The size of the most frequent nanoparticles is also supposed to be modified due to the spectral shifts of LSPR band corresponding to sodium citrate reduced AgNPs when lemon juice, green tea and mulberries extract were used. XRD and SEM-EDS analysis provided useful data in the characterization of crystallinity and granularity of the colloidal nanoparticle suspensions. Further analyses – TEM, AFM are needed to reveal with better accuracy the morphology and size distribution of the AuNPs and AgNPs. SANS (Small Angle Neutron Scattering) investigation is expected to provide more specific data on the structural features of the fluid samples synthesized by us.

References

- [1] A. Bhat, L. W. Edwards, X. Fu, D L. Badman, S. Huo, A. J. Jin, Q. Lu Appl Phys Lett. 109 (26) (2016) 263106
- [2] M. M. Alkhulaifi et al., Saudi J Biol Sci 27(12) (2020) 3434- 3441

Characterization of pure and nickel doped manganese hexacyanoferrate cathode materials

Mariam Maisuradze^{1,}, Min Li¹, Giuliana Aquilanti², Jasper Rikkert Plaisier², Corneliu Ghica³,
László Temleitner⁴, and Marco Giorgetti¹*

¹ Department of Industrial Chemistry "Toso Montanari", University of Bologna, Viale del Risorgimento 4, 40136 Bologna Italy

² ELETTRA Sincrotrone Trieste S.C.p.A., Elettra - Sincrotrone Trieste S.C.p.A., 34149 Trieste, Basovizza, Italy

³ National Institute of Material Physics (NIMP), Strada Atomistilor 405, Măgurele 077125, Romania

⁴ Budapest Neutron Center (BNC), 1121 Budapest, Konkoly-Thege Miklos st. 29-33, Hungary

* mariam.maisuradze3@unibo.it

Energy production as well as its storage is a complex and challenging task, especially nowadays, when the demand is constantly increasing. Batteries play a crucial role due to their ability to reversibly store and release energy when needed. Aqueous zinc-ion batteries (ZIBs) have a large perspective in this field, because of high abundance and safety of zinc, also metallic zinc is an ideal anode material with high theoretical gravimetric and volumetric capacity and low electrochemical potential. One of the promising cathode materials for ZIBs are Prussian Blue (PB) and its analogues (PBAs). They are a large family of transition metal hexacyanoferrates with general formula of $A_xM[Fe(CN)_6]_{y-1} \cdot zH_2O$, with open framework structure, redox-active sites and strong structural stability. Among simple PBAs, manganese hexacyanoferrate (MnHCF) has a high specific capacity and redox plateaus at high voltage. However, its severe crystal Jahn-Teller distortion effect, which affects its longterm cycling capability. Nickel is one of the elements which is used to relax the Jahn-Teller distortion in MnHCF. Also, the atomic radius of Mn is almost equal to the atomic radius of Ni, which means that with the replacement inside the structure, the framework will remain in the good order. In our group defective MnHCF and 10% and 30% nickel-doped MnHCF was synthesized.

According to the powder X-ray diffraction (PXRD) MnHCF has a monoclinic structure with space group: P21/n, while Ni-doped samples are cubic, with the space group of Fm-3m. However, with PXRD it is hard to identify the exact position of water molecules inside our material. Neutron powder diffraction (NPD) will be a useful tool in our study, because it has high sensitivity towards the light elements in the structures and it can help us to identify the position of water.

From MnHCF powder electrodes were made and coin cell batteries were assembled with metallic Zn as an anode and ZnSO₄ as an electrolyte. While electrochemical characterization on cycling voltammetry it was observed that certain reduction peaks were disappearing and new ones arising, which suggests of possible structural change. Later X-ray absorption spectroscopy also confirmed it by edge jump decrease of Mn edge and increase of Zn edge in aged electrodes, which can be as dissolution of Mn during cycling and Zn taking its place inside the structure. Neutron technics will be extremely useful here as well, as neutron beam carries no electric charge and has the ability of deeper penetration, so neutron scattering can be done on intact, exhausted coin cells, before dismantling them and detecting any structural changes in aged samples.

Structural investigations of 3D printed UV curable polymer-based sensors

C. Mendes-Felipe^{1,2,}, V.I. Petrenko^{1,3}, S. Lanceros-Mendez^{1,3}, M. Sangermano²*

¹ BCMaterials, Basque Centre for Materials, Applications and Nanostructures, 48940 Leioa, Spain

² Dipartimento di Scienza Applicata e Tecnologia (DISAT), Politecnico di Torino, 10129 Torino, Italy

³ Ikerbasque, Basque Foundation for Science, 48009 Bilbao, Spain

* cristian.mendes@bcmaterials.net

Multifunctional composites are essential for a large variety of applications, including printed electronics and responsive structures and devices, such as magneto- or piezoresponsive, among others. Usually obtained by a combination of functional fillers and an appropriate polymer, these materials allow the development of smart devices for the Industry 4.0 and the "Internet of Things" concepts [1]. These polymer composites are increasingly being implemented by additive manufacturing, also called 3D printing, in a variety of shapes, taking advantage of the synergistic combination of their inorganic and organic constituents, and giving rise to a variety of multifunctional responses. The polymer matrix offers advantages in terms of processability, while the filler usually allows to enhance one or more physico-chemical properties [2]. Among the different preparation methods, UV curing or photopolymerization, defined as polymerization reaction that converts a polymeric liquid composition into a solid material by irradiation with UV light, emerges as a suitable process for multifunctional composites preparation. It presents a series of advantages, such as fast and room temperature curing, reduced emission of volatile organic compounds, improved accuracy of the printed pattern and space and energy efficiencies [3].

Despite the enormous efforts devoted to the development of UV curable composites, relevant experimental drawbacks in terms of the limitation of the amount of filler added to the polymer has been identified, as well as in the deterioration of the mechanical properties [2]. The typical analysis carried out using Fourier Transformed Infrared Spectroscopy (FTIR), thermogravimetric analysis (TGA) or Scanning Electron Microscopy (SEM) show similar results independently to the filler content in functional composites, which hinders the proper interpretation of the observed behaviour of these materials [4]. Thus, learning about the filler dispersion in UV cured polymers, the polymer-filler interactions, the precise determination of the polymer-filler interface effects and the 3D cured polymer network structure by scattering techniques, and namely by small-angle neutron and X-ray scattering methods, is essential for a proper understanding of the main macroscopic properties of UV cured functional composites and, therefore, to tailor next generation of functional materials with well-defined macroscopic response.

References

[1] Policia, R., et al., *Advanced Electronic Materials*, 2019; 5(12):1900280.

[2] Nardi, T., et al., *Polymer*, 2013; 54:4472-4479.

[3] Mendes-Felipe, C., et al., *Advanced Materials Technologies*, 2019; 4:1800618.

[4] Mendes-Felipe, C., et al., *Compos. Part C*, 2021; 5: 100143.

Higher metal-insulator transition temperature and signature of second order magnetic phase transition in NdNiO₃ nanoparticles

Subir Roy^{1,2,}, Rajesh Katoch¹, R. B. Gangineni³, and S. Angappane¹*

¹ Centre for Nano and Soft Matter Sciences (CeNS), Jalahalli, Bangalore-560013, INDIA

² Manipal Academy of Higher Education (MAHE), Manipal-576104, INDIA

³ Department of Physics, School of Physical, Chemical and Applied Sciences, Pondicherry University, Kalapet, Puducherry-605 014, India

* roy.subir1991@gmail.com

The correlation between the structural and the physical properties of the rare earth nickelates (RNiO₃) are remained fundamentally fascinating to study the underlying physics. The temperature-dependent metal-insulator transition (MIT) and the magnetic phase transition in RNiO₃ provide a remarkable opportunity to understand and control these phenomena. Here, we report a way to tune the MIT as well as the magnetic phase transition of NdNiO₃ by reducing the particle size to the nanoscale. NdNiO₃ nanoparticles of various sizes have been synthesized by an aqueous solution-based chemical method. The size distribution and the morphology of the nanoparticles are studied by FESEM and TEM. The structural study from x-ray diffraction data shows the formation of orthorhombic nanocrystals of NdNiO₃ with the Pbnm space group. Further analysis of x-ray diffraction revealed the higher octahedral distortion, characterized by the reduction in Ni-O-Ni bond angle with the reduction of particle sizes. The temperature-dependent resistivity study shows the particle size dependent MIT at certain temperature TMI, which are higher compared to its bulk value and it increases with the lowering of the particle size. Further study of the magnetic susceptibility shows a magnetic phase transition at a temperature (Neel temperature TN), lower than the TMI, which indicates the existence of second order magnetic phase transition in the NdNiO₃ nanoparticles. The higher TMI and the origin of second order magnetic phase transition are attributed to the higher NiO₆ octahedral distortion and the bandwidth narrowing of the nanocrystalline NdNiO₃, which results in higher charge transfer gap compared to the bulk NdNiO₃.

Monte Carlo modelling of the carbon-oxygen logging measurement

József Gábor Szűcs^{1,}, László Balázs¹*

¹ ELTE Eötvös Loránd University, Institute of Geography and Earth Science, Department of Geophysics and Space Science, 1117 Budapest, Hungary, Pázmány Péter sétány 1/C

* szjgabor@student.elte.hu

Borehole geophysics has an essential role in the oil and gas industry. Analysing the changes of natural and artificially generated physical fields in time and space, the most important reservoir rock properties such as porosity, permeability, fluid saturation etc. can be estimated. Many of the methods used in borehole geophysics are based on neutron and/or photon reactions, including the subject of this study, the carbon-oxygen ratio (C/O) measurement. C/O tools use neutron generators (usually DT) in order to produce high energy neutrons in pulses. The gamma photon flux created through the inelastic scattering of these high energy neutrons is measured energy selectively using several scintillation detectors (sampling the axial distribution of the gamma flux at 2 or 3 volumes). Utilizing carbon (4.45 MeV) and oxygen (6.13 MeV) energy peaks on the measured gamma photon energy spectrum, the carbon-oxygen ratio in the studied medium is calculated, which can be used for hydrocarbon saturation determination for both the reservoir rock, and the borehole. Due to its advantageous properties, C/O logging is a rapidly growing part of borehole geophysics. In contrast to other methods of oil saturation estimation (e.g. electric resistivity logging) the C/O measurement is independent of water salinity, moreover, the small size of C/O tools makes it possible to use them in cased wells. (In order to preserve the borehole, it must be surrounded with steel pipes (casing) which kept in place by an outer cement sheet). In our work we carried out the modelling of the carbon-oxygen measurement with the Monte Carlo method using the MCNP transport code. These simulation results can be used to derive the interpretation diagrams (for the basic petrophysical effects) and to investigate the role of the side effects (corrections). We have simulated the high energy particle fluxes around the tool, and studied the most important model parameters that influence C/O ratios: detector distance from source, oil saturation, reservoir lithology, porosity, casing.

Aggregation of binary mixtures of sodium deoxycholate and sodium cholate in aqueous solutions with the addition of 6% propanol and 6% isopropanol

Vesna Tepavčević^{1}, Gorana Puača¹, Ana Pilipović, Zita Farkaš-Agatić, Kosta Popović, Mihalj Poša¹*

¹ University of Novi Sad, Faculty of Medicine, Department of Pharmacy, Hajduk Veljkova 3, Novi Sad, Serbia

* vesna.tepavcevic@mf.uns.ac.rs

Sodium dexycholeate (SD) and sodium cholate (SC), above a certain (total) concentration (cmcmM), in aqueous solution form binary mixed micelles. It is already known that, in the temperature interval $T = (278.15 - 298.15)$ there are synergistic interactions between SD and SC, in their mixed micelles. [1]. In this research, effects of adding 6% (v/v) propanol and 6% (v/v) isopropanol to aqueous solutions of SD and SC, mixed in different molar ratios ($\alpha = 0, 0.2, 0.5, 0.8$ and 1), were examined regarding the critical micelle concentration values (cmc), at different temperatures (278.15 K, 283.15 K, 288.15 K, 293.15 K, 298.15 K, 303.15 K and 308.15 K). Both additives reduced the cmc values of SD and SC in their aqueous solution. Mixed micelles of SD and SC also had reduced the cmcmM values in aqueous solutions which contained propanol and isopropanol additives, compared to their cmcmM values in aqueous solution without additives. The cmc values of SD were lower in aqueous solutions with 6% isopropanol than in aqueous solutions with 6% propanol, at all temperatures. As for SC, there were no significant difference in its cmc values between the propanol-containing solutions and the isopropanol-containing solutions, at all temperatures. In the binary mixed micelles having 20% and 80% molar ratios of DC, the cmcmM values were lower in aqueous solutions with 6% propanol than in aqueous solutions with 6% isopropanol, at all temperatures. In the mixed micelles with 50% molar ratio of DC, the cmcmM values were higher in aqueous solutions with 6% propanol than in aqueous solutions with 6% isopropanol, at all temperatures. The size, shape and aggregation number of the examined mixed micelles should be investigated by small angle neutron scattering, in order to further explain the obtained results.

References

- [1] Poša M, Pilipovic A. Effects of additives (methanol and NaCl) from aqueous surfactant solutions on the micellisation of sodium deoxycholate and sodium cholate binary mixture in the temperature interval $T = (278.15-318.15)$ K: The molar excess Gibbs energy and the molar Gibbs energy of the micelle formation. *The Journal of Chemical Thermodynamics*. 2020; 150:106179.

Characterization of lanthanide environments in amorphous systems and investigation of chemical durability of conditioned radioactive waste

István Tolnai^{1,}, Margit Fábrián¹*

¹ Centre for Energy Research, Konkoly-Thege Miklós St. 29-33., Budapest, 1121, Hungary

* tolnai.istvan@ek-cer.hu

The reprocessing of spent nuclear fuel generates high-level radioactive wastes (HLW) containing mainly long-lived isotopes in different forms and quantities. Based on their structural and mechanical properties borosilicate glasses are one of the best matrix forms for the immobilization of radionuclides. HLW solidification processes called vitrification receiving greater attention worldwide. Stabilizing high-level radioactive waste for disposal in a geological repository requires adequate data evolution for slow and long water/glass interaction in order to develop mathematical models for predicting and foreseeing the performance of the immobilizer glass matrix. The term of chemical durability describes the resistance of the matrix form to corrosion and dissolution caused by aqueous solutions. This phenomenon can be characterized by the rate of dissolution or by elemental release.

New glass compositions will be synthesized using lanthanide mixtures as they are considered as minor actinide surrogates based on their very similar chemical properties, therefore understanding the effects of lanthanide addition to a borosilicate glass structure is of great importance in view of waste management. $Ce^{4+,3+}$ will be used for modelling $Pu^{4+,3+}$, while Nd^{3+} is a model for Am^{3+} and Eu^{3+} for Cm^{3+} . The atomic structure of the samples and the incorporation of the $Ce^{4+,3+}$, Nd^{3+} and Eu^{3+} ions into the borosilicate glass matrix will be investigated by neutron and X-ray diffraction in combination with Reverse Monte Carlo (RMC) and X-ray absorption measurements. Using RMC modelling, the atomic pair correlation functions will be determined, providing structural data for the short- and medium-range order.

For the chemical durability tests, the samples are planned to be tested on a different timeframe in the order of days to month to gain information from the water/glass interfaces. Different conditions (temperature, time) and methods are also part of the tests. For deeper understanding of the dissolution and corrosion rate of the matrix, Boda Claystone Formation will be used in the experiments which is a planned host rock for the geological repository for HLWs. Chemical analysis of the leachates is important to further improve the understanding of corrosion processes for this purpose ICP-OES measurements will be performed.

Neutron Bragg-edge tomography for phase transformation of metallic materials

Khanh Van Tran^{1,}*

¹ Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

* khanhtv@tlu.edu.vn

Investigation of 3D phase transformation distributions of practical components is very important, especially under heavy loading conditions. While e.g., electron-based techniques can provide great details about a small-sized specimen, one key strength of neutron-based techniques is the investigation of representative sample sizes on the macro- and mesoscale. Neutron Bragg-edge imaging is a new method that is already studying contrast images with high-quality, e.g., for mapping phase distributions and compositions, lattice strain, and texture. Yet, investigations focus so far on radiographic projections, and tomographic reconstructions are limited to a single or a few wavelengths only. In this presentation, we not only report that sensible spectroscopic data can be recorded and displayed on a voxel by voxel basis for a three-dimensional representation in the form of attenuation coefficients, but also that it can be evaluated such that phase fractions can be carried out with higher precision than possible previously. The presented results include data obtained using the double crystal monochromator set up to reveal localized phase transformations in samples made from metastable stainless steel under plastic deformation load on the cm- length scale.

Unveiling the Drug Delivery Systems using X-ray and neutron techniques

Fabiano Yokaichiya^{1,}*

¹ Universidade Federal do Paraná

* fabiano.yokaichiya@gmail.com

The use of X-ray and neutron techniques, especially with the advent of large synchrotron light sources, nuclear reactors and "spallation sources" dedicated to scientific research, offer unique possibilities in the complementary use of its radiation for structural analysis in the advances of material engineering and provides information about the microstructure in regions of the material close to the surface and throughout the volume in a non-destructive manner. The objective of this presentation is the study of drug delivery systems such as cyclodextrins, poloxamers, solid lipid nanoparticles (SNL), nanostructured lipid carriers (NLC), self-emulsive drug delivery systems (SNEDDS) and hybrid systems for biological applications (medical and agriculture applications) such as anesthetics, high blood pressure control, colitis and cancer using X-ray and neutrons techniques. The presentation will focus on small-angle X-ray (SAXS) and neutrons (SANS) scattering techniques in order to characterize the drug carrier systems, and show the changes that these systems undergo with the addition of drugs, as a function of temperature (and also pH). The results from all these studies aim to improve the formulation of the drug carrier systems, their efficiency to act in the diseases and to minimize the side effects that most of the drugs can produce in other organs of the body.

25th October, 2021

Poster presentations

Characterization of electronic waste with neutron and X-ray based techniques

Noémi Anna Buczkó^{1}, Boglárka Maróti¹, László Szentmiklósi¹*

¹ Nuclear Analysis and Radiography Department, Centre for Energy Research, Eötvös Loránd Research Network, 29-33 Konkoly-Thege Miklós street, Budapest, Hungary

* buczko.noemi@ek-cer.hu

The recycling of electric and electronic waste is an important aspect of the circular economy. An analytical methodology needs to be developed for the determination of the valuable and/or hazardous elements in such waste. Multi-elemental neutron-based techniques, i.e. prompt gamma neutron activation analysis (PGAA), instrumental neutron activation analysis (INAA), and in-beam NAA have a lot of advantages, which can make suitable these techniques for the task. In this work, neutron-based techniques were used to determine the bulk elemental compositions of memory cards from personal computers. At first, non-destructive analysis was performed on the intact, structured samples. It was validated with the same samples after grounding and homogenization. The limitations in the applicability of the faster, cheaper, and more accessible handheld X-ray fluorescence spectroscopy (XRF) also were identified. The elements measured by more than one technique were used for the cross-validation.

A combination of PGAA, in-beam NAA, and instrumental NAA was found to be suitable to quantify the most valuable and/or hazardous elements present in printed circuit boards (PCBs) and integrated circuits (ICs), such as Au, Ag, rare earth elements, Br, Cd, etc. PGAA successfully identified the main or minor components (e.g. H, C, Si, Cl, Cu, Ni, Ca, Ti, Al, and Sn). Amongst the valuable elements, Ag, B, Sb, and Gd were identified. Cd and Br, both hazardous elements, were measured and a low detection limit for Hg was determined. It was proven that in-beam NAA measurements can decrease the detection limit of some valuable or hazardous elements (e.g. Au, Br, Sb, W, etc.). Au contents of both PCBs and ICs were successfully quantified with in-beam NAA. For Cu, Br, Au, and Mn the calculated masses were in agreement at a $k=2$ confidence interval compared to the PGAA and in-beam NAA results. INAA was suitable to measure the Au, Ag, Sb, Co, Sc, Sr, Hf, La, Ce, Eu, Tb, and Yb in low concentration, all of which have high importance in the circular economy. Good agreement was found in the element ratios determined with PGAA and INAA for the elements that were measurable by both techniques. Nevertheless, concentrations measured with PGAA were systematically higher. To match the results of the two methods needs further investigation. With XRF, the following elements were determined at various parts of the memory cards: Al, Si, Ti, Ni, Cu, Sb, Sn, Pb, and Ag. Pb contents that were not quantified by the nuclear analytic techniques, were successfully identified by the Olympus Delta handheld XRF equipment. The measured concentrations were significantly different compared so far to nuclear analytical techniques in the case of ground samples. There is no matrix-matched factory calibration method in the evaluation software of the handheld XRF device, which is suitable for such polymer matrices. The establishment of a new matrix-matched calibration is planned in the future.

Preliminary study of neutron spectra for "LvB" Compact Neutron Source

Ha Shuai^{1,2,}, Eszter Dian^{1,3}, Ferenc Mezei¹*

¹ Mirrotron Ltd., Budapest, Konkoly-Thege Miklós út 29-33. 1121 Hungary

² Eötvös Loránd University, Budapest, Pázmány Péter sétány 1/A. 1117 Hungary

³ Centre for Energy Research, Budapest, Konkoly-Thege Miklós út 29-33. 1121 Hungary

* Shuai.Ha@mirrotron.com

The number of Compact Accelerator-driven Neutron Sources (CANS) are increasing rapidly in recent years, to compensate the significant reduction of neutron beam time due to the close of many reactor-based neutron sources in the following decade. Among these CANS projects, the "LvB" project developed in Martonvásár, Hungary led by Mirrotron Ltd is the first CANS project in Central Europe. Currently, the RFQ linac of this project is able to accelerate proton beams to 2.5 MeV, to take advantage of the large cross section with a broad resonance of ${}^7\text{Li}(p,n){}^7\text{Be}$ reaction centered at 2.25 MeV. So far, spectra and angular distributions of neutrons produced by ${}^7\text{Li}(p,n){}^7\text{Be}$ reaction with 2.5 MeV proton beams and solid lithium target has been studied by many researchers. It was found that the energies of produced neutrons range from 0 to 800 keV. Most of the produced neutrons are emitted to the forward direction, while some of them (backward neutrons) are emitted along the direction opposite to the incident proton beams. These backward neutrons may go back to the bulk of RFQ linac and cause radiation due to neutron activation. To evaluate this backward-neutrons induced radiation from RFQ linac preliminarily, we simulated the angular distribution and spectra of neutrons produced by 2.5 MeV proton beams bombarding on a 100 μm thick solid Li target with Monte Carlo method. The simulated angular distribution and spectra of produced neutrons are in good agreement with previous results in Ref [1,2].

References

- [1] R. Reifarh, M. Heil, F. Käppeler, R. Plag: "PINO – a tool for simulating neutron spectra resulting from the ${}^7\text{Li}(p,n)$ reaction" NIMA 608 (2009) 139
- [2] W. B. Howard, Accelerator-Based Boron Neutron Capture Therapy, Massachusetts Institute of Technology, PhD thesis 1997

Citrate coated superparamagnetic iron oxide nanoparticles for magnetically controlled immune therapy

Amal Nasser^{1,2,}, Artem Feoktystov¹, Oleg Petravic³, Xiao Sun⁴, Harald Unterweger⁵,
Rainer Tietze⁵, Asmaa Qdemat³*

¹ Forschungszentrum Jülich GmbH Jülich Centre for Neutron Science JCNS

² Department of physics, Technical University Munich(TUM), 85748 Garching, Germany

³ Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institute PGI-4, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

⁴ Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

⁵ Department of Otorhinolaryngology, Head and Neck Surgery, Section of Experimental Oncology and Nanomedicine (SEON), Else Kröner-Fresenius-Stiftung-Professorship, Universitätsklinikum Erlangen, Erlangen, Germany

* a.nasser@fz-juelich.de

Superparamagnetic iron oxide nanoparticles (SPIONs) are a very promising vehicle for biomedical applications such as drug delivery, imaging and magnetic hyperthermia. In magnetic drug targeting (MDT), particles are accumulated in a certain region of the body using a magnetic field gradient. The response of the nanoparticles to the external magnetic field strongly depends on the particle crystalline structure, defects and phase composition (magnetite, maghemite, wüstite, etc.). Also the aggregation behaviour of SPIONs is crucial for proper utilization and is also determined by interface properties. Different approaches of interface modification are used to obtain stable particles in biological media, where the most promising way for water-based solutions are electrostatic and steric stabilization. The coating molecules are used simultaneously as binding moieties for pharmacologically active substances. With the application of an external magnetic field, drugs bound to the nanoparticle surface can be concentrated in the region of interest in the human body. The bioavailability of drugs can thus be enhanced, which greatly increases the efficacy of the therapy and reduces side effects. With regard to future in vivo applications in humans or animals, SPIONs have to be coated with a cyto- and immunocompatible layer.

Etioplasts are more susceptible to salt stress than chloroplasts and etio-chloroplasts of wheat (*Triticum aestivum* L. cv. Mv Béres)

Roumaïssa Ounoki^{1,}, Adél Sóti¹, Richard Hembrom^{1,*}, Renáta Ünnepe², Éva Sárvári³, Katalin Solymosi¹*

¹ Department of Plant Anatomy, Eötvös Loránd University, Budapest, Hungary

² Neutron Spectroscopy Department, Centre for Energy Research, Budapest, Hungary

³ Department of Plant Physiology and Plant Molecular Biology, Eötvös Loránd University, Budapest, Hungary

* roumaïssaounoki@gmail.com

Plants are subjected to numerous abiotic stresses which adversely influence their growth, metabolism and productivity. Among them, salinity stress is one of the most detrimental factors for plant growth and yield. High soil salinity causes ion imbalance and osmotic stress in plants. It is well-known that salt treatment, together with light, creates oxidative stress in plants. Plastids are semi-autonomous organelles of plant cells responsible for many crucial metabolic processes, for instance chloroplasts are responsible for photosynthesis (i.e., carbon, sulphur and nitrogen autotrophy in plants). In the absence of light, dark-grown angiosperm plants are unable to synthesize chlorophylls and their plastids cannot differentiate into chloroplasts but are instead developing into etioplasts. Many literature data report ultrastructural changes in chloroplast structure under salt stress (e.g. increased stacking of grana or swelling of the intrathylakoidal space, damage of envelope membranes), while others did not find any ultrastructural alterations. Our aim was to study and understand the molecular and ultrastructural background of the swelling of the prothylakoid membranes in the etioplasts and compare it with other plastid types. Therefore, in this work, 2-cm-long excised leaf segments of 11-day-old light and dark grown wheat (*Triticum aestivum* L. cv. Mv Béres) seedlings or etiolated wheat seedlings greened in low light for 16 h (and thus having etio-chloroplasts or young chloroplasts) were floated on various solutions (Hoagland as control, salt shock treatment and an isosmotic polyethylene glycol, PEG-6000 solution) in the dark or in light for 4 h. The effects of salt stress on chloroplast structure could be compared critically using small-angle neutron scattering (SANS) and transmission electron microscopy (TEM). In the etioplasts, we found swelling of the prothylakoid lumen, appearance of envelope invaginations using TEM, while in the chloroplasts or young chloroplasts no such swelling was observed. In contrast, in green leaves treated for 4 h in light, we observed a decline in the granum repeat distance values both with TEM and SANS. We also noticed significant decrease in the maximal and actual quantum efficiency of photosystem II, relative chlorophyll content (SPAD index) in dark and in the light-grown wheat floated in 4h light and in the greening seedlings, as well as slight alterations in the organization of chlorophyll-protein complexes as revealed by 77K fluorescence spectroscopy. These data indicate that the etioplasts are more sensitive to salt shock than chloroplasts or developing chloroplasts (etio-chloroplasts), and that the specific ionic components of the stress play a more important role in this process.

This work was financed by the National Research, Development and Innovation Office (grant OTKA FK 124748), the János Bolyai Research Scholarship of the H.A.S. (to K.S.), and the Stipendium Hungaricum scholarship for R.O. and R.H.

Investigation of the supramolecular organization of polyurethane-based multiblock copolymers using small-angle neutron and X-ray scattering

A.A. Pavlova^{1,2,*}, A.N. Bugrov^{3,4}, R.Yu. Smyslov^{2,3}, Yu.E. Gorshkova⁵, V.V. Volkov⁶, N.V. Tsvigun⁶,
A.E. Baranchikov⁷, G.P. Kopitsa^{2,8}

¹ Petersburg Nuclear Physics Institute NRC KI, Gatchina, Russia

² Saint Petersburg State University, Saint-Petersburg, Russia

³ Institute of Macromolecular Compounds Russian Academy Of Sciences, Saint-Petersburg, Russia

⁴ Saint Petersburg Electrotechnical University "LETI", Saint-Petersburg, Russia

⁵ Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Moscow district, Russia

⁶ FSRC "Crystallography and Photonics" of the Russian Academy of Sciences, Moscow, Russia

⁷ Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Moscow, Russia

⁸ Institute of Silicate Chemistry of the Russian Academy of Sciences, Saint-Petersburg, Russia

* teslagirl17@gmail.com

Segmented polyurethane ureas (PUU) are widely used in the world today as coatings, adhesives, membranes, sealants, heat-shrink packaging, damping and heat-insulating materials. The widespread use of PUU in such areas is possible due to their ability to microphase separation into hard and soft segments [1, 2]. In this work, as a soft segment in the synthesis of multiblock polyurethane ureas, were used polycaprolactone diols with molecular weights of 530 and 2000 g/mol, and result of the reaction between aromatic diisocyanates and diamines were formed as a hard block. This work aims to investigate relationship between the domain structure and thermomechanical properties, phase separation and morphology of PUU using small-angle neutron scattering (SANS) method. SANS measurements were performed at the YuMO spectrometer (IBR-2, JINR, Dubna, Russia). From the analysis of experimental data, it was shown that with increasing length of aliphatic segments in the structure of the polyurethane ureas don't affect on the size of the hard phase domains, but increases the distance between domains. It was found that the portion of hard segments does not affect the size of domains, but the chemical structure of the aromatic part can be influence to the domain structure. In view of the fact that symmetric diisocyanates promote denser packing of the hard segments, it leads to the enlargement of the domains from units of aromatic nature.

References

- [1] C. Prisacariu Polyurethane elastomers from morphology to mechanical aspects, Verlag Wien. Springer (2011)
- [2] K. Gissel, B. Helge // J. Macromol. Mater. Eng., № 3 p. 288, 265–271. (2003).

**Monocomponent micelle formation of the cationic surfactant
(1-tetradecyl)trimethylammonium bromide in the water solution containing
Poloxamer 188**

Kosta Popović^{1,}, Mihály Pósa¹*

¹ Department of Pharmacy, Faculty of Medicine, University of Novi Sad, 21000 Novi Sad, Serbia

* kosta.popovic@mf.uns.ac.rs

At greater concentrations of surfactants in the water solution micellar colloids begin to form in the bulk of the solution. Micelles have a role in development of pharmaceutical formulations as transport systems based on their potential to increase bioavailability of medical substances and enhance their pharmacokinetic profile. Block copolymers represent an ingredient in pharmaceutical products which makes possible the interactions between them and surfactants. A possibility of associates forming between surfactants and copolymers in concentrations lower than CMC (critical micelle concentration) decreases possible side effects and enhances applicability. The aim of the experiment is the examination of associates formation and parameter determination in the micellar system of the cationic surfactant (1-tetradecyl)trimethylammonium bromide (TTABr) in the presence of the copolymer Poloxamer 188. By various analytical methods, the critical micelle concentrations of the cationic surfactant, as well as the interaction parameters in the copolymer-surfactant system, is determined with spectrofluorimetric, conductometric and tensiometric measurements. In the presence of copolymers parallel processes of micellar formation are replaced with association process between surfactants and the copolymer which creates a new equilibrium. We can also conclude from calculated Gibbs free energy of micellization that the surfactant water solutions containing Poloxamer P188 create micelles that are more thermodynamically stable than solutions without the copolymer. Interactions between surfactants and copolymers can be investigated and used, making products more stable and less harmful, with surface tension modifications and side effects decreased. Small angle neutron diffraction would be used to measure the size of the surfactant micelle in the water solution compared to the surfactant micelle in the water solution containing copolymer Poloxamer 188 (copolymer P188 does not form micelles in the water solution, but it decreases the surface tension of the water solution). These measurements are required to determine whether the copolymer would stabilize the hydrophilic micelle surface by some form of molecular interaction (which would increase perceived micelle size obtained by small angle neutron diffraction) or if the copolymer would only affect the 2D interface between the air and the water solution containing the surfactant. If the latter is true, copolymer P188 would then only get incorporated in the air-liquid interface of the surfactant water solution where it interacts with surfactant monomers shifting the equilibrium toward the monomer association in the water solution (in this case the micelle size remains unchanged), and the CMC value of the surfactant in the water solution would decrease compared to the surfactant water solution without the copolymer.

E8 Spectra of Quasi-one-dimensional Antiferromagnet BaCo₂V₂O₈ under transverse magnetic field

Bella Lake¹, Konrad Puzniak^{1,}, Nazmul Islam¹, Karin Schmalzl², Jie Ma³, Jianda Wu⁴*

¹ Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, D-14109 Berlin, Germany; Technische Universität Berlin, Berlin, Germany

² Karin Schmalzl, Institut Laue Langevin, 6 rue Jules Horowitz, BP 156, F-38042 Grenoble, France}

³ Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Shenyang National Laboratory for Materials, Science, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China

⁴ Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai, 200240; China, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, 200240, China

* konrad.puzniak@helmholtz-berlin.de

In the poster presentation we report on inelastic neutron scattering (INS) measurements on a quasi-1D antiferromagnet BaCo₂V₂O₈ in a presence of transverse magnetic field applied along the (0,1,0) direction. Combining results of inelastic neutron scattering experiments and theoretical numerical simulations iTEBD, we can precisely study the E8 excitations appearing at $B_{c1D} = 4.7$ T, which is the one-dimensional quantum phase critical point (1D QCP). In consequence, three dispersions: m1, m2 and m3 have been observed. The energy scan at $Q = (0,0,2.0)$, reveals a match between the data and the theoretical prediction of energies of three E8 excitations.

Study of protection and detection materials used in nuclear medicine: Case of Iridium-192 Therapy center, Gamma Camera and PET-Scan

Achraf Radi^{1}, Péter Zagyvai², László Szentmiklósi²*

¹ Óbuda University, Budapest

² Centre for Energy Research, Budapest

* achraf.radi@gmail.com

Nuclear physics will continue to be an economic issue and lead to more societal areas such as electricity generation and industry. In particular, nuclear medicine, observing metabolic processes became possible thanks to the radioactive markers gamma emitters and positron. These elements not only allow selective targeting of diseased cells but the visualization of biochemical processes of disease indicators.

The techniques based on these materials have diversified and expanded considerably in recent years. Thanks to their essential utility installation crossed the presence only in centres with cyclotron to be distributed in other hospitals. Nevertheless, the use of these radionuclides requires protection precautions and special procedures from production to use.

To determine the radiation protection measures and optimize detection means for a centre that is planning to install a PET -scan machine and Iridium-192 therapy plus a Gamma Camera already exist, we based on the code based MCNPX on the Monte Carlo method.

The aim of our work is on the one hand to determine the biological shielding radiation in different rooms to ensure ambient dose rates allowable in nearby rooms. On the other hand, we try to model the response of some sparkling crystals to optimize the detection of radiation used.

Role of dopants on the phase stabilization and magnetism of Magnetic Shape Memory Alloys

N.A. Río-López^{1,}, P. Lázpita², A. Pérez-Checa^{1,3}, I. Zabala¹, J. Feuchtwanger^{2,4}, F. Plazaola², V.A. Chernenko^{1,2,4}, J.M. Porro^{1,4}*

¹ BCMaterials, Basque Center for Materials, Applications & Nanostructures, 48940 Leioa, Spain

² Department of Electricity and Electronics, Faculty of Science and Technology, University of the Basque Country, 48080 Bilbao, Spain

³ Tecnalia, Basque Research and Technology Alliance (BRTA), Mikeletegi Pasealekua 2, 20009 Donostia, Spain

⁴ Ikerbasque, Basque Foundation for Science, 48009 Bilbao, Spain

* natalia.rio@bcmaterials.net

Shape memory alloys, SMAs, are an interesting class of smart materials characterized by the Shape Memory Effect: a thermally-induced recovering process of their original shape after suffering from a pseudoplastic deformation in their low-symmetry, low-temperature state, commonly known as martensite. The so-called Martensitic Transformation, MT, is responsible for this effect. The MT involves a phase transition between two solid-state phases: the austenite, which is a high symmetry, high temperature phase; and the already mentioned martensite. The origin of the MT embodies a thermoelastic transformation, where a temperature change and/or the application of a mechanical stress leads to a change in the crystal structure of the alloy. The mechanical stress generated as a result leads, in turn, to a lattice deformation by twinning in the martensite. These crystallographically identical twin variants, initially randomly oriented, can be aligned upon the application of an external uniaxial stress. Magnetic Shape Memory Alloys, MSMA, are a particular type of SMAs that, due to their magnetic nature, exhibit Magnetic Field Induces Strains, MFIS. That is, the application of a magnetic field in a particular direction leads to an increase in the volume fraction of the twin variants whose easy-axis is aligned with the field, hence elongating the sample in the direction perpendicular to the applied field. A mechanical compressive stress can be applied to recover their original shape.

The applications in which MSMA can be used are related to these two effects, i.e. to their shape-changing property, this being greatly conditioned by the structure, atomic order and magnetic state of the MSMA. Therefore, the characterization of MSMA is crucial for pushing forward the current application limitations of the MSMA. Among the wide range of available characterization tools, neutron diffraction techniques stand out in acquiring advanced knowledge about the structure and magnetism of these alloys. In our particular case, Powder Neutron Diffraction experiments have been performed in order to elucidate the crystal structure of Ni₅₁Mn_{28-x}Ga₂₁Y_x MSMA, where the doping element Y is either Co or Fe, and x=0,1,3,5. The analysis of the diffractograms collected in the martensite phases of the MSMA shows that the non-doped alloy presents a mixture of modulated orthorhombic and tetragonal phases, the Co-rich samples tend to stabilize a non-modulated tetragonal phase, and the Fe-rich samples tend to stabilize an orthorhombic phase. Further to this, the atomic site occupancies and their relation with the magnetic properties of the MSMA have been studied in the aforementioned alloy series.

Quantitative detection of trace elements and heavy metals in coastal sediments using Neutron Activation analysis (preliminary results)

G. Halaris¹, P.K. Rouni^{1,}, M.J. Anagnostakis¹, E.P. Hinis¹*

¹ Nuclear Engineering Department, School of Mechanical Engineering, National Technical University of Athens, Building K, Zografou Campus, Iroon Polytechniou 9 Zografou, 15780, Athens, Greece

* prouni@mail.ntua.gr

Subject of this work is to detect metals and metalloids in marine sediment samples from Larymna, a coast close to industrial area (mainly aluminum production). The samples are irradiated using a 10Ci, Neutron source (Am-Be) located in a 1m³ water basin and then they are analyzed with gamma-spectroscopy using a Xtra-Ge detector. Each sample is placed in a 24mL water tight holder and is activated according three scenarios:

Scenario i) 1h irradiation to detect the short-lived radionuclides,

Scenario ii) a 4days irradiation for the medium ones and

Scenario iii) 20days irradiation to detect the ones with longer half-life.

The irradiated samples were analyzed using gamma-spectroscopy in XTraGe detector.

The analysis of the activated sample using γ -spectroscopy is based in the calibration factor estimated using a sample prepared from a certified SRM, which is irradiated and analyzed according the same 'scenario' as the unknown samples.

Using the NIST 2702 (marine sediment) the following major and trace elements were identified and quantified in the sediment samples from Larymna coast: Al, Mg, V, K, Mn, Na, Mo, Sb, Hf, Zn, Cr, As, Hg, Co, Ga, La, Sm, Ce, Cs, Fe, Sc, Th.

References

[1] T. K. Peppas et al., J. Hazard. Mater. 255-262, 181 (2010)

Amino acid encoded Metal-Organic Framework Adsorbents for Heavy Metals

Ainara Valverde, Gabriel I. Tovar-Jiménez, Dimas Torres, Maria I. Arriortua, Guillermo Copello, José M. Laza, José Luis Vilas-Vilela, Roberto Fernández de Luis*

¹ BCMaterials (Basque Center for Materials, Applications & Nanostructures)

* ainara.valverde@bcmaterials.net

Metal-Organic Frameworks (MOFs) have emerged as highly promising porous and crystalline materials to address heavy metal pollution, overcoming the adsorbing capacities and kinetics of classic adsorbents [1]. MOFs are formed by easily tunable inorganic and organic building blocks arranged in a porous and ordered fashion, creating a crystalline structure with large surface areas. Among all the broad variety of MOFs, Zr (IV) based ones, like MOF-808, have attracted the attention of the scientific community because of their great water stability, even in acidic conditions. However, the majority of Zr-MOFs show little selectivity towards heavy metal ion capture [2], which can be overcome encoding –SH, –NH₂ or –COOH functionalities into their structures. In these work, cysteine, histidine and citric acid have been post-synthetically anchored to the uncoordinated positions of Zr hexanuclear clusters of MOF-808, in order to increase its adsorption affinity over metal cations with different acidities. In fact, MOF-808 has six uncoordinated positions per cluster where formate molecules are found. Amino acids and natural acids can easily replace formate anions mimicking their binding mechanism to the cluster through the carboxyl groups [3]. Final encoding provides the pores of MOF-808 with amino acid residual groups able to act as metal-adsorption sites similar to the ones found in many metalloproteins active cores.

References

- [1] P. Kumar, A. Pournar, K. Kim, *Progress in Materials Science* 2017, 86, 25–74.
- [2] Y. Peng, H. Huang, Y. Zhang, *Nature Communications*, 2018, 9, 1–9.
- [3] S. S. Dhankhar, C. M. Nagaraja, *New J. Chem*, 2019, 43, 2163–2170.