KMM-VIN European Virtual Institute on Knowledge-based Multifunctional Materials AISBL

KMM-VIN Newsletter

Issue 23, Winter 2020

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EDITORIAL

The European Virtual Institute on Knowledge-based Multifunctional Materials (KMM-VIN) is an international non-profit association (AISBL) based on Belgian law with the registered seat in Brussels and a branch in Warsaw, Poland. It was established in 2007 as the major deliverable of the Network of Excellence project KMM-NoE of the EU 6th Framework Programme.

KMM-VIN is a self-sustainable European network of universities, R&D institutes and industrial companies which was created to promote and facilitate cooperative research on advanced structural and multifunctional materials. Research activities of the network comprise materials processing, characterisation of microstructure and properties, and modelling.

Joint research activities of the KMM-VIN members are being conducted within five Working Groups: WG1. Materials for Transport, WG2. Materials for Energy, WG3. Biomaterials, WG4. Materials Modelling and Simulation, WG5. Graphene/2D Materials. The industry sectors targeted by the KMM-VIN WGs are Transport, Energy and Healthcare.

Integration of research activities is supported through the KMM-VIN Research Fellowship programme for PhD students and young researchers.

Thematic scope of KMM-VIN R&D encompasses:

- metals and alloys
- advanced ceramics
- intermetallics and shape memory alloys
- composites of metal, ceramic, or polymer matrices
- coatings, layered materials, surface modification
- biomaterials and bioinspired materials
- graphene and 2D materials
- joining of advanced materials
- modelling and simulation of materials.

Besides the networking activities, KMM-VIN offers services for external customers such as integrated R&D solutions, access on market conditions to laboratory equipment, database of KMM-VIN materials and members' expertise, customised Specialised Courses, participation in KMM-VIN Industrial Workshops.

The purpose of KMM-VIN Newsletter is to inform about KMM-VIN activities, but also to serve as a source of information for the KMM-VIN members between the annual meetings in Brussels. Therefore, it has a more elaborated form than a typical newsletter providing relatively detailed information about the research being conducted within KMM-VIN Working Groups. This Newsletter issue summarises the main activities of the KMM-VIN in the second half of 2020 and the planned actions and events for the near future.

In year 2020 the networking activities, such as Industrial Workshops and the Mobility Programme, were strongly affected by the COVID-19 pandemic, as commented upon in "Latest News". A remedy for the mobility restrictions was sought by offering the KMM-VIN Research Fellowship holders and their hosts more flexibility in arranging the research stays. Research cooperation between the network members has been conducted mainly on a bilateral basis, as reported in "News from the Working Groups".

In the column "European Projects & Cooperation" a concise information is provided on selected European projects in which two or more KMM-VIN members are involved, Also, recent documents of the European Technology Platform on Advanced Engineering Materials and Technologies (EuMaT ETP) are highlighted. KMM-VIN has closely cooperated for many years with EuMaT on research priorities for advanced materials that were proposed to the EU funded programmes.

Within the "Research Fellowships, Courses and Trainings" column the results of the 2020 2nd call for KMM-VIN Research Fellowships for young researchers and PhD students are provided. Also, a list of Specialised Courses which can be offered by KMM-VIN members to external clients is presented.

Professional achievements of KMM-VIN members, such as scientific awards, recognitions, and promotion to high professional positions are reported in "Personalia".

The up-to-date register of the KMM-VIN members and the contact details of the KMM-VIN office are provided at the end of the Newsletter.

More information about KMM-VIN can be found on the website: http://www.kmm-vin.eu

Katarzyna Kowalczyk-Gajewska, Editor

LATEST NEWS

PARTNERSHIP

The KMM-VIN association is currently composed of 61 members: 31 core and 30 associate from 14 European States. Among them, 54 are institutions (research centres, universities, large companies and SMEs) and 7 are individual members. The size of the network has not changed since the last General Assembly meeting in February 2020.

KMM-VIN is open for new members from academia and industry interested in cooperative research within the thematic scope of the five WGs. Applications for membership are being collected on a continuous basis. Information on the accession procedure can be found on http://kmm-vin.eu (NETWORK). Answers to specific questions can be obtained by contacting the KMM-VIN CEO at Michal.Basista@kmm-vin.eu. The final decision on accession is taken once a year by the General Assembly at the annual meeting in Brussels.

FORTHCOMING EVENTS

The General Assembly 2021 and the annual technical meetings of the Working Groups will be held **online** on February 22-24, 2021, according to the following schedule (all hours in Brussels time):

- **WG2**. Materials for Energy (**EMEP**): Feb. 22, 2021 (Monday) 13:00-17:00
- **WG2**. Materials for Energy (**non-EMEP**): Feb. 23, 2021 (Tuesday) 10:00-12:00
- **KMM-VIN AISBL General Assembly**: Feb. 23, 2021 (Tuesday) 13:00-17:00
- **WG1**. Materials for Transport: Feb. 24, 2021 (Wednesday) 9:00-10:30
- **WG3**. Biomaterials: Feb. 24, 2021 (Wednesday) 10:30-11:30
- **WG4**. Materials Modelling and Simulation: Feb. 24, 2021 (Wednesday) 11:30-12:30
- **WG5**. Graphene/2D materials: Feb. 24, 2021 (Wednesday) 12:30-13:30.

The EMEP Management Committee (**EMEP MC**) will meet online on Feb. 22, 2021 (Monday) 10:30-12:00.

The KMM-VIN Governing Committee and Board of Directors (**GC & BoD**) online meeting is scheduled on Feb. 23, 2021 (Tuesday), 10:00-12:00.

Due to the COVID-19 outbreak the KMM-VIN Industrial Workshops 9 and 10 (IW9, IW10) have been moved to new dates. However, these new dates depend, obviously, on how the situation with the COVID-19 is going to develop.

9th KMM-VIN Industrial Workshop (IW9) on Materials for Energy in Turin is scheduled on **May 17-18, 2021**. It will soon be decided whether the IW9 will be held online or moved again to another date, hoping to have it in traditional (non-virtual) form. The aim of IW9 is to gather a mixed audience of researchers and industrial players in the field of energy and to show the new opportunities offered by advanced materials (see the IW9 leaflet at http://kmm-vin.eu/workshops/).

10th KMM-VIN Industrial Workshop (IW10) on "Design and modeling of innovative biomaterials and bioinspired materials for industrial applications" – the new dates are **January 25-26, 2022** (see "News from WG4" for more details).

THERMEC'2020 – the 11th International Conference on Processing & Manufacturing of Advanced Materials - Processing, Fabrication, Properties, Applications, http://www.thermec2020.tugraz.at) will be hold in an online format on **May 9-14, 2021**. It is being organised by the colleagues from the TU Graz: Christof Sommitsch as the General co-Chair, and Cecilia Poletti as the Program co-Chair.

ICTAM 2020+1 – 25th International Congress of Theoretical and Applied Mechanics has been postponed by one year and will be held from 22nd to 27th August 2021, in Milan. The organisers hope to hold a "real" congress but a fully virtual and a hybrid format are being also considered. For updates, please visit the ICTAM website: https://www.ictam2020.org/

SolMech2020 – 42nd Solid Mechanics Conference originally scheduled on September 7-10, 2020 has been cancelled. According to the SolMech organisers, it has not yet been decided if the conference will be held in 2021 or 2022. For the conference updates please check: http://solmech2020.ippt.pan.pl

EUROMAT 2021 – will be held on September 12-16, 2021 in Graz, either as a traditional or virtual conference, depending on the travel restrictions. Christof Sommitsch (TUG) is the scientific chairman. For more information, please visit the conference website: https://www.euromat2021.org

3rd EMMC Workshop online - the 3rd International Workshop of the European Materials Modeling Council (EMMC) will take place on March 2-4, 2021 in a digital format. For more information and registration please visit 3rd EMMC International Workshop

13th Call of the KMM-VIN Research Fellowship Programme will be open right after the General Assembly meeting in February 2021. Thanks to the expected savings from the online organisation of the KMM-VIN annual meetings 2021, the budget for the 13th Call may be higher than in 2020, depending on the General Assembly decision.

WHAT'S NEW IN WORKING GROUPS

Working Groups (WGs) constitute the internal research structure of KMM-VIN. Collaborative research supported by the KMM-VIN Research Fellowship programme, preparation of project proposals, and organisation of Industrial Workshops are currently the core activities carried out within the Working Groups. Since the internal collaborative projects within WGs receive no funding from KMM-VIN budget they are being formed bottom-up by the WG members without any imposed research agenda or work model from KMM-VIN. Therefore, the results of the collaborative work within WGs are dependent on the members' commitment and the leadership of WG coordinators. In fact, each WG operates in a slightly different way with different intensity.

At present KMM-VIN is composed of five WG, as listed below.

WG1. Materials for Transport

Coordinators:

Pedro Egizabal, Fundación Tecnalia (TECNALIA), Donostia/SanSebastian, Spain

Thomas Weissgärber, Fraunhofer Institute for Manufacturing and Advanced Materials, (FRAUNHOFER-IFAM DD), Dresden, Germany

WG2. Materials for Energy

Coordinators:

Monica Ferraris, Politecnico di Torino (POLITO), Italy

Christof Sommitsch, Graz University of Technology (TUG), Austria

WG3. Biomaterials

Coordinators:

Aldo R. Boccaccini, Friedrich-Alexander Universität (FAU), Erlangen-Nürnberg, Germany

Christian Hellmich, Technische Universität Wien (TUW), Austria

WG4. Materials Modelling and Simulation

Coordinators:

Katarzyna Kowalczyk-Gajewska, Institute of Fundamental Technological Research of Polish Academy of Sciences (IPPT), Warsaw, Poland

Andrés Diaz-Lantada, Universidad Politécnica de Madrid (UPM), Spain

WG5. Graphene/2D Materials

Coordinators:

Peter Hansen, Ammanford, United Kingdom

Antonios Kanellopoulos, University of Hertfordshire (UH), Hatfield, United Kingdom

Any member of KMM-VIN (core or associate) can join any WG upon prior consent from the WG coordinators, with the exception of the WG2-EMEP (a subgroup of WG2. Materials for Energy), where special accession rules apply (cf. http://kmm-vin.eu/members_area/wg2/ after login).

New WGs can be formed on themes not covered by the existing WGs, if requested by a group of minimum 7 members.

NEWS FROM WG1: MATERIALS FOR TRANSPORT

The collaborative activities among WG1 participants have continued during the last 6 months in spite of the obvious obstacles aroused by the COVID-19 pandemic and the difficulties to have access to research facilities.

IMIM and TECNALIA have continued their collaboration on the development of nanoreinforced aluminium alloys. The last activities are now addressed to compare the in-situ process developed by IMIM with the ex-situ stir casting route that is being studied by Tecnalia. nTiC reinforced aluminium alloys are being produced in order to compare the feasibility of both production processes as well as the performance of the obtained materials. It is foreseen that a researcher from IMIM visits TECNALIA next year to progress in this collaboration in the frame of the 2020 call of the KMM-VIN Research Fellowships.

The collaboration between research groups of VSB TU Ostrava and IMIM in the project related to the effect of severe plastic deformation on aluminium based composites continues, even though the activities in the last months have been delayed due to situation created by the COVID-19.

A new round of brainstorming session for further collaborative projects will be opened by coordinators in January 2021 in order to identify new opportunities of collaborations among WG1 members that can be discussed and get crystallized during the next KMM-VIN General Assembly meeting.

Internal Collaborative projects

Development of aluminium based nanocomposites

There is still running the fruitful collaboration between IMIM and TECNALIA in investigation of matrix composites reinforced with ceramic nanoparticles. The most recent scientific activity consists in the in-situ production of aluminium-based composites with (Ti, W)C particles and their microstructural characterization. The research was aimed at finding answers to two questions: what is overall microstructure of in-situ cast composite and how a content of W in (Ti,W)C solid solution influence on microstructure of (Ti,W)C/Al composite, especially at the interface between matrix and particles. In this work, composite Al/10 wt.% (Ti,W)C were produced in-situ via casting process by Self-propagating High-temperature Synthesis (SHS) in bath. As the starting materials for production of the composite elemental powders of Ti, C, W were used as the substrates for reaction formation of (Ti,W)C solid solution and Al powder as moderator of this reaction. The powders were mixed, then compacted and finally green compact was put into induction furnace with molten aluminium where an SHS reaction occurred, forming the composite suspension, which was cast to the mould. Fig. 1 presents SEM BSE microstructure showing a homogeneous distribution of fine ceramic particles (bright) and pores (dark) whose content was calculated as 6% applying the image analysis method.

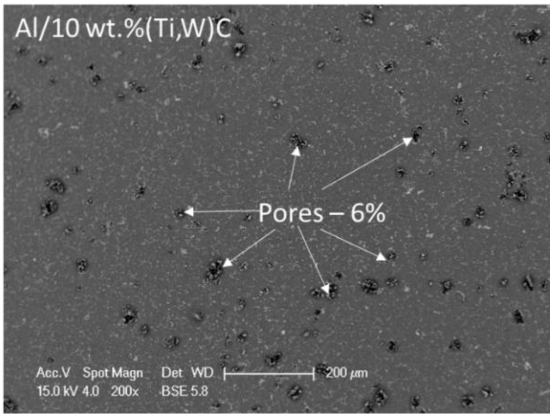


Fig. 1*. SEM BSE microstructure showing homogenous distribution of fine ceramic particles (bright) and pores (dark) (courtesy of IMIM).*

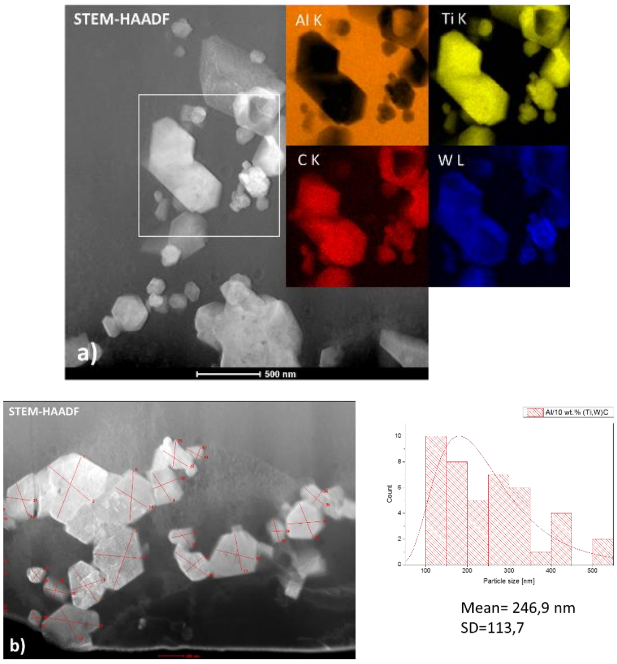
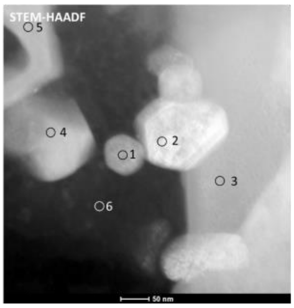


Fig. 2*. STEM-HAADF microstructures showing mapping of elements distribution and results of particle size measurements (courtesy of IMIM).*

Chemical composition of the composite was determined by use of STEM-HAADF microstructure and EDS analyses. Fig. 2a presents STEM HAADF microstructure and elemental mapping of distribution of elements performed at indicated area. One can see in the aluminium matrix the faceted particles consisting of Ti, W and C. What is interesting, the tungsten is located only in ceramic particles, but not in the matrix what indicates that synthesis process was performed properly. Also, the STEM HAADF images were used for particles size determination (Fig. 2b) by the secant method. The mean particles size was estimated as 246.9 nm with the lognormal distribution.

Fig. 3 presents another STEM-HAADF microstructure taken at a higher magnification and quantitative result of chemical composition performed for the particles and matrix. One can see that content of W in particles ranges from 2.5 to 10 wt.%, and there is no tungsten in the matrix as was previously shown by the elemental mapping. Additionally, at the point 3 the phase containing Al, Fe and Si was determined, which is usually formed as a result of contamination of pure aluminium with these elements.



p1

Element	Weight %	Atomic %
Al(K)	27.43	41.79
Ti(K)	66.14	56.76
W(L)	6.42	1.43

p2

Element	Weight %	Atomic %
Al(K)	8.56	15.36
Ti(K)	81.08	81.91
W(L)	10.34	2.72

p3

Element	Weight %	Atomic %
Al(K)	58.27	73.57
Si(K)	1.58	1.92
Ti(K)	0.16	0.11
Fe(K)	39.96	24.38
W(L)	0.00	0.00

p4

Element	Weight %	Atomic %
Al(K)	6.97	12.27
Ti(K)	86.88	86.13
W(L)	6.14	1.58

p5

Element	Weight %	Atomic %
Al(K)	1.67	2.99
Ti(K)	95.80	96.34
W(L)	2.51	0.65

p6

Element	Weight %	Atomic %
Al(K)	99.50	99.92
Ti(K)	0.00	0.00
W(L)	0.49	0.07

Fig. 3. *STEM-HAADF microstructure taken at the higher magnification and quantitative result of chemical composition performed for the particles and matrix (courtesy of IMIM).*

The observation in bright field (BF) and selected area electron diffraction (SAED) allowed to identify the shape of particles and their crystal structure. Fig. 4 presents a set of BF microstructures and corresponding SAED images for two different places of sample. In both cases there are faceted particles of a size of about 300 nm with zone axes [111] and [110] respectively of regular fcc crystal structure. The (Ti,W)C particle with [110] zone axis adjacent with the aluminium matrix have the contrast indicating close Bragg conditions. Therefore, this region was chosen for high resolution investigations.

Fig. 5 presents HREM image and corresponding FFT and IFFT images performed in indicated areas. The interface between aluminium matrix and (Ti,W)C particles consists of several Moire patterns formed as twisted each other crystal with the same orientations and close values of lattice parameters. Beside the areas with the Moire patterns, the regions with clear cross-grating of crystallographic planes can be distinguished, which corresponds to the [011] zone axis of Al matrix and also [011] zone axis of (Ti,W)C particle. In the interface region on the FFT image, additional diffraction spots located closer to the central spot are present which correspond to the Moire fringes.

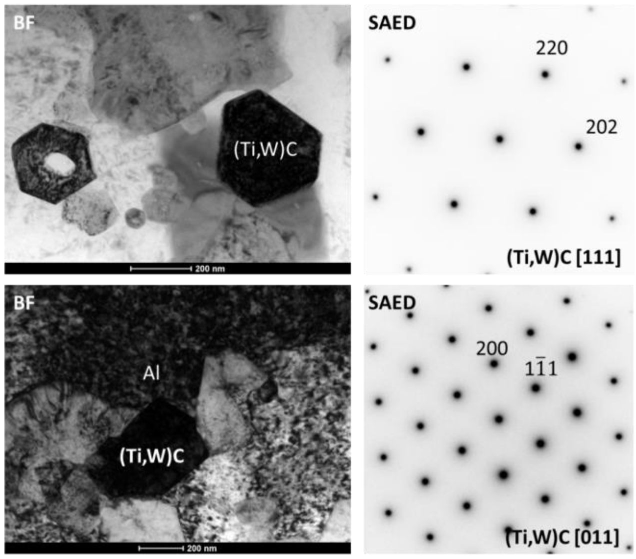


Fig. 4. *Set of BF microstructures and corresponding SAED images for two different places of sample (courtesy of IMIM).*

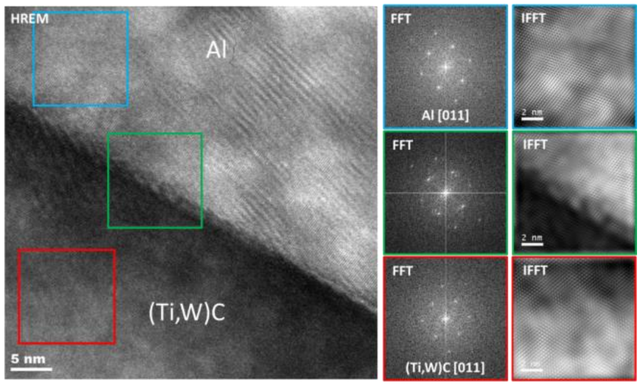


Fig. 5*. HREM image and corresponding FFT and IFFT images performed in indicated areas (courtesy of IMIM).*

Since the matrix and the reinforcing particles have an identical crystal structure and a similar lattice parameter, using the FFT images of the matrix and particles with the same zone axis [011], and using the relationship of lattice constant (a) of a cubic lattice and lattice spacing dhkl of plans hkl the lattice parameters of these phases and the lattice mismatch can be determined (Fig. 6). Accurate measurements of the interplanar spacing for (111) planes of the Al matrix and (Ti, W) C particles have shown that the lattice parameters of these phases are aAl = 4,117Å and a(Ti,W)C = 4.401Å, respectively, and the lattice mismatch between them is 6.9%.

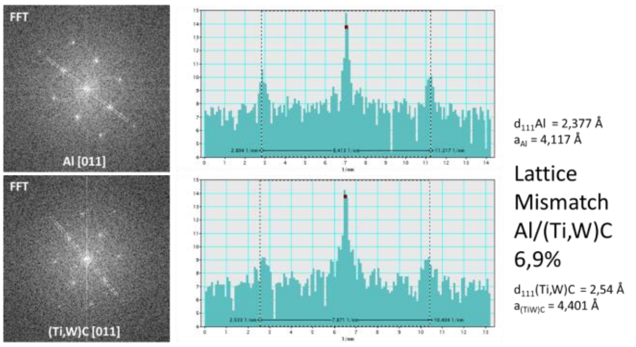


***Fig. 6**. Result of determination of lattice parameters and lattice mismatch between aluminium matrix and (Ti,W)C particle (courtesy of IMIM).*

The microstructural investigations of in-situ cast Al/10 wt.% (Ti,W)C composite showed that it has porosity of 6%, homogenously distributed in the aluminium matrix faceted (Ti,W)C particles of about 250 nm in size. High resolution electron microscopy investigations allowed to determine the lattice parameters of aluminium matrix (aAl = 4.117 Å) and (Ti,W)C particles (a(TiW)C = 4.401 Å) and the lattice mismatch at a level of 6.9%.

New projects. The collaboration between IMIM and TECNALIA contributed to a common research project titled "Economically friendly Al / TiC nanocomposites", which will be submitted in on Small Grant Scheme (funded by the Norwegian Financial Mechanism 2014-2021). The Small Grant Scheme is dedicated to female scientists in technical sciences. Principle Investigator will be Anna Wójcik from IMIM, the participation of scientists from the Polish company Innerco and the Czech Republic from VSB from Ostrava is also planned. The project concerns aluminium-based composites fabricated in a two-stage process including casting and further plastic deformation, and heat treatment to obtain good quality composites, with homogeneous distribution of TiC particles and enhanced mechanical properties.

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News from AGH-UST

1) ESTEEM3 - Integrated infrastructure network of electron microscopy facilities providing free access for the academic and industrial research community in materials science to the most powerful TEM techniques available at the nanoscale.

esteem3

The ESTEEM3 project, in which AGH-UST is one of the partners, gives a possibility of a Transnational Access (TA) to the most advanced Transmission Electron Microscopy (TEM) installations offering world-class expertise in many different fields of electron microscopy. ESTEEM3 is a European project funded by the European Commission's Horizon 2020 programme. It is a network of European laboratories and SMEs in electron microscopy. The main objective of ESTEEM3 is to facilitate access to electron microscopes in Europe.

The project, which takes over from ESTEEM1 and ESTEEM2, started in January 2019 for 4.5 years. TA is the central feature of the project and allows European and International researchers to access state-of-the-art European facilities of electron microscopy. Thus, researchers can apply in the laboratory of their choice from a list of 15 facilities in Europe for all what is necessary to perform planned investigations: Sample preparation, Transmission electron microscopy (TEM) and also Data analysis. Only user groups that are allowed to disseminate the results, they have been generated under the action, may benefit from the access, unless the users are working for SMEs. Access for user groups with a majority of users not working in an EU or associated country is allowed but limited to 20% of the total amount.

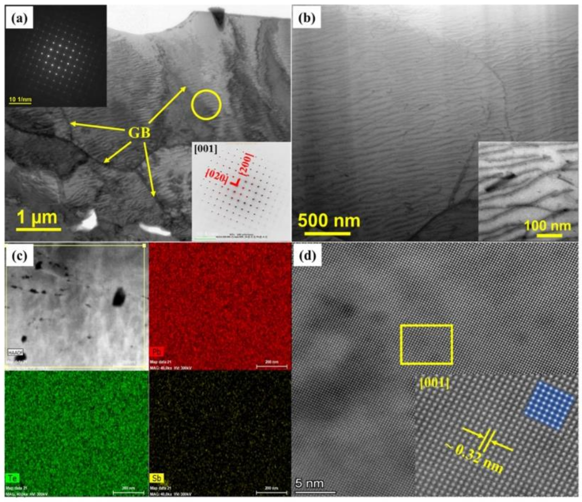

***Fig. 7**. Grain boundaries in PbTe materials studied utilizing the TEM technique on the atomic scale (courtesy of AGH-UST).*

One of the example of the investigations, performed within the projects is the research dedicated to the investigation of thermoelectric materials: the effect of Sb impurity as well as grain boundaries on the thermoelectric properties of PbTe materials. The grain boundaries was studied utilizing the TEM technique on the atomic scale (Fig. 7). A number of crucial factors affecting on the thermoelectric performance were clarified: HRTEM confirmed the polycrystalline nature of the investigated samples with the presence of sharp grain boundaries and TEM investigation clarified the origins of heat and charge transport in the n-Pb1-xSbxTe material. More detailed information can be found in [1].

[1] T. Parashchuk, I. Horichok, A. Kosonowski, O. Cherniushok, Piotr W., G. Cempura, A. Kruk, K. T. Wojciechowski, Insight into the transport properties and enhanced thermoelectric performance of n-type Pb1-xSbxTe, *J. Alloys Compd*. (in the revision stage)

Project website: www.esteem3.eu

This project has received funding from the European Union's horizon 2020 research and innovation programme under grant agreement n°823717

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2) Microstructural changes of Inconel 718 during high-temperature exposure

Inconel 718 is a Ni-based superalloy that belongs to a group of precipitation strengthened alloys. It exhibits excellent high temperature properties, such as high strength and corrosion resistance even up to 649 °C. The above-mentioned properties cause that Inconel 718 is a widely used material for parts of aircraft and land-based turbine engines.

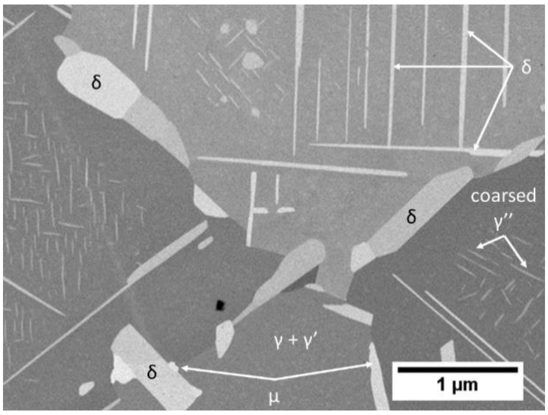

Fig. 8. SEM-BSE image of Inconel 718 after isothermal hold 760°C / 500 h (courtesy of AGH-UST).

In the present work, the microstructure evolution of Inconel 718 after 500 h of isothermal holding at 760 °C was studied. Microstructural observations were performed using Zeiss Merlin Gemini II field emission scanning electron microscope equipped with Quantax 800 energy dispersive X-ray spectroscopy microanalysis system. Moreover, to determine both the morphology and spatial distribution of γ'' precipitates, the FIB-SEM tomography using Zeiss Neon CrossBeam 40EsB scanning electron microscope equipped with focused ion beam was performed.

Fig. 8 shows the microstructure of Inconel 718 after 500 h of thermal exposure at 760 °C. The influence of the elevated temperature has led to a coarsening of enriched in Nb and Ni (Fig. 9a) δ phase precipitates present on grain boundaries. Another effect of the isothermal holding was a coarsening of main strengthening phases (spheroidal Al-enriched γ' (Fig. 9b) and disc-like shaped Nb- and Ni-enriched (Fig. 9a) γ'') within γ phase grains. Moreover, on the above-mentioned δ precipitates, enriched in Mo and W (Figs. 9c-d) μ phase nucleated. Furthermore, a certain amount of γ'' phases precipitates transformed to plate-like δ phase precipitates present inside γ grains. Three-dimensional visualizations of FIB-SEM reconstructed volumes of Inconel 718 are shown in Fig. 10a-c. Fig. 10b presents the shape of δ phase precipitates and spatial distribution of γ'' precipitates. In Fig. 10c, a morphology of coarsed γ'' precipitates can be observed.

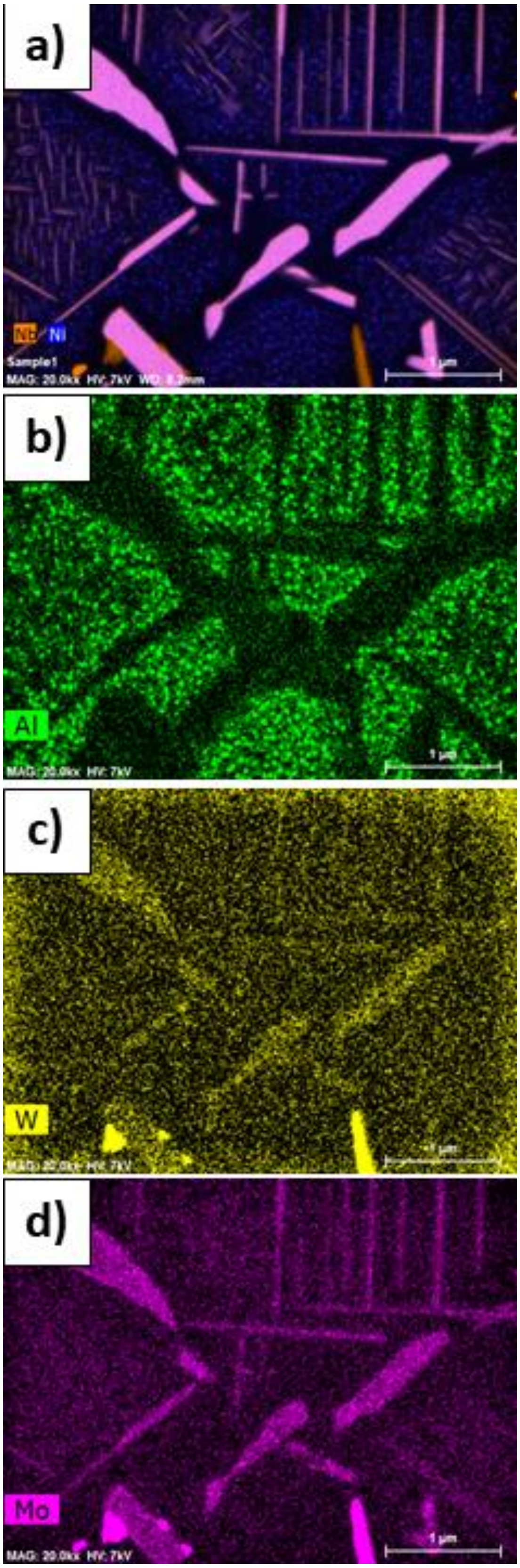

Fig. 9. SEM-EDXS maps of selected elements a) Nb (orange) + Ni (blue), b) Al, c) W, d) Mo (courtesy of AGH-UST).

Future work will focus on detailed microstructural studies of specimens isothermally held for 1 – 250 h.

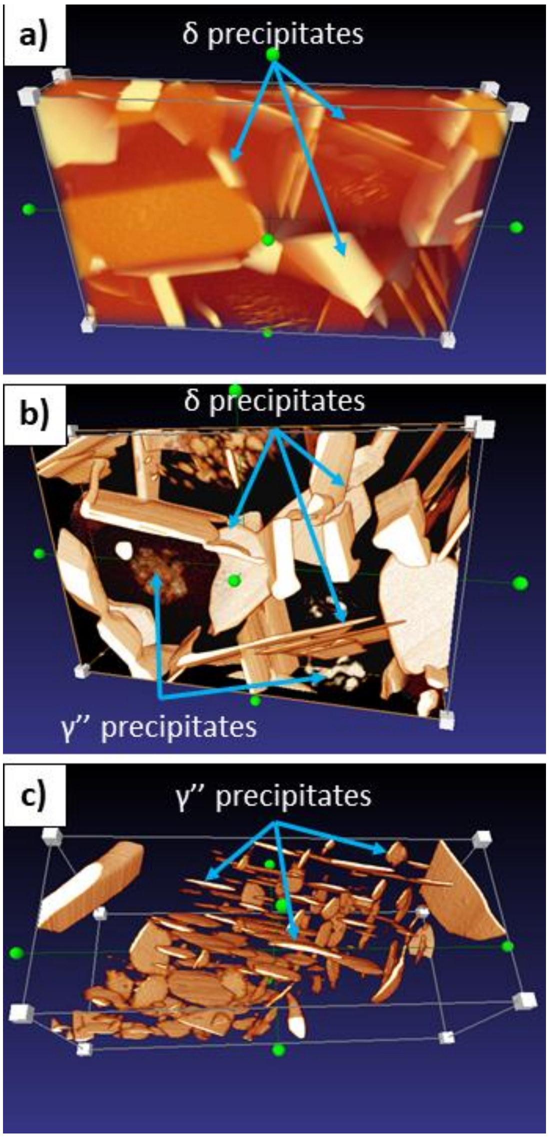

Fig. 10. *a) 3D visualization of the isothermally held Inconel 718 microstructure, b) tomographic reconstruction of δ phase precipitates, c) tomographic reconstruction of γ'' precipitates (courtesy of AGH-UST).*

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3) Discontinuous precipitation during aging of Ni-Fe-Cr-Al alloy

Haynes® HR-224® (HR224) is a wrought Ni-Fe-Cr-Al alloy having a superior oxidation resistance when compared with similar heat-resistant alloys. A potential application of this alloy includes heat recuperators, fuel cells, automotive catalytic converters and heat shields and other heavily oxidizing environments. Although, several studies reported outstanding environmental resistance of HR224 alloy, there was a lack of information regarding the bulk material microstructure and its potential for further strengthening via heat treatment. In our study, we subjected HR224 alloy to 2-hour long aging treatment between 600-1100°C. The results of tensile tests showed increase of mechanical properties (tensile strength and yield strength) between 600-800°C, when compared with as-received material.

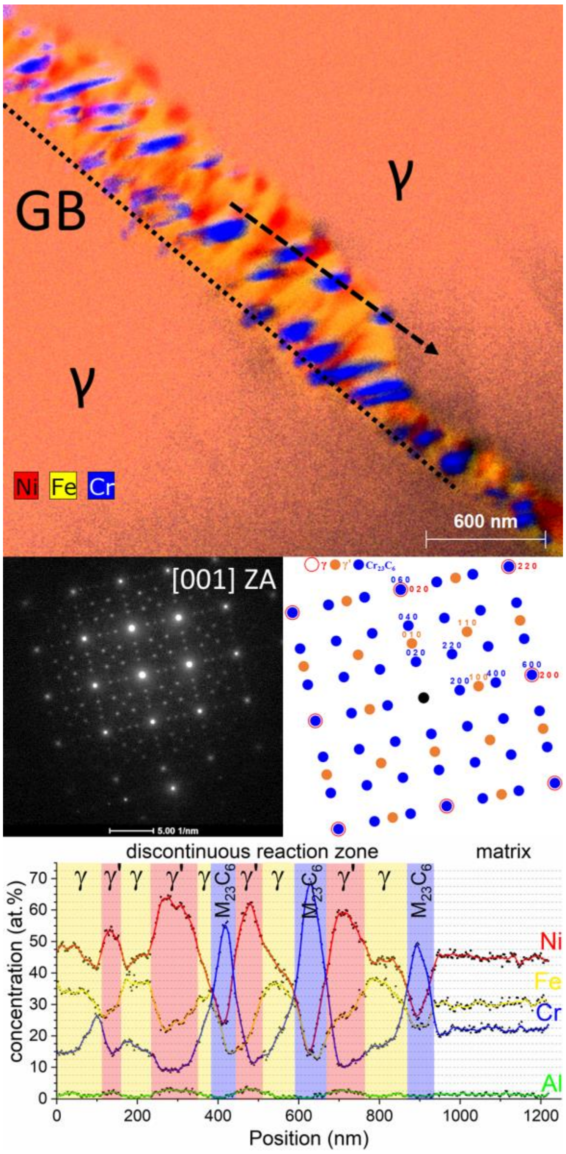

Fig. 11. *Overlayed STEM-EDXS elemental distribution map of Ni, Fe and Cr of discontinuous precipitation zone at the grain boundary in HR224 alloy aged for 2 hrs at 700 °C. Black dashed arrow indicates position for EDXS linescan showed at the bottom of the figure. In the middle selected area electron diffraction pattern is showed, along with the solution for γ, γ' and Cr23C6 phases in a [001] zone axis. (courtesy of AGH-UST).*

Moreover, microstructural investigations revealed presence of discontinuous precipitation zone formed at the grain boundaries within the aforementioned temperature range. The TEM analysis showed that within the discontinuous precipitation zone three phases were present, which was a deviation from a classical model where two-phase discontinuous precipitation product is formed. The three phases were identified as a Fe-rich γ phase, γ'-Ni_3Al phase and Cr-rich $M_{23}C_6$ carbide. Interestingly, chromium carbides showed cube-on-cube orientation relationship with the γ matrix, which explains to some extent the increase in mechanical properties.

Fig. 11 shows overlayed STEM-EDXS elemental distribution map of Ni, Fe and Cr at the grain boundary, where discontinuous precipitate was formed. Black arrow indicated the acquisition position of EDXS linescan of elements distribution showed at the bottom of the image. In both STEM-EDXS map and linescan clear separation between three phases can be distinguished. The figure is completed by selected area electron diffraction pattern taken within the discontinuous zone, along with the solution for the diffraction pattern.

More information about this study can be found in recent publications [1–2]. It is worth mentioning that the study was conducted in collaboration with KMM-VIN members: Wojciech Polkowski and Adelajda Polkowska from Łukasiewicz Research Network – Krakow Institute of Technology.

[1] A. Polkowska, S. Lech, W. Polkowski, Microstructure and mechanical properties of Ni-Fe-Cr-Al wrought alumina forming superalloy heat-treated at 600-1100°C, *Mater. Charact.*, (2020), 110737; https://doi.org/10.1016/j.matchar.2020.110737.

[2] S. Lech, W. Polkowski, A. Polkowska, G. Cempura, A. Kruk, Multimodal discontinuous reaction in Ni-Fe-Cr-Al. alloy, *Scr. Mater.* (to appear in 2021)

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News from IMBAS

Institute of Mechanics is involved in two projects, both funded by the Operational Programme Science and Education for Smart Growth and co-financed by the European Union through the European Regional Development Fund: Project BG05M2OP001-1.001-0008 Creation and development of centres of excellence “National Center for Mechatronics and clean technology” as a partner, and Project BG05M20P001-1.002-0011 Creation and development of centres of competence “Mechatronics, Innovation, Robotics, Automation, Clean Technology – MIRACle” as a coordinator. Within the scope of these projects two laboratories will be established in the Institute: Laboratory for mechanical tests and express diagnostics and Laboratory "Monitoring, nondestructive control, testing and characterization of mechatronic systems".

The Laboratory for mechanical tests and express diagnostics belongs to the Centre of excellence “National Center for Mechatronics and clean technology” and will be established in partnership with the Institute of Metal Science, equipment, and technologies with Hydroaero-dynamics Center “Acad. A. Balevski”. This laboratory will be equipped with Split Hopkinson bar, known also as SHPB, for analysis of material behaviour at high deformation rates (102-104s^{-1}). This apparatus is expected to become an important component in the optimization of the technologies for creating materials of appropriate dynamic properties for unique mechatronic products.

Another important equipment will be Complex for determination of mechanical characteristics and crack resistance in static and dynamic conditions in wide temperature range. The complex envisaged to be purchased will provide the possibility to determine the fracture toughness of the materials tested under different type of loadings, including critical cracks opening and crack growth rate, with high accuracy of the data obtained from the tests due to its high digitalization and automation degree. All these tests will expand the knowledge about the mechanical characteristics and exploitation reliability of components and units of mechatronic systems, including those in the field of transportation and energy.

The Laboratory "Monitoring, non-destructive control, testing and characterization of mechatronic systems" belongs to the Centre of competence “Mechatronics, Innovation, Robotics, Automation, Clean Technology – MIRACle” and will be engaged in experimental research, analytical and numerical modelling of the processes of operation, deformation and destruction of structural elements and systems (including MEMS) of high-tech multi-functional composite materials with a polymer or metal matrix with the presence of discontinuities and defects, such as cracks, layers (including thin coatings), openings, inclusions at macro, micro and nano level under various loads, and assessment of their critical values.

The intended for purchasing equipment, climatic chamber-system for analysing noise and vibration taking into account climatic factors, low and high frequency ultrasonic scanning system, a system for measuring the time of distribution of ultrasonic waves, apparatus based on eddy-current method, acoustic emission and high-precision optical system, will improve the understanding of the properties of the materials used for manufacturing the basic elements, components, assemblies and equipment incorporated into mechatronic units, industrial machines, devices, systems and bio-mechatronic products and products that will enhance their operational reliability and extend the life cycle, including the responsible structures and components in the field of transport and energy.

Increasing the accuracy in determining the characteristics of parts and components will allow design and manufacture of high-tech products and products with improved physical and performance properties that can meet today's requirements for reliability and infallibility of mechatronic systems running in aggressive environments at loads with various types and duration.

This equipment would allow for expanding the range of carried out testing and non-destructive evaluation of the microstructure, stress condition, physical and mechanical properties and defectiveness of materials with wide practical applications and will provide a more complete picture of the mechanical characteristics of classic and newly developed materials, and of the operational reliability of the components produced from them, parts and assemblies incorporated as part of a mechatronic unit, including parts, components and systems in the fields of transport and energy.

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NEWS FROM WG2: MATERIALS FOR ENERGY

There are two thematic subgroups in WG2 called "EMEP" and "non-EMEP". The EMEP partners follow the work model and research programme of the former COST proposal "Engineered Micro- and nanostructures for Enhanced long-term high-temperature materials Performance" (EMEP). The internal work programme EMEP consists of Work Topics (WT): WT1. Advanced Materials Modelling & Design, WT2. Materials Development and Manufacturing (A. Pipework and Tubing, B. Castings, C. Forgings), WT3. Materials Process Development and WT4. Testing and Validation.

The non-EMEP subgroup deals with other topics related to energy materials, especially the low-carbon energy materials. The WG2-EMEP is coordinated by Christof Sommitsch (TUG), whereas the WG2-non-EMEP by Monica Ferraris (POLITO).

News from POLITO and FRAUNHOFER IKTS

A new oxidation protective coating for titanium suboxide (TiOx) thermoelectrics

POLITO and FRAUNHOFER-IKTS are currently collaborating on the development of a resistant glass-ceramic coating for titanium suboxide (TiO_x). Protective coatings are crucial to manufacturing reliable and durable thermoelectric modules.

A new $Y_2Ti_2O_7$ based glass-ceramic was successfully designed, characterised and tested as an oxidation protective coating for TiO_x thermoelectric material up to 600 °C (Fig. 12). The coating exhibited excellent thermo-mechanical and chemical compatibility with the substrate and the heat-treatment, selected for the coating deposition, led to a glass-ceramic with improved refractory properties (an increase of ~270°C of the dilatometric softening temperature was observed after the parent glass devitrification).

Oxidations tests on coated and uncoated thermoelectrics were carried out at 600°C for 120 h in oxidising conditions. The XRD pattern of the uncoated substrate following the oxidation test shows that it completely oxidised to TiO_2. In contrast, the XRD pattern of the coated thermoelectric material after the oxidation test is identical to that of the as-sintered sample, thus confirming the effectiveness of the T1 glass-ceramic to protect the TiO_x material.

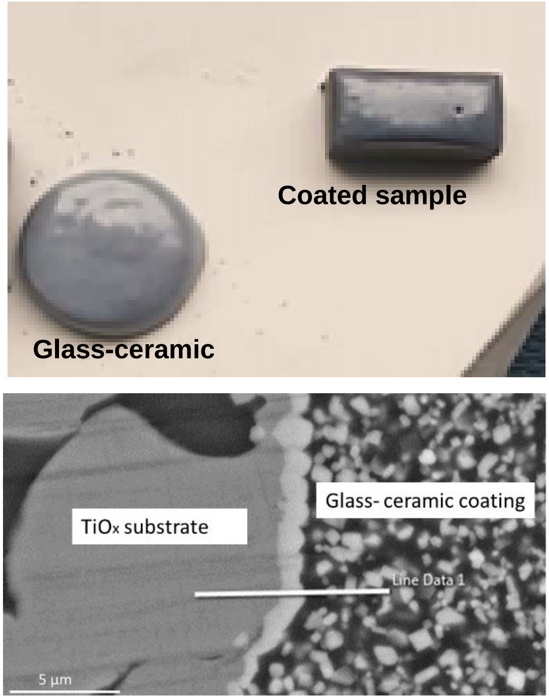

***Fig. 12**. A new Y2Ti2O7 based glass-ceramic tested as an oxidation protective coating for TiOx thermoelectric material up to 600 °C (courtesy of POLITO).*

POLITO team: F. D'Isanto, F. Smeacetto and M. Salvo (*milena.salvo@polito.it*), FRAUNHOFER-IKTS: H.-P. Martin. Further characterizations were carried out at UH (A. Chrysanthou) and IMRSAS (R. Sedlák, M. Lisnichuk).

News from AGH-UST

The Fe–Ni–Cr–Al–Mo–TiCp composites fabricated by three-dimensional plasma metal deposition on low-alloy steel

Metal matrix composites (MMCs) are widely known for combining beneficial properties of two materials classes; metals and ceramics. As the matrices for refractory composites, Ni-based alloys, and austenitic stainless steels are favored because they have high strength and ductility at service temperature, as well as strong resistance to hot corrosion and oxidation. Reinforcement particles are chosen, considering their reactivity with matrix, wettability, thermal expansion coefficient, and density. The carbides, intermetallics, nitrides, borides, and silicides could be particles reinforcing the metal matrix, and they are inserted into the matrix as irregular blocks, spherical particles, whiskers, and long fibers.

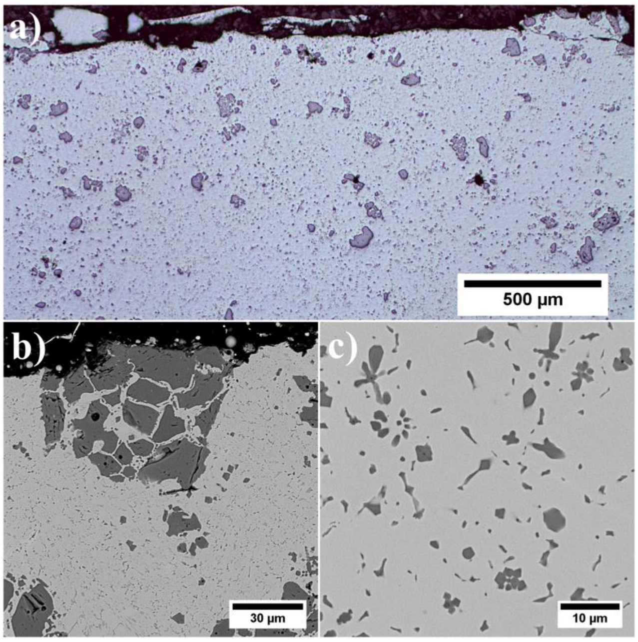

Fig. 13. Microstructure of Fe-Ni-Cr-Al-Mo-TiC$_p$ composite: a) distribution of the particles: b) large particle near the surface; c) small particles in the composite's volume (courtesy of AGH-UST).

The composites fabricated by three-dimensional plasma metal deposition on low-alloy steel are characterized by irregular distribution of titanium carbides (Fig. 13). Large particles are present close to the external surface due to the acting buoyancy effect, while in the interior, the particles with an equivalent radius around 0.2–0.6 µm dominate. On the edges of TiCp, two types of secondary precipitates are present, the first enriched in S and the second one in Cr (Fig. 14). High-temperature exposure during the deposition process resulted in the reaction of TiC$_p$ with the matrix, which led to the formation of nano-size $M_{23}C_6$ and $TiOSO_4$ precipitates (Fig. 15).

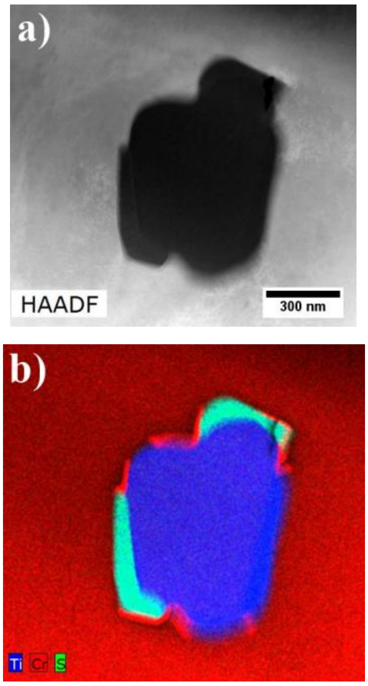

Fig. 14. a) Microstructure of single TiC particle; b) distribution map of the Ti, Cr and S (courtesy of AGH-UST).

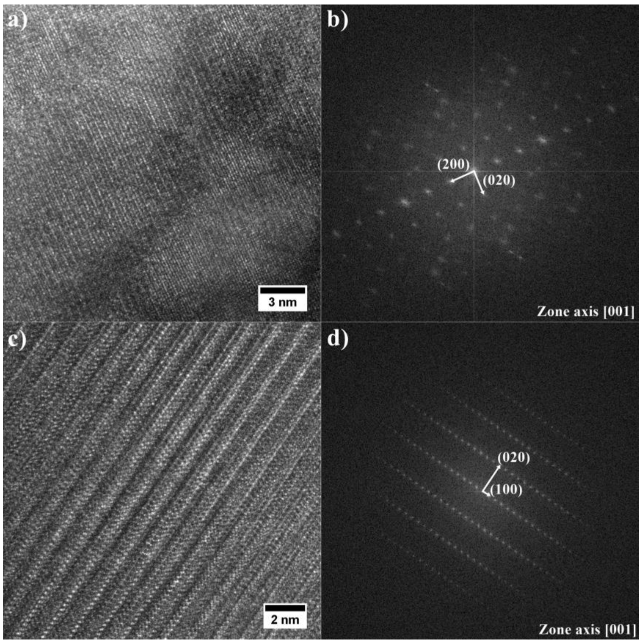

Fig. 15. Secondary phase structure in atomic scale resolution with the corresponding diffraction peaks calculated by fast Fourier transformation (FFT): a-b) $M_{23}C_6$; c-d) $TiOSO_4$ (courtesy of AGH-UST).

An investigation was carried out in cooperation with the Chair of Welding Engineering of the Chemnitz University of Technology. The cooperation has been supported by the Polish National Science Centre (Preludium 13) under grant 2017/25/N/ST8/02368 and DAAD (Research Grants-Short-Term Grants, 2019). More details can be found in [1].

[1] Ł. Rakoczy, K. Hoefer, M. Grudzień-Rakoczy, B. Rutkowski, M. Goły, T. Auerbach, R. Cygan, K. Gordon Abstoss, A. Zielińska-Lipiec, and P. Mayr. Characterization of the microstructure, microsegregation, and phase composition of ex-situ Fe–Ni–Cr–Al–Mo–TiCp composites fabricated by three-dimensional plasma metal deposition on 10CrMo9–10 steel. *Arch. Civ. Mech. Eng.*, 2020, 20, 127. doi.org/10.1007/s43452-020-00132-z

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News from IOD

A tangible example of cooperation between the WG2 partners is the recent submission of a proposal to the M.ERA-NET Call 2020. Together with IK4-TEKNIKER and other companies and R&D centres, the Foundry Research Institute (IOD) (new name: Łukasiewicz - Krakow Institute of Technology) has submitted a proposal entitled “Additive manufacturing and Projected Parts by using Recycled Powder from scraps” (RePoParts) to the M.ERA-NET 2020 Call. The proposal had passed to the 2nd stage of evaluation and the auhors were invited to submit a full proposal (now under evaluation). A brief project description is given below.

The development of new materials for European and world industry is of paramount importance. However, it requires eco-friendly new production technologies to protect the natural environment, preserve critical natural resources, and to reduce CO_2 emission.

Classic methods of producing advanced engineering materials often involve high CO_2 emission and degrade the natural environment due to the need for raw materials in the production process. The objective of the "RePoParts" project is to use metallic scraps containing highly valuable elements such as: Cr, Ni, Mo, V to produce powder for additive manufacturing (AM) technologies (i.e. LMD, SLM) and for coating deposition (i.e. HVOF). The powder obtained in the project will have a wide range of applications in High-Speed AM and thermal spray technologies. It will be used to produce new types of materials and new smooth and thin coatings for innovative components with a low carbon footprint.

The project results will significantly impact science, economy and the society by applying a more sustainable, circular economy approach in the solutions proposed. Furthermore, the project will positively contribute to the protection of the environment (reduction of waste, reduction in mining activities, reduction in CO_2 emissions), advancing the competitiveness of the European science and industry through the introduction of new technologies into the market.

Project partners: Lukasiewicz - Krakow Institute of Technology (T. Dudziak) – project coordinator, Progresja, GESCRAP, DELASER, STERN, La Rochelle University, TEKNIKER (subcontractor)

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News from POLITO

POLITO would like to invite you to a "virtual visit" of our new research centre on joining technology at Politecnico di Torino, J-TECH@POLITO: you are welcome for "in person visit" as soon as possible. We are open for collaboration starting now ... just let us know!
https://www.youtube.com/watch?v=bS_f5g82hDY&feature=youtu.be

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NEWS FROM WG3: BIOMATERIALS

From FAU to IPM

(KMM-VIN Research Fellowship, call 2020)

Evaluation of mechanical properties of electrophoretically deposited zein/bioactive glass composite coatings for biomedical applications

In the framework of the KMM-VIN Research Fellowship programme, Zoya Hadzhieva, PhD student of Aldo R. Boccaccini at the Institute of Biomaterials (FAU), visited the Institute of Physics of Materials, ASCR, Brno, Czech Republic (IPM) to conduct research under the supervision of Ivo Dlouhý.

Organic-inorganic composite coatings, which mimic the composition of natural bone by combining biopolymers and bioactive ceramics, are gaining increasing attention for bio-functionalization of orthopedic and dental implants. Following the expertise gathered at the Institute of Biomaterials at FAU [1], bioactive and biodegradable composite coatings based on the natural polymer zein and SiO_2-CaO-P_2O_5-based bioactive glass particles (BG) doped were developed by electrophoretic deposition (EPD) on titanium substrates. The materials are being developed in the framework of the project “Beethoven Classic 3“ in collaboration with AGH-UST (Principal Investigator: T. Moskalewicz).

The adhesion strength of the coatings was analyzed at the Faculty of Mechanical Engineering, Brno University of Technology, by using a CSM Instruments scratch tester. A Rockwell indenter having a 200 μm tip radius was moved 5 mm over a coating surface with linearly increasing normal load (from 1 to 10 N) at a loading rate of 9 N/min and speed of 5 mm/min. The critical load (Lc), at which the coatings started to fail, was obtained by light microscopy observations, acoustic emission and friction force signals. SEM and EDX analysis were performed to assess the coating removal from the substrate after the scratch test. In addition, the hardness of the coatings was determined by using a CSM Instruments nano-indentation tester equipped with a Berkovich diamond indenter. Loading and unloading rates were kept at 100 mN/min with a holding time of 15 s. In order to verify the obtained results, two maximal loads of 35 mN and 50 mN were applied.

The scratch results (Fig. 16) showed that the addition of BG particles in the zein matrix increased the critical load of the coating and reduced the frictional force. The highest critical load was measured for zein/BG coatings, while no statistically significant differences were observed for coatings containing different types of BG particles. These observations are in accordance with nanoindentation measurements as zein/BG coatings showed higher hardness in comparison to the other deposits. Further collaboration between FAU and IPM will focus on investigating the mechanical performance of novel multicomponent zein-based composite coatings.

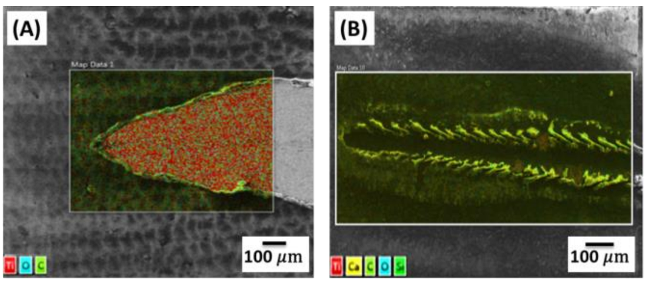

Fig. 16. *Images showing a scratch made by a Rockwell diamond tip (radius: 200 μm) on a chitosan-based coating at low and high magnifications (courtesy of FAU).*

[1] N. Meyer, L. Rivera, T. Ellis, J. Qi, M. Ryan, A. R. Boccaccini. Bioactive and antibacterial coatings based on zein/bioactive glass composites by electrophoretic deposition, *Coatings*, 8, 27, 2018. https://doi.org/10.3390/coatings8010027

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News from FAU

New EU project at the Institute of Biomaterials

A new EU consortium with participation of the FAU Institute of Biomaterials (Principal Investigator: Aldo R. Boccaccini) focusing on tendon regeneration has been awarded a 4.1 M€ grant from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Innovative Training Networks European Joint Doctorates (MSCA-ITN-EJD) (grant agreement No 955685). The project "Perspectives for Future Innovation in Tendon Repair" (**P4 FIT**) will train a new generation of 15 early stage researchers (ESRs) in the interdisciplinary fields of biomaterials, nanomedicine, drug delivery and tissue engineering. The **P4 FIT** project brings together world-renowned academic and non-academic EU institutions, covering key basic and technological disciplines to launch a unique European joint doctorate. The inter-disciplinary, inter-sectoral, and international high quality educational environment will deliver innovation-driven training and research leadership, grounded in excellence, to provide innovation in tendon medicine to tackle the urgent societal/economic healthcare demand determined by the worldwide growing incidence of tendinopathy. **P4 FIT** also involves 21 partner organizations, 10 academic and 11 non-academic institutions from across Europe and it will enable cross-disciplinary research. This four-year project will begin in January 2021.

News from AGH-UST

Electrospun fibers patches as an oil carrier for skin treatment

Skin diseases affect people all over the world regardless the age. Atopic dermatitis is one of the most common skin problems. Different treatments can be applied, oral administration of antibiotics or steroids, but also topical therapy. As a PhD student I work in the project "Nanofiber – based sponges for atopic skin treatment" funded by Foundation for Polish Science, led by Urszula Stachewicz. In this project we produce poly(vinyl butyral-co-vinyl alcohol-co-vinyl acetate) (PVB) nano and microfibers via electrospinning, characterize their morphology, mechanical properties and porosity by 3D reconstruction.

Moreover, the biocompatibility was assessed, and the results showed great potential for fibers in biomedical applications. In the examination of PVB fibers interaction with oils, we noticed that oil spreading and release depends on the fiber diameter and their morphology. Additionally, the preliminary skin test with nano- and microfibers patches with oil were performed to show the potential applicability of our research approach. Our study has been selected for the front cover in the ACS Applied Bio Materials [1], as showed in Fig. 17.

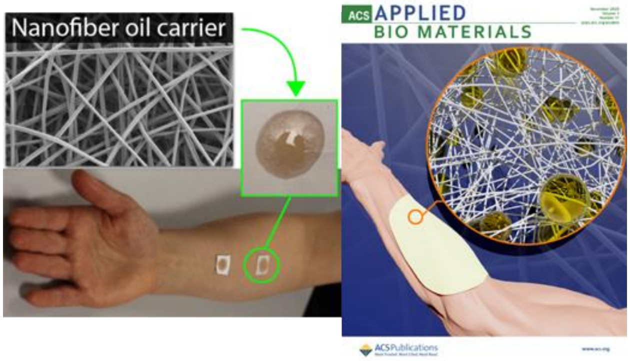

Fig. 17. *Electrospun PVB fibers as an oil carrier. On the left: scheme of skin test. On the right: front cover of ACS Applied Bio Materials adopted from [1] (courtesy of AGH-UST).*

[1] Z. J. Krysiak, Ł. Kaniuk, S. Metwally, P. K. Szewczyk, E. A. Sroczyk, P. Peer, P. Lisiecka-Graca, R. J. Bailey, E. Bilotti, and U. Stachewicz, "Nano- and Microfiber PVB Patches as Natural Oil Carriers for Atopic Skin Treatment," *ACS Appl. Bio Mater.*, 3(11), 7666–7676, 2020, doi: 10.1021/acsabm.0c00854

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NEWS FROM WG4: MATERIALS MODELLING AND SIMULATION

10th KMM-VIN Industrial Workshop on "Design and modeling of innovative biomaterials and bioinspired materials for industrial applications" (Reminder)

The IW 10 will be held at the Technical University of Vienna, from 25 to 26 January 2022.

Co-chairs: Christian Hellmich (TUW, IW10 local organiser), Katarzyna Kowalczyk-Gajewska (IPPT), Andrés Díaz Lantada (UPC).

The workshop is the tenth in a series of industrially oriented workshops organized by KMM-VIN in collaboration with leading research centres and industries. The most recent advances in material science and technology with high industrial potential are presented in this series. These workshops provide a unique opportunity to start and intensify the communication and cooperation between scientists and engineers for reshaping several industrial sectors with the help of knowledge-based multifunctional materials. The 10th KMM-VIN Industrial Workshop will cover the following topics:

- Design and modeling of biomaterials for medical devices and other biomedical applications.

- Design and modeling of bioinspired materials for industrial applications.
- Multi-scale / multi-physical modeling of the synthesis, processing and application of biomaterials and bioinspired materials.
- Modelling methods of microstructure-property relationship for hierarchical materials.
- Artificial intelligence-aided design of innovative biomaterials and bioinspired materials.
- Manufacturing hierarchical biomaterials and bioinspired materials towards final applications
- Promotion of knowledge-based biomaterials and bioinspired materials for enhanced industrial performance.
- Cases of success in different industrial sectors: health, energy, transport, space, construction and

All participants are invited to present a poster or oral presentation to show and discuss their work on materials modelling and process simulation. Invited keynote speakers will present research directions and recent breakthroughs in the aforementioned topics.

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News from IPPT

Core-shell model and atomistic estimates of elastic properties of nanocrystalline metals

Recently in IPPT the research on modelling elastic properties of nanocrystalline materials has been conducted in the frame of the National Science Centre project OPUS no. 2016/23/B/ST8/03418.

In a series of three papers [1-3] the anisotropic core-shell model of a nano-grained polycrystal was formulated and verified. As it was demonstrated, the approach enables estimation of the effective elastic stiffness of nanocrystalline metals of cubic and hexagonal crystal lattice symmetry. In the approach the bulk nanocrystalline material is described as a two-phase medium with different properties for a grain boundary zone (GBZ) and a grain core (Fig. 18a). While the grain core is anisotropic, the boundary zone is isotropic. The first problem addressed in the studies was the proper assessment of the thickness of GBZ and its elastic properties. Next, predictions of the proposed mean-field model were verified with respect to simulations performed with the use of the Large-scale Atomic/Molecular Massively Parallel Simulator, the Embedded Atom Model, and the molecular statics method. Polycrystal structures were generated using the Voronoi tessellation method. All calculation samples were approximately cubes (Fig. 18b). The size of the samples was chosen so that: small sample contained only an amorphous structure representing the grain boundaries, an medium sample of about 0.5 million atoms and a large sample of about 4 million atoms. The effect of the grain size on the overall elastic moduli of nanocrystalline material with random distribution of orientations was analyzed. The simulations were performed at the Interdisciplinary Centre for Mathematical and Computational Modeling of Warsaw University (ICM UW) and the computing cluster GRAFEN at Biocentrum Ochota.

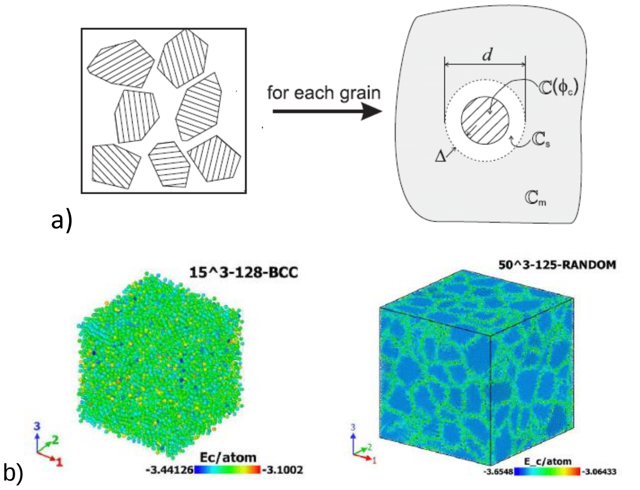

Fig. 18. *a) Schematic of core-shell model; b) Visualization of selected atomistic computational samples and cohesive energy Ec (eV/atom). (Courtesy of IPPT).*

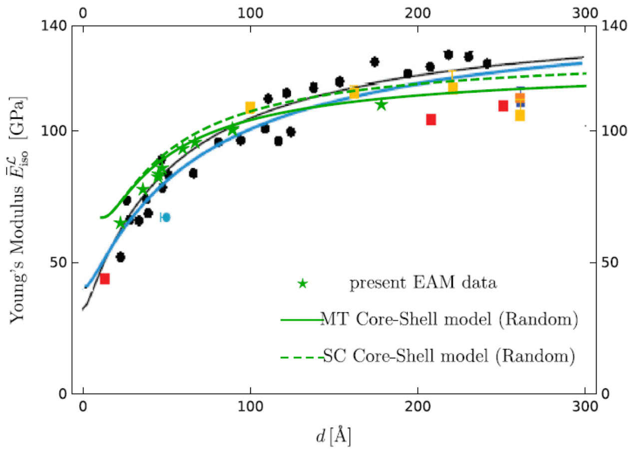

Fig. 19. *Young's modulus of nanocrystalline copper acquired in atomistic simulations for ten polycrystalline samples (green stars) and by the two variants of core-shell model (green line) as a function of the average grain diameter. Additionally, results of other experimental and atomistic studies reported in Gao et al. (2013), Comput. Mater. Sci., 79 , 56–62 are shown. (Courtesy of IPPT).*

In [1] the two-phase core-shell model was proposed in two variants. The model is size dependent and the basic length scale parameter is the thickness of a core coating (see Fig. 18a), representing the grain boundary zone. According to the study this thickness can be specified by a cutoff-radius of the corresponding atomistic potential used in the molecular static simulations. First, the model was applied to nanocrystalline copper. For this metal it was proposed to take local bulk modulus and smaller modulus of two shear moduli of a single crystal as parameters describing isotropic properties of GBZ. The model results were then with an agreement with atomistic simulations. For both approaches the shear modulus of nanocrystalline copper, similarly to Young's modulus (Fig. 19), decreased with the grain size, while the bulk modulus showed negligible dependence on the grain diameter. In [2] the model was verified for a set of crystals of cubic symmetry.

Materials selected for analysis differed in the lattice geometry (face-centered cubic vs. body-centered cubic) as well as the value of a Zener factor: a ratio of two shear moduli defining elastic anisotropy of a cubic crystal. Outcomes of molecular simulations indicated that, while the assumption of the thickness of grain boundary zone is still valid for each of analysed materials, the assumptions concerning the stiffness of boundary zone, which were made for nanocrystalline copper, cannot be transferred on other cubic metals. Specifically, it was observed that the bulk modulus may vary with a grain size and the shear modulus of a boundary zone can be equated with none of two modulus of a single crystal. Therefore it was proposed to identify the shell properties separately using the atomistic simulation results for samples with very small grains. When the shell thickness and properties were identified in the described way, obtained mean-field estimates were in a satisfactory qualitative and quantitative agreement with the results of atomistic simulations for all considered cubic metals. Interestingly, it was found that the dependence on grain size varies quantitatively with the Zener factor: stiffness moduli increase (resp. decrease) with the grain size if the Zener factor is higher (resp. lower) than one.

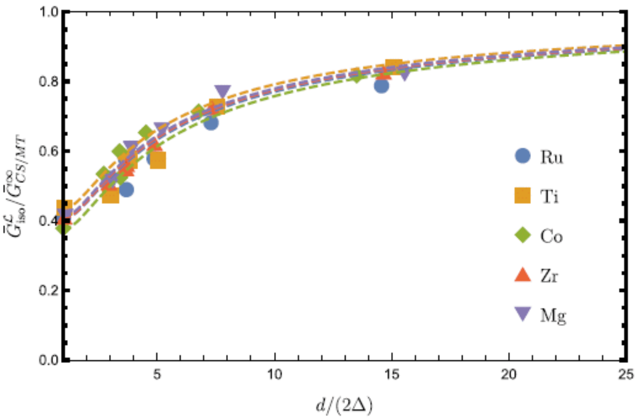

Fig. 20. *The shear modulus (scaled by a respective value for a coarse-grained polycrystal) as a function of the average grain diameter d (scaled by double cut-off radius) for 5 hcp metals: Ru, Ti, Co, Zr and Mg - the results of atomistic simulations (markers) as well as the core-shell model predictions (dashed line) (courtesy of IPPT).*

In [3] the core-shell model is extended to estimate the effective elastic stiffness of nanocrystals of hexagonal crystal lattice symmetry (hcp). For analysis six metals of hcp lattice geometry were selected for which the verified EAM potentials were available in the literature. All of them, as concerns elastic stiffness of ideal single crystal, are characterized by relatively low non-coaxiality angle and the same relation between Zener-like anisotropy factors. For each metal atomistic simulations were conducted on seven generated samples of polycrystalline materials with randomly selected orientations. Samples varied by the average grain size, so that the averaged grain diameter took values between ca. 1 nm to 20 nm. Similarly to cubic metals, the smallest sample served to identify the average properties of the grain boundary zone. It was found that for five out of six studied metals (Ru,Ti,Co,Zr,Mg) the elastic bulk and shear moduli increase with a grain size (Fig. 3). The reverse trend is observed for rhenium (Re). Rhenium exhibits the strongest anisotropy among considered metals, although the correlation between the anisotropy degree and the variation of stiffness moduli with grain size is not clear. The predictions of a core-shell model were in agreement with the atomistic simulation results. More details can be found in references [1-3].

The developed core-shell model can be extended to estimate a non-linear response of a nanocrystalline material and specifically the yield strength. Atomistic simulations may serve to validate such an extension.

[1] Kowalczyk-Gajewska K., Maździarz M., Atomistic and mean-field estimates of effective stiffness tensor of nanocrystalline copper, *Int. J. Eng. Sci.*, DOI: 10.1016/j.ijengsci.2018.04.004, 129, 47-62, 2018.

[2] Kowalczyk-Gajewska K., Maździarz M., Effective stiffness tensor of nanocrystalline materials of cubic symmetry: the core-shell model and atomistic estimates, *Int. J. Eng. Sci.*, DOI: 10.1016/j.ijengsci.2019.103134, 144, 103134-1-24, 2019.

[3] Kowalczyk-Gajewska K., Maździarz M., Elastic properties of nanocrystalline materials of hexagonal symmetry: the core-shell model and atomistic estimates, *Int. J. Eng. Sci.*, DOI: 10.1016/j.ijengsci.2020.103393, 157, 103393-1-21, 2020.

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News from the EuMaT Modelling Group

RoadMap on Modelling. Within the modelling and characterization working group WG1 of EuMaT, the RoadMap on Modelling has been published and is available under the link:
https://zenodo.org/record/4272033#.X9cIrnqg82w

Financing opportunities for modelling activities (including characterization) will be included in next M-ERA.NET call for proposals. Batteries stakeholders are trying to identify modellers for developing batteries. Registration: https://emmc.eu/register/

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NEWS FROM WG5: GRAPHENE/2D MATERIALS

News from UH

Development of new graphene enriched composites

Published Work. The unpresented circumstances that we all had to face this past year had a significant impact on our research progress which inevitably was slowed down. Nonetheless, together with colleagues from the Universities of Sunderland and Northumbria we completed our work on the development of new graphene/epoxy nanocomposites and the study of cure kinetics, thermal and mechanical properties [1]. In this work, new graphene/polymer nanocomposites were prepared using graphene nanoplatelets (GNPs) and the epoxy system Epilok 60–566/Curamine 32–494. The GNPs were first dispersed into the curamine hardener using bath ultrasonication, followed by the addition of the epoxy resin. The cure kinetics were studied by DSC under non-isothermal and under isothermal conditions. The kinetic parameters of the curing process were determined using the non-isothermal Kissinger and Ozawa-Flynn-Wall models.

The degree of curing increased with the addition of GNPs, while the activation energy decreased by 13.7% for the primary amine reaction and by 6.6% for the secondary amine reaction with epoxy groups as obtained from Kissinger. An increase in thermal stability by the addition of GNPs was identified in the range of 360–580°C using TGA. In terms of mechanical properties, addition of an optimum amount of 0.5%wt of GNPs in the hardener improved the Young's Modulus by 37%. Nanoindentation measurements showed 9.4% improvement in hardness at 0.7%wt.

Extension of Facilities. Over the past year, at the Materials and Structures research group at the University of Hertfordshire we have also extended our research facilities in the field of innovative construction materials. Our new testing capabilities include:

- A small scale robotic-arm controlled screw-extrusion 3D printer for additive manufacturing of cement-based materials and ceramics. Graphene is an integral part of this work as we explore the possibility of using as nano-reinforcement of the printed matrices.
- An automated programmable carbonation chamber for performing rapid carbonation evolution tests on ceramics and cement-based materials.
- An automated climatic chamber for conditioning and freeze-thaw testing on all types of materials.
- A high precision isothermal calorimeter for assessing hydration and curing kinetics in ceramics, cement-based materials and composites.

[1] S. Rehman, S. Akram, A. Kanellopoulos, A. Elmarakbi, P.G. Karagiannidis, Development of new graphene/epoxy nanocomposites and study of cure kinetics, thermal and mechanical properties, *Thermochim. Acta.* 694 (2020). doi:10.1016/j.tca.2020.178785

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News from Łukasiewicz Research Network – Institute of Microelectronics and Photonics (Łukasiewicz-IMiF, formerly ITME)

Ongoing intensive research into graphene on silicon carbide physics leads to new scientific findings. Researchers from Łukasiewicz-IMiF prove its potential in high-temperature magnetic field detection. Their technology of graphene-based Hall effect sensors (Fig. 21) enters the stage of industry-supported validation. The sensors are operational up to 500 degrees Celsius and address the requirements of space instrumentation and magnetic confinement fusion reactors. Already recognised with Gold Medal during the Seoul International Invention Fair 2019 they offer excellent platform for innovative R&D activities in the field of smart metering, electric vehicles and magnetic measurements under particles irradiation. In cooperation with scientists from Faculty of Materials Engineering and Technical Physics, Poznan University of Technology, Łukasiewicz-IMiF is targeting the development of high-temperature electronic components for magnetic diagnostics in extreme environmental conditions.

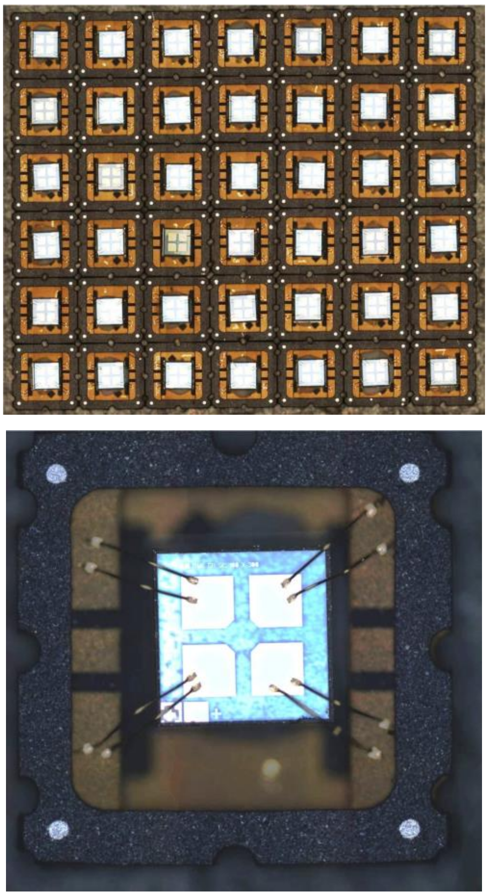

Fig. 21. *Graphene-based Hall effect sensors developed in Łukasiewicz-IMiF (courtesy of Łukasiewicz-IMiF).*

More details available at:
www.researchgate.net/profile/Tymoteusz_Ciuk

EU PROJECTS and COOPERATION

In several EU projects two or more KMM-VIN members are currently involved as partners. Three examples of the ongoing projects are briefly presented below.

BIONECA COST Action: "Biomaterials and advanced physical techniques for regenerative cardiology and neurology" (2016-2021). This COST action involves three KMM-VIN members: UNIVPM (coordinator), AGH-UST and TUW as project partners.

NICRRE: "Innovative Ni-Cr-Re coatings with enhanced corrosion and erosion resistance for high temperature applications in power generation industry" (2017-2021). This MERA-Net consortium is composed of four KMM-VIN members: ITME (coordinator), IPPT, WUT and IMRSAS. The project has entered the last year of execution. The new NiCrRe coatings deposited by the HVOF technique on steel panels are now being tested in a boiler installed in a power plant in Poland.

OntoCommons:"Ontology-driven data documentation for industry commons", a CSA H2020 project coordinated by TUW, with TEKNIKER and UPM among the 18 project partners. The project started on November 1, 2020 for a duration of three years. OntoCommons aims to lay the foundations for standardising the format of data and ensure interoperability so that it will be easier to use and distribute data in the manufacturing sector and the material science field. To achieve its aims, OntoCommons will coordinate a wide range of EU stakeholders for developing an ontology commons ecosystem that comprises a set of ontologies and tools following specific standardisation rules.

EuMaT ETP. KMM-VIN maintains working contacts with the European Technology Platform for Advanced Engineering Materials and Technologies (EuMaT). Our representatives are members in the EuMaT Steering Committee: Pedro Egizabal (TECNALIA), Arnaldo Moreno (ITC) and Michal Basista (IPPT). Amaya Igartua also serves as the co-secretary of the EuMaT ETP. It is a bottom-up created platform whose main role is to integrate the materials research community and the EU industry in the process of establishing of R&D priorities concerning advanced materials and technologies, and expressing them towards the EU Commission. Recently, a number of interesting documents have been worked out and published by EuMaT. The readers of this Newsletter are invited to have a look at Latest News on the EuMaT website https://www.eumat.eu. The most important one is the Role of the materials for Post-COVID Society that has also been published by the EU Commission.

KMM-VIN RESEARCH FELLOWSHIPS, COURSES and TRAININGS

KMM-VIN Research Fellowships 2020 (II Call)

The KMM Mobility Programme offers Research Fellowships on a competitive basis for PhD students and early stage researchers from the KMM-VIN members to do research at other KMM-VIN member institutions.

Joint publications of the fellowship holder and the host are expected as a result of the KMM-VIN Research Fellowship within 12 months after the research stay completion. The up-to-date published papers resulting from KMM-VIN RF stays are listed on http://kmm-vin.eu/fellowships/. More information on KMM-VIN Research Fellowships is available in the Members' Area of KMM-VIN website.

Due to the COVID-19 outbreak, the number of applications for KMM-VIN Research Fellowships in the 12th call opened in February 2020 was lower than usual (4 applications). Therefore, an additional call (Part II of the 12th call) was opened in August 2020. There were 8 applications submitted in that call, which were reviewed by the Research Fellowship Committee, consisting of the Chair of the KMM-VIN Mobility Programme and of the Coordinators of the KMM-VIN Working Groups. Five applications were awarded with in total 5.5 person months (financed by the regular KMM-VIN budget).

The following applicants were granted the research fellowships in Part II of 12th Call of KMM-VIN RF:

Applicant	**Host**	**Duration** (months)	**Start date** (provisional)
G. Imbir (IMIM)	F. Baino (POLITO)	1.0	1.02.21
M. Grudzień-Rakoczy (IOD)	P. Hvizdoš (IMRSAS)	1.0	1.12.20*
F. Miller Branco Ferraz (TUG)	P. Macioł (AGH-UST)	1.0	1.11.20*
A. Wątroba (AGH-UST)	A. Boccaccini (FAU)	1.5	15.01.21*
M. Saqib (FRAUNHOFER-IKTS)	L. Orazi (UNIMORE)	1.0	1.04.21

* - postponed due to the COVID-19.

KMM-VIN Specialized Courses

KMM-VIN offers customer-tailored Specialized Courses in the fields of materials design, processing technologies, fundamentals of chemical and physical processes, thermodynamics of complex materials, characterization of materials microstructure and properties, modelling of material properties and response to in-service conditions. The courses entail lectures, practices and case studies. They can be delivered at company's premises, at KMM-VIN members' location, or as e-learning.

These courses are designed for experienced staff members, who want to improve their skills in a selected field, but also for non-experienced employees, who would like to gain basic knowledge in the field. The courses are offered on a continuous basis upon individual arrangement with the interested parties. The fees depend on the type and extent of the course and can be agreed upon with the customers on case by case basis. More information on the courses can be found on KMM-VIN webpage (a detailed booklet to be downloaded) using the following link: http://kmm-vin.eu/for_industry/courses_and_trainings/

Interested companies can contact the coordinator of KMM-VIN trainings, Arnaldo Moreno (ITC) amoreno@itc.uji.es

Current list of Specialised Courses

MATERIALS

- Adhesive bonding (LU)
- Biomaterials (FAU)
- Development and applications of micro-structured and micro-textured materials (UPM)
- Light alloys and composites (IOD)
- Materials for energy systems and advanced steam power plants (AGH-UST)
- Materials for aerospace (AGH-UST)
- Materials science and technology (POLITO)
- Nanomaterials for biomedical applications (FAU)
- Nickel based superalloys (AGH-UST)
- Sustainable use of materials (LU)

PRODUCTION PROCESSES

- Automotive body materials (UH)
- Colloidal processing (FAU)
- Electrophoretic deposition (FAU)
- Foundry (TECNALIA)
- Heat treatment of welded joints (IS)
- International / European Welding Engineer / Technologist / Specialist (IS)
- International welder (IS)
- Plastics processing technology (LU)
- Rubber compounding and processing (LU)

CHARACTERIZATION TECHNIQUES

- Joining of dissimilar materials and mechanical tests of joints (POLITO)
- Electron microscopy (AGH-UST)
- High-temperature materials characterization in liquid and semi-liquid states (IOD)
- Material characterization via depth sensing indentation tests (IMBAS)
- Microstructural analysis and characterization by microscopy and tomography (AGH-UST and TECNALIA)
- Stress analysis of texturized materials by X-ray diffraction technique (IMIM)
- Testing methods for materials at high temperature and in aggressive environments (IOD)

MODELLING TOOLS

- Advanced multiphase and multi-scale material modelling (IMBAS)
- Design and modelling of micro-structured and micro-textured materials (UPM)
- Fracture mechanics of piezoelectric composites (IMBAS)
- Modelling and numerical simulations of multiphase composites (IMBAS)
- Sintering of metal-ceramic composites: modelling of the process, measurement and prediction of residual stresses (IPPT)
- Tissue engineering: biomaterials and cardiovascular systems (BIOIRC)

RISK MANAGEMENT

- Risks in Industry (R-TECH)
- Asset/plant Oriented Risk Management (R-TECH)
- Health, Safety, Security and Environment (R-TECH)
- Risk Governance (R-TECH)
- Risk Based Inspection (R-TECH)

PERSONALIA

Peter Hansen – new job role

Peter is now Director and shareholder in a new company called Hive Composites Limited. Peter spent 24 years working at MERL (which became part of Element Materials) followed by several years at Haydale Graphene Industries and then as a consultant running his own company. He has now joined forces with former colleagues from Haydale. Hive Composites Ltd is based in Loughborough, UK and offers industrial services including designing, developing, testing and certifying new composite materials, processes and products including:

- Next generation composite battery boxes for electric vehicles
- High pressure, spoolable thermoplastic composite pipelines for oil, gas & water
- Composite signposts, 5G masts and streetlight poles
- Electrically resistant composite structures for electricity transmission
- Multi-functional composites and adhesives for aerospace and space (deicing, tooling, conductive adhesives …)
- In-situ polymerising liquid thermoplastic resins.

Hive Composites Ltd have been successful in bidding for contracts in the area of nano-technology, mainly in the aerospace and automotive sector, and projects are underway to develop multi-functional materials using CNT based materials available in several different formats including suspensions, yarns and sheets for electrical adding conductivity, fire protection and damage detection in composite structures.

KMM-VIN Core Members

Institutions

1.	**AGH-UST**	AGH-University of Science and Technology, Krakow, Poland
2.	**BioIRC**	Bioengineering Research and Developing Centre, Kragujevac, Serbia
3.	**FAU**	Friedrich-Alexander Universität Erlangen-Nürnberg, Germany
4.	**FRAUNHOFER**	Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., Germany
	- IFAM	Fraunhofer Institute for Manufacturing and Advanced Materials, Bremen,
	- IFAM-DD	Fraunhofer Institute for Manufacturing and Advanced Materials, Dresden,
	- IWM	Fraunhofer Institute for Mechanics of Materials, Freiburg
	- IKTS	Fraunhofer Institute for Ceramic Technologies and Systems, Dresden,
5.	**IK4-TEKNIKER**	Foundación TEKNIKER, Eibar, Spain
6.	**IMBAS**	Institute of Mechanics, Bulgarian Academy of Sciences, Sophia, Bulgaria
7.	**IMIM**	Institute of Metallurgy and Materials Science, Polish Academy of Sciences, Krakow, Poland
8.	**IMRSAS**	Institute of Materials Research, Slovak Academy of Sciences, Kosice, Slovakia
9.	**INTA**	Instituto Nacional de Técnica Aeroespacial, Torrejón de Ardoz, Spain
10.	**IOD**	Foundry Research Institute, Krakow, Poland
11.	**IPM**	Institute of Physics of Materials, Brno, Czech Republic
12.	**IPPT**	Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland
13.	**ITC**	Instituto de Tecnología Cerámica - AICE, Castellón, Spain
14.	**ITME**	ŁUKASIEWICZ-Institute of Electronic Materials Technology, Warsaw, Poland
15.	**MCL**	Werkstoff-Kompetenzzentrum-Leoben Forschungsgesellschaft m.b.H. (Materials Centre Leoben), Leoben, Austria
16.	**POLITO**	Politecnico di Torino, Torino, Italy
17.	**R-TECH**	Steinbeis Advanced Risk Technologies GmbH, Stuttgart, Germany
18.	**TECNALIA**	Fundación Tecnalia, Donostia-San Sebastian, Spain
19.	**TUD**	Technische Universität Darmstadt, Darmstadt, Germany
20.	**TUG**	Graz University of Technology, Graz, Austria
21.	**TUW**	Technische Universität Wien, Wien, Austria
22.	**UH**	University of Hertfordshire, Hatfield, Herts, UK
23.	**UNIVPM**	Università Politecnica delle Marche, Ancona, Italy
24.	**UPM**	Universidad Politécnica de Madrid, Madrid, Spain
25.	**WRUT**	Wroclaw University of Technology, Wroclaw, Poland
26.	**WUT**	Warsaw University of Technology, Warsaw, Poland

Individual members

1.	**Katarzyna Pietrzak**	Warsaw, Poland
2.	**Michał Basista**	Warsaw, Poland
3.	**Krzysztof Doliński**	Warsaw, Poland
4.	**Michał Urzynicok**	Koszęcin, Poland
5.	**Peter Hansen**	Ammanford, UK

KMM-VIN Associate Members

Institutions

1. **BEG** Böhler Edelstahl GmbH & Co KG, Kapfenberg, Austria
2. **BSGA** Böhler Schweißtechnik Austria GmbH, Kapfenberg, Austria
3. **CSM** Centro Sviluppo Materiali S.p.A., Rome, Italy
4. **GE Power** General Electric Power Ltd, Rugby, UK
5. **UNIMORE** Università degli Studi di Modena e Reggio Emilia, Italy
6. **UNIPER** Uniper Technologies Limited., Coventry, UK
7. **ENS P-S** Ecole Normale Supérieure Paris-Saclay, France
8. **ETD** European Technology Development Ltd, UK
9. **ETE** Energietechnik Essen GmbH, Essen, Germany
10. **EU-VRi** European Virtual Institute for Integrated Risk Management, Stuttgart, Germany
11. **GSC Ltd** Goodwin Steel Castings Ltd, Hanley, UK
12. **IMSETHC** Institute of Metal Science, Equipment and Technologies with HydroAerodynamics Centre of the Bulgarian Academy of Sciences, Sofia, Bulgaria
13. **IS** ŁUKASIEWICZ-Instytut Spawalnictwa, Gliwice, Poland
14. **LU** Loughborough University, Loughborough, UK
15. **MPA** Materialprüfungsanstalt Universität Stuttgart, Germany
16. **NOMASICO** Nomasico Ltd, Nikosia, Cyprus
17. **NUIG** National University of Ireland, Galway, Ireland
18. **NTUA** National Technical University of Athens, Athens, Greece
19. **SIEMENS** Siemens AG, München, Germany
20. **SSF** Saarschmiede GmbH Freiformschmiede, Völklingen, Germany
21. **SWG** Schmiedewerke Gröditz GmbH, Gröditz, Germany
22. **TUBAF** TU Bergakademie Freiberg, Germany
23. **UCM** Universidad Complutense de Madrid, Spain
24. **UL** University of Limerick, Limerick, Ireland
25. **VAGL** Voestalpine Giesserei Linz GmbH, Linz, Austria
26. **V&MD** Vallourec & Mannesmann Tubes, V&M Deutschland GmbH, Düsseldorf, Germany
27. **VTT** VTT Technical Research Centre of Finland, Espoo, Finland
28. **VZU** Výzkumný a zkušební ústav Plzeň s.r.o., Plzeň, Czech Republic

Individual members

1. **Peter Mayr**, Munich, Germany
2. **Alex Lanzutti**, Udine, Italy

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