

Report on 1st Co-creation Workshop of NanoMECommons project: *“Materials characterisation challenges to support the industry transition in the digital era”*

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Authors:

Nadja Adamovic, TU Wien (Austria) and EMMC President

Miguel Banares, CSIC (Spain) and CHARISMA coordinator

Bojan Boskovic, Cambridge Nanomaterials Technology (UK) and EMCC Organisational Management Board

Małgorzata Celuch, QWED Sp. z o.o. (Poland) and EMMC Model Development Focus Area Co-Chair

Costas Charitidis, National Technical University of Athens (Greece), NanoMECommons coordinator and EMCC Organisational Management Board

Donna Dykeman, ANSYS (UK) and EMMC Associate Member

Gerhard Goldbeck, Goldbeck Consulting Ltd (UK) (NanoMECommons WP1 Leader) and EMMC Executive Secretary

Gerard Kada, Keysight (Austria) and NanoBAT coordinator

Ioannis Kakogiannos, IRIS (Spain) and NanoPAT coordinator

Athanasios Katsavrias, National Technical University of Athens (Greece) and NanoMECommons coordination team

Ferry Kienberger, Keysight (Austria) and NanoBAT coordinator

Georgios Konstantopoulos, National Technical University of Athens (Greece) and NanoMECommons project manager

Elias Koumoulos, CEO at IRES (Belgium) and EMCC Organisational Management Board

Mirco Kröll, BAM (Germany) and i-Tribomat testbed representative

Argiris Laskarakis, AUTH/LTFN (Greece) and RealNano project manager

Stergos Logothetidis, AUTH/LTFN (Greece) and RealNano coordinator

Nikolaos Nikoloudakis, National Technical University of Athens (Greece) and NanoMECommons coordination team

Rui de Oliveira, BASF (Germany) and researcher scientist in BASF

Nello Li Pira, CRF (Italy) and Global Materials R&I and Roadmap manager, Materials Engineering Methods & Tools

Alan Ryder, NUIG (Ireland) and Pat4Nano coordinator

Marco Sebastiani, University Roma Tre (Italy) and EMCC Organisational Management Board

Dionysios Semitekolos, National Technical University of Athens (Greece) and NanoMECommons coordination team

Alexandra Simperler, Goldbeck Consulting Ltd (UK) and EMMC Associate Member

Nikolaj Zangenberg, DTI (Denmark) and EASI-STRESS coordinator

Contents

1.	Background	4
2.	Session: Interoperability - Standardisation - Harmonisation	6
2.1	Overview of characterisation, modelling and standardisation activities on Residual stresses	6
2.2	Overview of characterisation, modelling and standardisation activities on Raman spectroscopy	6
2.3	Discussion - Can our communities find ways to compare “materials” so one could confidently say, when two specimens are identical?	8
2.4	Process Analytical Technologies - Real-time monitoring of particle suspensions for Industry	8
2.5	Real-time process monitoring for digital production processes	9
2.6	Discussion - Do our communities consider meso and nano materials in-depth?	10
2.7	In line 4D characterisation to address nano-manufacturing challenges	11
2.8	Discussion - Directions in modern (4D) characterisation to support emerging manufacturing challenges in Industry	13
2.9	Benefits of novel tools open to Industry from Open Innovation Testbeds	14
2.10	Discussion - Make industry more confident; demonstration of the benefits of novel tools and concepts.	17
3.	Session: Think Digital - entry to a new era	18
3.1	EMCC - Bridging digitalisation needs for characterisation in Industry – CHADA	18
3.2	Discussion - Bringing digitalisation of characterisation closer to Industry needs - Make CHADA interoperable and machine readable	21
3.3	EMMC - MODA and CHADA integration and exploitation to Industry	22
3.4	Discussion - MODA and CHADA; challenges and opportunities for integration and exploitation to industrial stakeholders beyond EU projects	25
3.5	Discovery of new knowledge by aiding interoperability and integration in an Open Innovation Environment	25
3.6	Discussion – Concepts/Objectives for Interoperability of characterisation and integration to an Open Innovation Environment for discovering new knowledge	27
4.	Session: Industrial Insights	28
4.1	Industrial perspectives on the utility of CHADA and MODA	28
4.2	Focused Automotive needs for new advanced materials and characterisation	30
4.3	Discussion - Evolution of materials in future vehicles: a new paradigm for the automotive components	32
4.4	Digital Infrastructures	32
4.5	Discussion – Building an industry-driven “innovation ecosystem” through the establishment of platforms for characterisation	35
5.	Brainstorming - Round Table session	37
6.	Conclusion and Outlook	42
	Acknowledgements	46
	APPENDIX 1: Event Agenda	47
	APPENDIX 2: Event Pictures	50

1. Background

This co-creation workshop event was organised by the H2020 project NanoMECommons¹ with the support of the European Materials Modelling Council (EMMC ASBL)² and the European Materials Characterisation Council (EMCC)³.

Industrial twin transition into industrial context is well-established and demanding process. The emerging changes in manufacturing and Industrial revolution worldwide includes automation, process adaptation, and characterisation tools (standards, SOPs, integration with modelling) to efficiently support the transition to Industry 4.0 and 5.0^{4,5,6}. Industry goals contain the circular and safe manufacturing by design, data-driven control and tailoring of materials towards waste reduction, which is evidenced by zero-defect manufacturing and real-time anomaly detection procedures. Additionally, the precise characterisation of materials is a key point to acquire this information while the needs for high speed and reliability remain a state-of-the-art topic. Reliability is often a concern and the catalyst in digitalizing the information, which comes to address the EC directive for Open and Reusable data⁷. Modelling, Artificial Intelligence and EU competitiveness are all dependent on the quality of data to establish accurate predictive models, intelligence in materials design, process automation and adaptation providing further high-quality products for Industry and Society end-users. Especially, data management and Open Data are expected to fulfil the ambition of reducing effort and resources needed towards product development and reduce duplication of work, which is also expected to reduce the energy demand derived by the use of digital infrastructures to support the Industry 4.0 needs. Thus, a common language and wider communication plans are required to raise awareness about the actions at European level via EC-funded projects, where currently EMMC and EMCC councils coordinate relevant activities for knowledge transfer across modelling/ontology and characterisation projects, respectively.

Examples of relevant actions from both councils towards the increment of manufacturing reliability are the standardisation activities for widely accepted data documentation for modelling and characterisation, MODA (CWA 17284, 2018) (de Baas, 2014) and CHADA (Sebastiani, Charitidis, & Koumoulos, 2019), respectively. Current efforts in Europe to support interoperability are realised in NanoMECommons project, where CHADA is being ontologized according to EMMO⁸ requirements, which was developed under the umbrella of EMMC to support the applied sciences cases where modelling and characterisation is required.

In this Workshop, the main objective is to aid and encourage synergies between existing NMBP characterisation projects, testbeds, EMMC and EMCC. As it is recognised nowadays, knowledge transfer and united efforts are crucial to support developments, which will be exploited and will improve Industry to various dimensions. Many new insights have been gained through the work

¹ <https://www.nanomecommons.eu/>

² <https://emmc.eu/>

³ <http://characterisation.eu/>

⁴ Deguchi, C. Hirai, H. Matsuoka, T. Nakano, K. Oshima, M. Tai, S. Tani, What Is Society 5.0?, Society 5.0: A People-centric Super-smart Society, Springer Singapore, Singapore, 2020, pp. 1-23.

⁵ M. Doyle-Kent, P. Kopacek, Industry 5.0: Is the Manufacturing Industry on the Cusp of a New Revolution?, Springer International Publishing, Cham, 2020, pp. 432-441.

⁶ A. Gabriele, The Made in China 2025 Plan, Enterprises, Industry and Innovation in the People's Republic of China: Questioning Socialism from Deng to the Trade and Tech War, Springer Singapore, Singapore, 2020, pp. 171-178.

⁷ <https://digital-strategy.ec.europa.eu/en/policies/open-data>

⁸ E. Ghedini, G. Goldbeck, J. Friis, A. Hashibon and G. J. Schmitz. The European Materials & Modelling ontology (EMMO). Available on <https://github.com/emmo-repo/EMMO>

performed in different European projects and the need for closer engagement with the activities of both councils is important to support the multidisciplinary character of integration of characterisation and modelling activities and provide innovative solutions to Industry. The following topics of the Workshop⁹ were discussed and the directions for standardisation and digitalisation according to emerging Industrial needs were defined and will be used for a structured consultation process to ensure a wider impact of the work which is being performed:

- Interoperability – Standardisation – Harmonisation
- Think Digital – entry to a new era
- Industrial Insights

The organization of the Workshop is connected to previous satellite event¹⁰ hosted by EuroNanoForum in May 2021. Costas Charitidis welcomed the audience, and the summary of the NanoMECommons Workshop objectives was presented. The first goal is to proclaim knowledge and share new ideas amongst academic scientists, researchers, engineers, and stakeholders from areas of nanotechnology, modelling and (nano-)characterisation. Another goal is to gain deep insights in the work performed in other characterisation NMBP projects and Open Innovation Testbeds⁸ and to establish synergies between them towards the goals of modelling, characterisation integration and interoperability of the new Horizon Europe¹¹ programme and the Open Innovation¹² (Pillar 3 in Horizon Europe). Moreover, a strong point was the opportunity to benefit from the presence of two European Councils, EMMC and EMCC to provide our community with the chance to engage with the innovative work performed and coordinated via those councils, as well as build collaborations towards Industrial Green and Digital transition. The ultimate vision of the Workshop is the production of novel insights and to make further steps towards innovation in characterisation and modelling objectives for a more Resilient Industry by improving also societal impacts. This report provides a summary of the presentations and discussions based on contributions by speakers and attendees.

⁹ <https://www.nanomecommons.net/wp-content/uploads/2021/12/1st-Workshop-Draft-Agenda-%CE%9DanoMECommons-v4.1.pdf>

¹⁰ <http://doi.org/10.5281/zenodo.4912683>

¹¹ Horizon 2020 is an EU Research and Innovation programme, that was running from 2014 to 2020.

¹² https://ec.europa.eu/info/horizon-europe_en

2. Session: Interoperability - Standardisation - Harmonisation

2.1 Overview of characterisation, modelling and standardisation activities on Residual stresses

Nikolaj Zangenberg from the Danish Technology Institute gave an overview presentation of the H2020 EASI-STRESS¹³ project activities and standardisation activities. The project will shed light on the Industrial problems related to residual stresses in materials manufacturing. This is an issue which is tackled using both characterisation and modelling tools; though, it remains for the scientific community uncertain and often termed as the known-unknown. This is the case especially for the metal industry, including automotive, energy, wind, additive manufacturing, and aerospace.

Currently, the safety considerations lead to the usage of quite high safety factors for manufactured components to prevent stress-induced failure. EASI-STRESS uses two neutron and two x-ray synchrotron facilities to access materials information in depth about stresses in the bulk of metal components to reduce the risk for failure and prolong the service life of the component during the use phase. These sophisticated and complex characterisation tools for internal stresses monitoring will be the subject for CEN standardisation activities in EASI-STRESS since standards are important for Industry, as they contribute to the successful Harmonisation of characterisation results. First in EASI-STRESS, a Technical Specification (TS) will be developed, which is considered to be an initial form of a standard. The Danish standardisation body (DANAK) is supporting the standardisation tasks in the project, which will contribute to the successful establishment of a standard. Current needs are on providing the required information of the sample preparation and guidelines for conducting a measurement. Moreover, it is also required the widely accepted calibration methods and reference samples. In addition, definitions about data collection and data management strategies, which are connected to the characterisation method, are a must to ensure the development of robust modelling tools.

By assuring the high quality of data, modelling of stress in materials, could accelerate the access to information about the material state, but the complexity of this problem requires the engagement of the modelling community. Some modelling efforts focus on extracting modelling data from the virtual representation of the characterisation procedure to validate the experimental results. One of the remaining challenges is about the use of models with high confidence in their prediction ability and turn over the current situation which is about depending on and trusting mostly the experimental characterisation data. More conventional methods are important but still are limited, since properties can be measured in the surface, or can be measured in a sample performing destructive testing. As such, another motivation for establishing modelling tools is to overcome these barriers which is a key step to convince Industry that these tools will provide added value.

2.2 Overview of characterisation, modelling and standardisation activities on Raman spectroscopy

Miguel Banares presented currently work being implemented in the H2020 project CHARISMA14. CHARISMA is focusing on Harmonisation of Raman spectroscopy and related work towards the industrial standardisation to establish characterisation tools for fast and precise material identification via universal Raman spectroscopy fingerprinting, which demonstrates high versatility. Raman spectroscopy is used widely since it is convenient, sensitive, providing valuable information about materials. Raman spectroscopy gives a lot of information about the molecular and crystalline structure

¹³ <https://easi-stress.eu/>

¹⁴ <https://www.h2020charisma.eu/>

in multiscale ranging from a few nanometers to macroscopic dimensions of the measured material.

Access to many databases is the main advantage for experimental validation, which further supports the spectra comparison, identification of compounds and even give the users the opportunity to share their data within the community. Even though Raman spectroscopy is widely used, signal variability remains the main challenge and the bias may be attributed to both user and equipment. Any fluctuations for a given sample could be dependent on the frequency, the intensity and can be even originated from the relative intensity of the peaks and baseline. Thus, the main issue remains the quantitative interoperability. In CHARISMA the big challenge is the Harmonisation of the output of various Raman instruments ranging from portable to high-end Raman systems, to manage and get a reproducible quantitative interoperable spectrum from any equipment.

To realise quantitative assessments, validations, or other operations of interest with the output spectra, current efforts in CHARISMA focus on demonstrating these capabilities on three very different applications. One of them is in catalysis and the fabrication of nanoscale materials, the second is about nanomarkers added to documents where there is the need of acquiring quantitatively interoperable information. In another demonstrator the focus is on the application of plastic to prevent the development of biofilm derived from bacteria, where it is possible to monitor changes in the molecular structure where it is needed to acquire accurate measurement. Accuracy is the focus, and a representative example of an application was given when supermarkets are verifying their material, they know whether these components are still active or not by using portable Raman spectroscopy. Another example is that of an additive that increases the durability of the raw meat by 50%, which could prolong the safe consumption period from two to maybe three weeks, hence it is very important to accurately detect the presence of biofilms, and certainty for preservation is of high interest. Conclusively, the motivation in CHARISMA is to enable the separation of all artefacts from different measurements so the resulted spectra can be quantitatively interoperable to correct and integrate the relative intensity of the peaks, the actual position of the peaks, the background, or any other effect.

In addition, in CHARISMA both the experimental part and the core of the software are investigated, which is dealing with spectra analysis algorithms so that the Raman characterisation of materials can be harmonised beyond working solely on the hardware and reference samples. By working on the algorithm and the protocols for spectral acquisition and all the computational quantitative analysis, is also possible to get into the chemometrics as well. The goal is to be able to correlate these random data with a specific state of processes or materials or identification or validation. Databases have a frontier role to accomplish this goal and in CHARISMA the FAIR¹⁵ approach is adopted across an Inter-laboratory consortium with 16 Raman systems with various laser lines, different kind of optics and configurations to compensate, correct and eventually harmonise all these random measurements from various systems. The measurement data are stored online via a big data streaming architecture to a platform and the programming interfaces applications enable access through different websites to handle spectra and to automatically apply corrections. From that point of view, the four key pillars of FAIR principles are critical to be able to create the appropriate ontology for the respective data so that all the information can be integrated. This is expected to be a great step towards success in CHARISMA by acquiring quantitative and interoperable Raman spectra for multiple applications. The documentation of the experimental workflows in the project is performed by using the CHADA structure which was developed in the H2020 project Oyster¹⁶. In the final remarks of the presentation, regarding standardisation activities it was shown that characterisation collaborations are already in place with VAMAS¹⁷ for harmonisation of testing and with a standardisation agency in Spain.

¹⁵ <https://www.go-fair.org/fair-principles/>

¹⁶ <https://www.cen.eu/news/workshops/Pages/WS-2020-010.aspx>

¹⁷ <http://www.vamas.org/>

2.3 Discussion - Can our communities find ways to compare “materials” so one could confidently say, when two specimens are identical?

Following the two presentations a short discussion revealed that challenges of CHARISMA and EASI-STRESS are quite similar in general. The debate is in harmonisation approaches and often the engagement of instrument manufacturers is required since the software is different. In some cases what is needed is to make changes in the firmware, where it is not always an easy task to engage the instrument manufacturers and for these reasons there are efforts in establishing partnerships with the main Raman manufacturer, coordinated by CHARISMA. Standardisation for safety applications has a big value and has already attracted instruments manufacturers interest if such a standard is possible to be implemented.

Another topic discussed is about providing guidance in sample handling, where specifically for biopharma Raman spectroscopy, signal is sensitive to humidity, which is one of the most critical issues in generating reproducible spectra. Guidance should also include possible error management strategies and subsequent analysis recommendations. Working with several standard reference materials was proposed, which helps to calibrate those effects. In the H2020 project Pat4Nano18, sample handling protocols are being developed towards this direction.

Beyond the standard materials, other materials are dependent on processing history. This is a factor affecting the measurement and all the other specifications as well. In these efforts, in Pat4Nano the engagement of the Joint Research Council in Galen, Belgium, was implemented to develop primary standards and secondary standards so that an approach is agreed to develop standards for wide variety different industries.

2.4 Process Analytical Technologies - Real-time monitoring of particle suspensions for Industry

Alan Ryder proceeded with an overview of developing real time technologies and tools for particle measurements in Pat4Nano. The motivation for real time monitoring of nano suspensions is related to the fact that their properties are largely determined by their size. Beyond the average size and the distribution of the sizes, also other factors play an important role in determining how a nanoparticle or nanomaterials suspension behaves when applied in real world cases. Features like the shape are also important, but other factors may not always be considered when particle size measurements are conducted such as: the chemical composition, the charge on the nanoparticles, viscosity, and refractive index. In addition, it is important to consider other parameters that are characteristic of the sample and affect the particle size measurement, which is one of the critical aspects to address within Pat4Nano. The main approach is about understanding the sample as a whole and how all the other characteristics have an impact on the measurements to determine which measurements are suited for which sample. An important challenge also is the particle size determination into an industrial relevant environment, particularly in the environments where someone is dealing with very highly concentrated suspensions of about 20-30, or even 50 wt.% nanoparticles.

Real time monitoring is expected to tackle the need of end users to be able to manufacture highly controlled suspensions, so that a highly defined analysis for a variety of different applications is required, especially for the manufacturing of inks and active pharmaceutical ingredients. The ultimate objective is to establish feedback loops to realise the precise control of manufacturing.

Another consideration for the harmonisation of characterisation is the influence of the interaction

¹⁸ <https://pat4nano.com/>

between the nanomaterial and the environment and how that affects the measurements in terms of the information that is extracted from a sample or single particles with adequate statistical relevance. This task requires complex descriptors that adequately describe the sample, the measurement and consequently, the information that is extracted, which can often be problematic. Another question on sampling is about how light scattering is affected by different particles, as well as the dynamic suspensions environment, which is often restricted by a limited number of techniques available that are suitable for measuring, especially in case of highly concentrated suspensions.

The ambition is to develop and use an integrated end user driven approach to exploit complementary particle size analysis technologies, aiming to serve inline and online real time monitoring of industrial manufacturing processes. In this direction Pat4Nano collaborates with two technology providers who supply relevant instrumentation while the project is constantly seeking for collaboration with new technology providers.

Another issue tackled is about ink suspensions, where it is needed to control the size distribution so that big particles are prevented from blocking the inkjet courts. Real world technologies can serve a wide range of other specialty materials used in green energy, battery, catalysis sector and so on. Efforts focus on the development of these tools to provide the ability of monitoring suspensions over a wide particle size range, from about 10 nanometers to 10 microns. Other capabilities include the extraction of the quantified particle size and distribution in real time and information of the chemical composition, which is in accordance with the needs of the end users. The end-user needs are constantly defined through information gathering exercises and are all inserted together in a series of databases. These repositories will be used to optimise the development of the instrumentation for seven individual particle sized technologies.

Validation is critical, and it is demonstrated to the end users that each technology addresses the corresponding purpose and can serve the manufacturing needs. Another objective is to combine multiple techniques together to provide combined information and feed into the technology development and vice versa to the end users. These online particle size analysis tools are expected to provide accurate process endpoint determinations, both inline and online, to gain a higher level of understanding of the processes in order to lead them to develop improved industrial manufacturing processes and materials.

2.5 Real-time process monitoring for digital production processes

Ioannis Kakogiannos presented the H2020 project NanoPAT¹⁹ ambition on developing process analytical technologies for industrial nanoparticle production. The main challenge is to acquire real-time information about nanoparticles which are used in end-products to enhance their properties such as colour, mechanical or chemical properties. The main qualities that affect performance depend on material and size. Currently, the main issue is that nanoparticles are much smaller than the wavelength of light and the actual “diffraction” limit. Different kind of techniques are employed in process analytical technologies for the determination of chemical production of nanoscale particles. The methodology to bridge this gap contains three novel complementary real time in situ particle size characterisation technologies, such as photodensity wave spectroscopy, optofluidic force induction and turbidity spectroscopy, which will be deployed for inline and online pilot process monitoring in different Industrial sectors and the manufacturing of silica, ceramic, hydroxyapatite, polymers and zeolite.

Innovative data elaboration techniques will be set up to identify by-design the most suitable nano characterisation. These tools will be integrated as an emerging solution to produce polymer

¹⁹ <https://www.nanopat.eu/>

dispersions which is expected to have a societal impact, including growth and job creation via post project Industrial commercialisation of the developed technologies. Wave spectroscopy is an inline technique which offers quantification of live absorption and light scattering in highly turbid, highly concentrated liquid dispersions that can perform well even under strong steering conditions. Another advantage of wave spectroscopy is that it is calibration free and it functions with optical fibre, where a fibre tip is inside the sample and emits light into dispersion in order to achieve a multiple light scattering which occurs as a photon density wave. Another technique is optofluidic force induction, which is a suitable high throughput counting method for real time process monitoring. Turbidity spectroscopy is a flexible optical technique for monitoring the evolution of suspending particles, which size ranges from approximately 100 nanometers up to 4200 nanometers with an acquisition speed up to one second.

In some cases, there is the need to perform real time monitorings and at the same time interconnecting them with other systems. Digital process monitoring incorporates different kind of protocols which are visualised in the developed Innopath platform. At the same time, Innopath platform is interconnected with the SCADA²⁰ systems and the ERP systems that are already installed in the industrial sites available in the consortium of NanoPat. The expected impact is to have quantifiable enhancement of the ability to control the quality and reliability, with consequent improvement of product lifetime and associated environmental impacts as well as to have a cross cutting, open innovation in improving different kind of technology providers including both RTOs and the end users. Strengthening the competitiveness and growth of companies will be combined with improvement of social acceptance of nanomaterials and nano safety, which is inline also with Nanosafety Cluster²¹ objectives.

2.6 Discussion - Do our communities consider meso and nano materials in-depth?

Pat4Nano and NanoPAT demonstrate complementarity and connection of the measuring methodologies of the particles. Especially, aiding the acquisition of their molecular state and relevant molecular insights was an important remark by a scientific point of view. A short discussion was regarding the Raman information that could demonstrate a complementary role, because usually water does not interfere and a lot of insight from particles samples can be obtained. A major question which remains unanswered is about the connection of different outputs from wet and dry monitoring techniques. In Pat4Nano, Raman spectrum is used just to identify the chemical composition and identify changes in the chemical composition, which is critical and relevant to particle size. In case the dispersion solvent changes, or if it is about a mixture of solvents in which a suspension is formulated, it may introduce changes in activity and refractive index. This is exemplified with a check on how light scattering intensity is affected. The quantification of the different components in the dispersion and the background may lead in the acquisition of big background signal.

Tyndall light scattering technique is important to provide intrinsic size information, so that background signal can be harvested and then interpretation in terms of particle size changes is implemented so that this change can be used for very subtle variant size analysis. By the utilisation of Raman and the scattered light from the background it is possible to use chemometrics and build robust models for particle size and particle size distribution. Another method is to look at the Rayleigh scattering and more specifically at the variation of the real scattered signal part and incorporate the measurement results in a more holistic approach for spectra normalization. Consequently, the size information is not acquired by a direct measurement. Size change information is collected and by coupling it with offline

²⁰ [https://inductiveautomation.com/resources/article/what-is-scada#:~:text=Supervisory%20control%20and%20data%20acquisition%20\(SCADA\)%20is%20a%20system%20of%20that%20allows%20industrial%20organizations%20to%3A&text=Directly%20interact%20with%20devices%20such,%2Dmachine%20interface%20\(HMI\)%20software](https://inductiveautomation.com/resources/article/what-is-scada#:~:text=Supervisory%20control%20and%20data%20acquisition%20(SCADA)%20is%20a%20system%20of%20that%20allows%20industrial%20organizations%20to%3A&text=Directly%20interact%20with%20devices%20such,%2Dmachine%20interface%20(HMI)%20software)

²¹ <https://www.nanosafetycluster.eu/>

measurements from DLS or other techniques, can lead to the development of models suitable for online process monitoring, which could be essentially readout programming spectra in real time, track the chemical composition, the evolution or change in the particle size. Also, nearly for every case of sample it is realistic to build a robust key metric model for particle size and size distribution and pull-out spatial information, which is essential for technology transfer to the end users. This approach could be an efficient alternative that could result to obtain the vast amount of information in the spectra, which is lost during background corrections.

Another point discussed is about how the characterisation information based on the method developed in both Pat4Nano and NanoPAT projects can be used to integrate some modelling approaches to gain deeper insights about materials, i.e., the main purpose of running the AI and the possible enabling mechanisms such as process adaptation/automation for product optimisation. In NanoPAT modelling activities are integrated in the project's digital platform; AI computing is performed for feeding data for further processing and support process adaptation by monitoring nanoparticles behaviour, which is realised by detecting patterns amongst process and materials descriptors. Currently, solely data driven approach will not perform at maximum level and incorporation of physics-based models and chemical metrics is also required to be coupled in the process to go beyond the SoA.

In Pat4Nano modelling activities are focused on light scattering and scatter characteristics of the different nanoparticle sizes, so that it can be predicted what the scatter will be like at the different wavelengths of the spectrum. Subsequently, it is possible to realise experimental validation. The fundamental aspect of modelling in case of Pat4Nano, and more specifically in case to chemometric modelling as a better alternative than AI or machine learning is connected to the fact that AI often functions as a black box approach. This requires better dissemination with Industry and is regarded as a shortcoming when modelling is communicated to regulators. AI operations in Pat4Nano stick with approaches that can attract regulators, such as principal component analysis, since partially least squares involved in calculations are explainable and statistically based, which is enabling for technology transfer into Industry.

2.7 In line 4D characterisation to address nano-manufacturing challenges

Argiris Laskarakis from the Nanotechnology Lab LTFN/AUTH presented the work performed in RealNano²² project, which is coordinated by Stergios Logothetidis, and the actual proceedings in fast 4D inline characterisation approaches. LTFN is a Digital Innovation Hub and has an internationally acknowledged excellence in the fields of thin film technologies which are organic, organic electronics, and nanobiotechnology large activities in metrology and computational modelling at the nanoscale, which are expected to revolutionise our lives in energy generation sector in transportation and automotive, and in food production plants. Fast and reliable in-line characterisation is expected to boost the efficiency and revolutionise the large area production and to efficiently support emerging manufacturing challenges in the industry. This has been the case for the collaborative work between LTFN and Organic Electronics Technologies (OET) end user for the reliable and intelligent manufacturing of Organic Electronic (OE) devices. Through this collaboration, AUTH and OET have developed unique pilot lines for the fabrication of OE devices by wet processing, printing, and gas transport processes (Organic Vapor Phase Deposition – OVPD).

Organic Electronic devices are complex 3D device architectures that consist of printed nano layers (organic semiconductors, semiconductors, transparent electrodes, plasmonic nanoparticles) which have thickness of between 30 and up to 150-200 nanometers. One of the main challenges is to ensure that this quality will remain the same. Organic Electronic devices with reproducible properties is

²² <http://www.realnano-project.eu/>

required to serve the needs of organic photovoltaics (OPVs), where it has to be the same covering surface amongst several thousands of square meters produced. Their efficiency is not so high as in respect to the crystalline silicon or amorphous silicon photovoltaics, but organic photovoltaics have several unique advantages that include flexibility, low weight, the capability to integrate curved surfaces, and of course it is the greenest PV technology because materials can be recycled. The concept and the motivation are to develop lab scale innovations, because new materials, new device concepts mainly occur in small scale devices. The idea is to go to large scale manufacturing innovations in materials and devices are exploited, since large scale manufacturers and transferring technologies to commercial products like for example solar buses or energy efficient windows could demonstrate a societal impact.

The Idea is to include robust and intelligent characterisation method inside the process itself and several production stages, including printing of different nano-layers. It is needed to integrate inline metrology to get information during the process without affecting the process flow. The generated data are managed and transferred to an intelligent system to process this data either by using logical correlations or by using artificial intelligence methods to understand what happens in the process; if a material fulfils the specifications that the user has preset (or if not) to provide specific information in the pilot line to adjust the experimental parameters in a closed loop. Materials informatics provide information about what happens with the material intrinsically and provide knowledge for predicting the effect of using specific materials inside the formulations and the expected specific output. At the level of device manufacturing with a specific performance, process informatics ensure that the process is reliable and is optimised. The outcomes realised contain the minimisation of the waste of materials and the number of defective sites in the materials.

An issue which became evident during the last years, is related to all the data that are generated by using 4D characterisation, which could not be usable in the as-generated state, for example in case of inline reflectometers amongst other metrology tools. Through open innovation environment databases, it is possible to obtain data and manage them using specific structure to be usable by other types of manufacturing tools. The most important is the in line optical metrology by Spectroscopic Ellipsometry (SE), Raman Spectroscopy, Photoluminescence, and other emerging photoluminescence-based technologies.

The most important feature of spectroscopic ellipsometry is the capability to measure during the rolling of the film. This can be a trivial task, because if you are trying to focus a light beam on a moving substrate that runs with several meters per minute, then it should be ensured that the information extracted from the material is reliable. Main concerns are about the vibrations from the hardware of the manufacturing facilities, and i.e. all the drums (R2R) are running very smoothly in order to get sufficient results.

4D characterisation contributes to get accurate information about the process reliability; for example, for the printed roll a constant thickness is required, which is monitored with SE and a precision at 40 nanometers range can be realised in data acquisition, and variations could be correlated to the misalignment of the head or to the instabilities of the rolling. By using this type of metrology, the main idea is to detect the quality of the material that is printed and overlapping areas. The material control platform could be set up and notify when it is required to stop the process or to advance the process by setting the reliability limits in the upper and lower values. By identifying exactly the out of boundaries points it is possible to isolate areas of the printed OPV and perform cleaning by eliminating the defective cells from the whole OPV device. Specific modelling procedures enable the detection of the distribution of the polymer, electron donor and electron acceptor of organic semiconductors in the printed films. So, in this way the morphology of the printed film can be controlled.

Another important aspect is to manage all metrology data, to curate data and to extract all the valuable parameters. Optical properties and thickness characterisation of roll-to-roll printed nano-layers corresponds to a data acquisition of about 50 MB of data per meter (considering only the SE technique). At pilot scale data management and curation is quite demanding, experts in the field such as ANSYS offer their expertise to serve the nano-manufacturing needs. For the management, organisation, formatting of those data is necessary to extract specific insights from these types of metrology control methods. The characterisation and modelling data documentation is aligned with widely accepted documentation protocols for indicating all these procedures. The implementation of metrology contains the preparation and description of the different characterisation and modelling activities using MODA and CHADA structures.

RealNano the project deals with the development of these metrology tools for real time nano characterisation, including Spectroscopic Ellipsometry, Imaging Photoluminescence, Laser Based Induced Current (LBIC), while in RealNano the fabrication of biosensors aims to the nano-detection of COVID antigens and proteins connected to cardiovascular disease, such as troponin. Other types of applications are about agriculture greenhouse photovoltaics, but also the integration of OPVs and OLEDs in automotive in cooperation with CRF manufacturer for integration into the interior and the exterior parts of the car. In RealNano and through the CORNET²³ project an open innovation environment has been created to support relevant developments.

While partnership in NanoMECommons and harmonisation activities for nanomechanics and Raman, and in other different sister projects OYSTER²⁴ and MAMMA²⁵, and including the participation in the open innovation testbeds it is supported the promotion of these activities and through services to the European industries for creating functional light surfaces for Organic Electronics. Complementary modelling activities take place in MUSICODE²⁶ project for the development of an operation and modelling platform that gathers different types of modelling structures and activities to couple with characterisation for the optimisation of organic electronics manufacturing.

The concluding idea was that it is important to have 4D characterisation to understand what happens during the process and to ensure that there is high reliability and ensure the quality and reliability of fabrication for advanced nanomaterials, as well as there is efficient use of resources in a pilot manufacturing lines, but also applicability in larger scale industrial manufacturing processes.

2.8 Discussion - Directions in modern (4D) characterisation to support emerging manufacturing challenges in Industry

The discussion focused on the participation of several EC-funded projects which may have led to the identification of specific needs for high-speed characterisation methods that could be incorporated for inline process monitoring. In general, it is identified that metrology is compatible with the characterisation metrology monitoring platforms that are adopted. The main condition to meet is that the tools incorporated in the production line do not to influence the process. It is important for an inline characterisation tool to provide robust, reliable, and fast data acquisition. Flexibility is another concern, to facilitate the adaptation, but also at the same time not to disrupt the process. It is not possible, for example, to integrate an electron microscope, but there are several spectroscopic tools that can be adjusted instead. Raman spectroscopy and electrical methods could be easily integrated. The integration of tools for assessing the nano mechanical properties could be a challenge, hence in this direction, there are several solutions available in the market for stopping the web for moving

²³ <https://www.cornet-project.eu/>

²⁴ <https://www.oyster-project.eu/>

²⁵ <https://www.mmama.eu/>

²⁶ <http://musicode.eu/>

during continuous production, i.e., by using dancer rollers in the line. Thus, the process could stop instantly the organic electronics foil for making a potential measurement and enhancing further these types of 4D characterisation tools to support production activities.

The next part of the discussion was around the need for establishing commonly accepted in line characterisation protocols in case there is a gap in current protocols/standards or if standardisation initiatives are required in case standard methods have not been established yet. Currently, RealNano, NanoMECommons and Musicode projects incorporate standardisation activities to answer current needs for single measurement tools or even standardise a combination of different characterisation tools. An indicative example is the transparent electrical properties measurement as a first tool and the subsequent use of a second tool for measuring the properties of the printed organic semiconductors. Afterwards, a widely accepted methodology to combine this information needs to be established to get added value through the synergy between the information from the two characterisation tools for the R2R pilot line, which is a dynamic system. It is not as simple as the case of a thin film that is grown just by using a single process of vacuum deposition. To combine the different steps of the deposition or printing with the integration of tools is enabling to gain insights from each one of these layers and assure the surface homogeneity, good adhesion between these layers. Developing a device is an additive process for the printing case, so it is important to extract information from specific stages during this additive procedure. These properties are determined by the homogeneous evaporation of the solvent during manufacturing and determine the homogeneity of the thickness profile of the printed analogous overlapping areas over several square meters.

2.9 Benefits of novel tools open to Industry from Open Innovation Testbeds

Mirco Kröll presented the work on Tribology, digitalisation, and the harmonised procedures developed in i-Tribomat²⁷ Open Innovation Testbed. The project develops procedures and shares ideas on how to deal with characterisation techniques and provide services to end users in different places and locations, which is realised by adopting a common and widely agreed procedures. i-Tribomat is active also via YouTube platform to enhance communication and spread the word amongst the interested parties and society.

A historical review was presented to show the impact of tribology in everyday life from the early years of humanity, where dealing with friction and wear was very common even in ancient Egypt; it was known that friction could be reduced, and the idea of using lubricant-like substances, to reduce friction and reduce the force required in several applications was familiar. It comes without saying that tribology is and will be an important property for the future as well.

Tribological behavior is always a system property, as are friction and wear as well. It was emphasised that it is not about dealing with the material characteristics, but with a system of at least two bodies, and the interfacial behaviour or even with their environment. There are many parameters that influence friction and wear. Every parameter needs to be dealt with friction and wear, which occur with and without motion. In addition, any motion adds to the variables, so that it is needed to describe the motion itself, and this is often itself an exhaustive process that needs many characterisation attributes to be determined. Therefore, tribology is important since friction exists everywhere and friction and wear cannot be eliminated, the community needs always to be confronted those factors in every application. In addition, from a strategic viewpoint, the European Green Deal²⁸ needs excellence in tribology as an important aspect to realise the long-term goals of carbon dioxide neutrality by 2050. Literature considers that tribological contacts consume 23% of the global energy

²⁷ i-tribomat.eu

²⁸ https://ec.europa.eu/info/strategy/priorities-2019-2024/european-green-deal_en#documents

produced²⁹. Friction is always an energy loss and at the same time the lifetime of products is limited by wear. Also, the need to replace any worn parts is always present, while at the same time, by optimizing the tribological context, it is possible to reduce the carbon footprint by 367 megatons. It is expected that a period of 15 years is required to deploy and optimise those tribological contexts.

These 370 megatons equal to 11% of the annual carbon dioxide emission of EU and this is indicative of tribology being a part of the picture of the carbon dioxide neutral Europe. In this direction, digitalisation work is performed on tribology sector within i-Tribomat project, where more than 950 attributes are collected not only describing the tribological test, but also the analytics which are involved to describe the tribological behaviour, the samples informatics before and after the tribological test, as well as statistics to describe the repeatability and reproducibility of the tests which have been conducted for those materials. Moreover, a description of the history of the samples is collected: where was a sample manufactured, details about the manufacturing, preparation, exposure history of the sample prior to any tribological test, and the subsequent analysis that has been conducted. All the information that is collected is complying to the FAIR principles, which can ensure that it provides the ability to reuse data in an unbiased way. In tribology it does not matter only which sample is resisting against motion, but also the counter body is of equal importance to the tribological system. So, in the i-Tribomat database the description corresponds to a system of more than one sample.

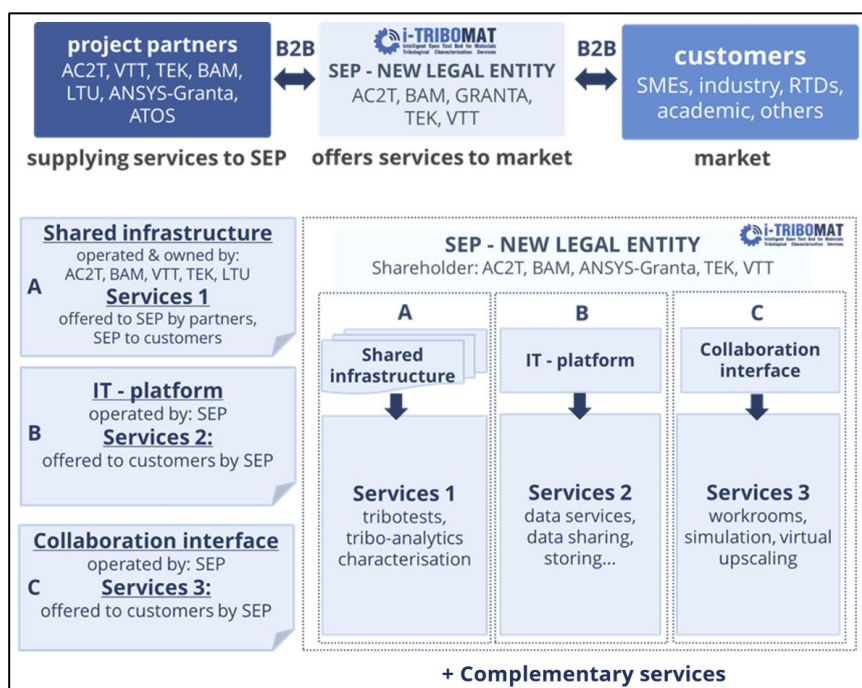


Figure 1. Structure and setup of i-TRIBOMAT.

In i-Tribomat the idea goes beyond a simple project, as it is intended to set up open innovative testbeds and businesses. A European Tribology Centre is funded, which is already a registered trademark, and the main services have been officially mentioned. The services contain shared infrastructures, data driven services via an IT platform, and a collaboration interface, which includes simulation and modelling services where a user can virtually upscale materials of laboratory model tests, while at the same time complementary services like patents, publication searches or the search for additional data beyond the i-Tribomat database are realised. The Consortium of i-Tribomat offers its services to the European Tribology Centre, so so that the latter becomes the bridging element

²⁹ Holmberg, K., Erdemir, A. Influence of tribology on global energy consumption, costs and emissions. Friction 5, 263–284 (2017). <https://doi.org/10.1007/s40544-017-0183-5>

between the customers and industry with the academic partners. It is like the one stop shop for providing tribological services to the to the European industry and European customers. This business is only possible when access is provided to fast digital tools and infrastructures. So, the European Tribology Centre is at the end of that a digital business. Cyber security and interoperability have been ensured to satisfy the needs of a digital business.

In i-Tribomat specific tools have been developed and exploited in three application areas, amongst them, bearings and gear boxes for wind turbines, symmetric seals and components. Characterisation tools amongst the shared infrastructure contains mainly tribometers which are used for testing materials in tribological contexts, while complementary characterisation tools are dependent on the capacities of the i-Tribomat partners i.e., roughness, hardness, chemical analysis and chemical composition determination, which are used to collect more insights of materials condition before and after the tribological test.

Over 250 experts are providing services and support for the industry to assist and find the right characterisation techniques, which is enabling for realizing the exploitation of these tools. Another benefit is that all these tools are connected via IoT technologies. That means that the Internet of Things idea is also coming to tribometers, and the communications is implemented directly with the database. Data can be directly uploaded without any need for manual input, which can preserve mistakes or other error origins, due to the direct connection of equipment to the database. The IT platform of i-Tribomat offers data driven and cloud services to customers, Industry, and RTOs, such as access to software tools, visualisation, and report creation, while information is distributed only digitally, which prevents any risk of the information being outdated. This is reinforcing IT competencies since commercial software is requiring licenses to access tools and services. In addition, another service is about the modelling and simulation collaboration interface, which is important to realise the tribology problems in a larger scale, which is the case for big components and what information Industry needs to access, since experiments are limited to measuring friction and wear.

Harmonisation procedures have been established in i-Tribomat to determine friction, which is commonly realised by the determination of the coefficient of friction as a direct measure of friction. The way, moment, and hysteresis in movement lead to different ways to calculate the coefficient of friction, i.e., the mean coefficient of friction averages the coefficient of friction and hysteresis, while other ways to measure the friction are much more complicated such as the energetic coefficient of friction and the geometric independent coefficient of friction. The harmonisation of characterisation output is something which is implemented to offer high quality services via a shared infrastructure and ensure that the test results are comparable, reproducible, while repeatability and high quality of data is acquired.

A current shortcoming in tribology is that the standards available are suboptimal. This fact highlights that there is still room for advances in the field. The Continuous Improvement Process is a standardised tool, which is part of the very well-known standard ISO 9001³⁰ and implemented in i-Tribomat for quality management issues. The PDCA tool – Plan-Do-Check-Act – is used for analysing and improving the results and derive best practices for the method applied from each partner. Another thing which has been taken into consideration are the costs of the services of this digital enterprise as well as improvement suggestions.

Best practices have been established for tribology tools, and what has been already achieved is the reduction of interlaboratory variation from the doubled value of standard deviation linked to existing standards and practices, to half the value upon harmonisation and application of improved standards. Efficient communication is realised via restful APIs for determining roughness where home grown

³⁰ <https://www.iso.org/standard/62085.html>

algorithms for statistics - written in Python or R - are implemented.

2.10 Discussion - Make industry more confident; demonstration of the benefits of novel tools and concepts.

The discussion tried to tackle a topic beyond the presentation context regarding inline characterisation services for Industry and any emerging challenges that should be overcome to realise the inline characterisation about the tribological characterisation. Currently, the inline property monitoring in Industry is implemented via sensor-based technologies, such as friction sensors or sensors about the quantification of energy lost by the machine. In fact, in an industrial line, it is not possible to measure what is happening between the surfaces with a tribometer and sampling is required to take apart the system to really investigate and to measure the wear volume via confocal microscopy.

There are approaches on how to measure actually inline in machines, i.e., while the machine is working, but limited only to Artificial intelligence approaches, for example, via vibrations correlation with the wear volume. Since the project solely focuses on tribological characterisation techniques, work on the development of new sensing systems, the harmonisation of inline sensors at industrial relevant environment and machine intelligence engagement for sensor-based systems, it is an orientation for future work to solve tribology challenges.

Regarding the novel digitalized tools to be used for characterisation in i-Tribomat platform, the possibility to support the simulation of characterisation was discussed – Digital labs – that describes the service life in demanding application environments, such as exposure to ageing factors and high temperatures. In fact, one of the three main services of i-Tribomat is about the collaboration interface which is only focusing on modelling and simulation, and this is very relevant to the specified needs for tribological performance characterisation and upon the exposure at high temperature and then data are used to establish models for the real application and to simulate extreme pressure or temperatures events.

3. Session: Think Digital - entry to a new era

3.1 EMCC - Bridging digitalisation needs for characterisation in Industry – CHADA

The collaborative presentation of Marco Sebastiani and Costas Charitidis took place to give insights related to EC funded projects OYSTER and NanoMECommons, and to present the identified gaps for Industry on behalf of EMCC. The three main messages of the presentation are related to new initiatives for the next years to come under the coordination of the European Materials Characterisation Council, the development of new standardised data formats in data structures, which started within OYSTER project and further developments are implemented within NanoMECommons and, finally, ideas for future activities in characterisation to fill the identified gaps, which could be addressed for example in future topics and the next work programme of the European Commission. The aim is just to promote discussion within the Workshop and interact fruitfully with many experts who can bring insights about the challenges in the near future for the materials, characterisation and modelling.

The EMCC encourages the adaptation of the materials modelling and characterisation manufacturing triangle schema. Currently, Oyster project has been aligned with this EMCC directive. The EMCC paradigm is based mostly on this triangle, and more specifically on the deeper integration and interaction among materials circular manufacturing, experimental characterisation, and modelling activities, which is the core engine for digitalisation and vice versa. Beyond the activities on digitalisation, standardisation it is also needed to establish a common language with Industry. Thus, this scheme ensures a balanced presence of a characterisation, modelling, and manufacturing, which could be included in all future topics related to materials, modelling, manufacturing, and characterisation, and ensure the high-level impacts from European projects.

In 2022 the EMCC will publish the new Roadmap and will move towards the next steps of the development of the CHADA structures. The current contributors are amongst the EC funded projects, which are affiliated to EMCC, which with the new technologies and numerous experts working on these technologies could be the basis for the development of a robust new roadmap, focused on these two main areas that should be strengthened: digitalisation and automation. Also, main priorities pay tribute to promoting safety and enabling the Green transition. This is a summary of the high-level goals of the Characterisation Council and future work will contain core activities to achieve the integration among manufacturing, modelling and characterisation. Emphasis should be given to digitalisation as the main core engine for innovation and then keeping working on the key activities, which include development of ontologies and harmonisation of testing procedures to enhance management, quality of data and deliver improved models, as well as the deployment of web platforms, which will exploit the modelling and characterisation tools.

An interesting initiative that could be realised in the next years is about establishing an effective and fruitful connection between INFRAIA-projects, so that large infrastructure activities of lower TRL and NMBR projects join forces to provide innovative technologies at a higher TRL level. Since all these projects work on advanced characterisation, it is important to align and establish a connection and improve communication between these two domains via the EMCC Roadmap. The idea came from Ennio Capria from ESRF and could try to use EMCC as a way to establish a clear connection. The outcome would be industrial application of the roadmap, which is a possible strategy for imminent implementation and could be a promising path to accelerate the progress on the digital and green transitions.

In the second part of the presentation NanoMECommons and Oyster projects were presented, which have some common activities on nanomechanical characterisation and the activities on the development of the CHADA structure and concepts. In NanoMECommons the main objective is the

harmonisation of nanomechanical testing procedure. In the project there is a series of industrial relevant case studies that have a common basis on the harmonisation of nanomechanical testing, in combination with other techniques like electron microscopy, diffraction, optical spectroscopy. What is expected is the development of widely accepted and reliable protocols for Industry. Another target is to move forward regarding the CHADA structure to develop an ontology which will make the CHADA interoperable among the different and multiple characterisation techniques. A representative example is the combination of nanomechanics with high resolution diffraction, amongst other technologies to serve industrial relevant and representative environments. Materials to be characterised in NanoMECommons contain superhydrophobic coatings for automotive, microelectromechanical systems and in particular radio frequencies applications, organic electronics, and additive manufacturing. There are a series of industrial players, amongst them large companies, small and medium enterprises. The final objective would be for each case study to develop an integrated and harmonised characterisation workflow based on different CHADA and interaction among the different characterisation, so the enabling and interoperable i-CHADA will be developed to move forward with the development of novel materials and manufacturing processes. For example, for the automotive application apart from conventional microscopy, several techniques will be combined including advanced nanoindentation mapping, X ray diffraction mapping and advanced atomic force microscopy to validate and develop new materials.

In the Oyster project, the focus is narrower with specific focus entirely on adhesion properties. Innovative protocols have been developed for the nanomechanical testing to feed the development of superhydrophobic materials for several applications, and the project is now going to be completed in the next few months. These are a couple of examples on superhydrophobic surfaces that have been developed, and the incorporation of the manufacturing, characterisation, modelling triangle, which aided the development of new materials and new characterisation methods. New methods correspond to measurement procedures to characterise adhesion and surface free energy by nanoindentation and by atomic force microscopy. Moreover, new multiscale models have been developed to describe the materials at a multi-scale level; atomistic to continuous to understand the effect of chemistry, topology and surface morphology on wettability and for different applications of the industrial partners. This is a representative example from OYSTER on a balanced approach among these three aspects, which was implemented and assisted by the internal engine of the open innovation environment, which is a platform entirely based on the development of new ontologies in this case for nanomechanical testing.

In Oyster standardisation activities took place via a CEN workshop, which was successfully completed, and a CWA agreement was published, which includes the material characterisation, terminology, metadata, and classification. This CWA contains a widely agreed and shared standard in an open document that was prepared thanks to the contribution from more than 60 experts. This document is published and open to public and could be the basis for the further development of the CHADA structure.

In this CWA, the experts practically agreed that the data documentation for any material characterisation should be defined according to four main classes specified for CHADA as well as the user case experiment, raw data and metadata, and the metrological chain definition. Within an individual experiment different steps may be refined, but any of these steps, such as the probe that was used for testing, the signal that is acquired at the time, the detector, the noise, and also other factors are contributing to the definition of the metrological chain. Then raw data, which is the set of data that come out of the experiment, and after the data analysis, the metadata are also refined. Methods development is not an easy task, and it was interesting to open a fruitful discussion with all the experts with different expertise from different communities during these CWA preparation meetings on how to make the data structure utility to facilitate working with different methods. The

CHADA templates can be used to define the main workflow, and the use of the other templates is about the detailed data documentation. All the instructions have been included in the CWA that was published, including the preparation procedures for these workflows but also the documentation procedure for each item of the workflow in the sublevels. So, the structured information with the maximum level of details leads to the completion of the data documentation.

Clearly now the main challenge is to collect more and more examples from the different projects. The main point now is to enable and provide interoperability among the different techniques by adding new features. This CWA can be the basis for this action, and it is important that it is realised a wider adoption and of these common documents for the new activities. For the new actions in this way it will be easy to make results compatible between one project and another, and to work towards a synergic action rather than individual project actions that sometimes are not effective at the end. A second priority is to implement CHADA documentation into web platforms.

For the third part of the presentation, some ideas were shared regarding the characterisation and digital and green transition were presented, as well as ideas on how the community can work together to define the new roadmap of EMCC. A couple of ideas were put together on what could be the next challenges for materials characterisation and how this could be made by interaction between and among different projects. The first idea would be trying to validate a universal characterisation data structure, which could correspond to a universal CHADA which can be made only by interaction among the projects. Another point would be also to establish a link between MODA and CHADA, so the models used for analysis are linked directly to the workflow. Thus, it is important to start interacting between modelling and characterisation to make data interoperable and to make more effective the application of advanced characterisation into modelling and vice versa. There are two main technical challenges; first, to improve the data driven AI representations, predictive modelling which is important for the digital transition. Another enabling activity is to improve the effectiveness by which data both coming from modelling and characterisation can be used to develop new products and new manufacturing processes. Finally, the development and standardisation of reliable, fast 3D and 4D characterisation methods is a priority, which can be supported by artificial intelligent toolboxes and the analysis of big data in large scale and high-throughput industrial characterisation level.

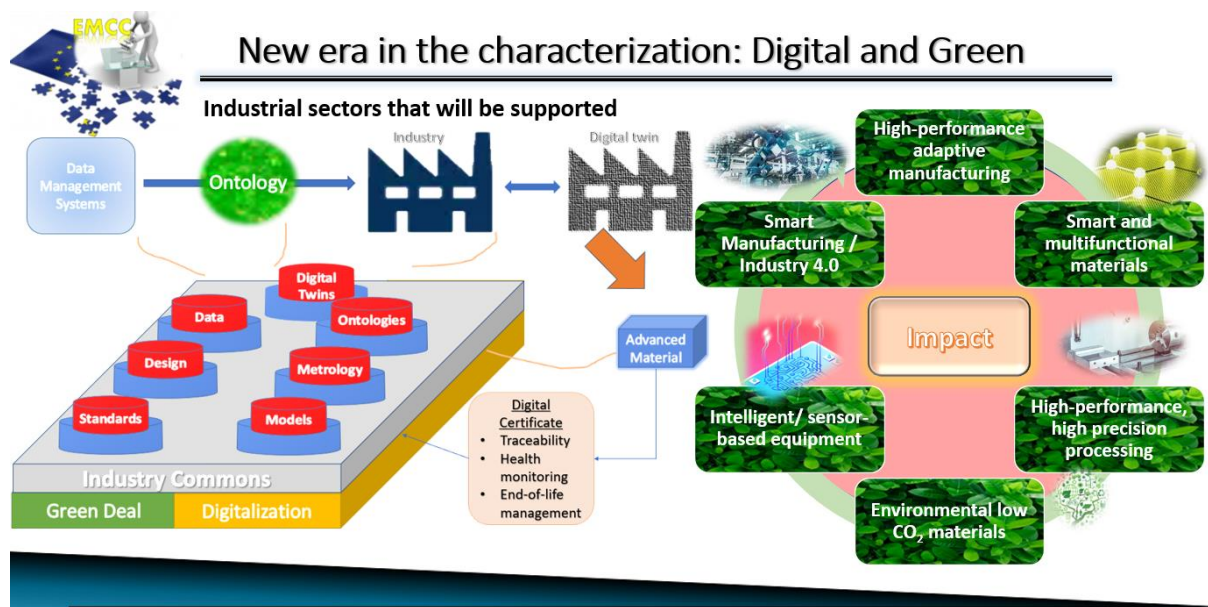


Figure 2. EMCC strategic priorities.

Orientations have been identified and can be used as ideas for new actions in the next future of the European Materials Characterisation Council. The first orientation would be working on integration

between modelling, simulation and process monitoring to enable new designs for faster time to market, and from concept to reality. Digitalisation and digital representation are expected to reduce the technological risk of innovative materials and products, and thus attract more investors, and could be enabling towards reduce, reuse, recycle of commercial materials. Regarding materials design, which is a dynamic process, could be supported by applying fit-to-purpose characterisation tools to assist the by-design development of materials and systems design with uncertainty quantification, management, manufacturing, trade-offs, analysis and risk assessment conducted in real time. The outcome of these technological directions would be to adopt digital technology and the products with lower environmental footprints and with improved efficiency. Then characterisation 4.0 could be integrated and smart testing that leverages simulation and characterisation standards, as well as multi objective optimisation approaches, to help minimise costly, time-consuming delays from excessive physical testing. Another possibility is to exploit interoperable platforms on the utilisation of manufacturing and the Green Deal activities. What remains unanswered is whether platforms can be designed to be interoperable. If the community can join forces to establish widely agreed common data structures, common architecture and data formats, this challenge could be addressed and make the platforms interoperable and give the capacity to support technology transfer and information exchange with Industry.

To summarize, the characterisation is now going into the twin Transition era, so it is clear that we really need now to work a lot on the integration between advanced characterisation and modelling and advanced manufacturing and the link between these should be probably the use of new digital tools that are open to everybody, and they can be used also to make Information exchange is easier between these different Domains.

3.2 Discussion - Bringing digitalisation of characterisation closer to Industry needs - Make CHADA interoperable and machine readable

The discussion focused on a possible and emerging need for education and training activities on the modern digitalisation skills. This could be enabling in the manner of bridging the knowledge gap between experts in characterisation and experts in digitalisation to accelerate and realise broader proceedings and innovation for Industry. This is a multidisciplinary field and many engineers, physicists, material scientists that are all involved could sometimes find a hard time to understand the digital terminology in depth and an indicative example could be the ontologies, the coding skillset that are required to build a platform and put it online. This need is very relevant in case the community has to accept the idea of future actions, which should always be multidisciplinary with experts from data science, from characterisation, modelling and manufacturing.

The training aspect is something that should be considered and covered by all projects because the community is not yet ready regarding the existing background for multidisciplinary. For example, experts in characterisation, with several years of experience under their belt will always feel much more comfortable when speaking about characterisation. This is not always the case when there is interaction and exchange of information on modelling, new digital tools and it is required to have a vision on future developments by a holistic aspect. It could be a fruitful idea as an additional orientation, at least to have these activities foreseen into the topics. This could be set up as a clear instruction that training of people to these new multidisciplinary approach to Manufacturing and materials development is important. Probably this can be another aspect of the roadmap of EMCC. Thanks to training activities in the end, education of new way of thinking probably is extremely important to bridge this knowledge gap. Of course, training activities could function also vice versa, because the software engineers may have difficulty to get deep into physics for example or the physics and mechanics during testing.

3.3 EMMC - MODA and CHADA integration and exploitation to Industry³¹

Nadja Adamovic, the president of EMMC presented the first part of the presentation devoted to MODA and CHADA, the main challenges and opportunities for integration and exploitation to industrial stakeholders beyond European projects. The background and motivation for this work was summarised. The situation one decade ago in both communities on materials modelling and characterisation was that there were multiple communities that were not well-networked together, which used multiple terminologies and there was no agreed classification or way of documentation. But, on the other hand, there was an increased industrial use that really produced the need for standards in documentation and interoperability of data following FAIR data principles. This is just one example from materials modelling community and MODA developments. Descriptions are defined by applications, phenomena, the scale, the software used or by a solver. There are multi levels in the description and this should be supported by a standardised tool to visualise and simplify the representations for the end user. Obviously for materials modelling but at the same time for characterisation as well, there is a need to develop a communication tool that captures and conveys publication of modelling and characterisation towards the wider audience and to present a complex characterisation and modelling process in a more visible, simplified and standardised way, so that the standardisation of the documentation is supported. These activities offer the potential also to be used in data management and as supplementary material in publications to ensure better quality control of publications. Another objective is to have also widely agreed terminology in the Community as a first step for digitalisation.

In 2015 the European Materials Modelling Council and the community started to develop templates for modelling data and there was a really large number of use cases, which is already provided on the website of the European Materials Modelling Council. In 2018 there was a CEN workshop agreement on the materials modelling, terminology classification and metadata. Similarly, EMCC have followed a very similar approach with CHADA and European projects use these templates in the description of characterisation process with a CWA agreement published in October of 2021. The collaboration of these two councils started many years ago, including joint presentations, events, collaborative input for the follow up work Programme Horizon Europe on the cooperation between materials, characterisation and materials modelling that was reflected in both Roadmaps. Within the International Workshop there was one relevant presentation on pairing up materials, modelling and characterisation that was done on behalf of European Commission by Javier Sanfelix and Yanaris Ortega, which also indicated the strategy and the need to collaborate on modelling and characterisation. All this effort resulted in one call that was published already in October 2021. EMMC organised one related brokerage event with participation of the European Commission that presented this open call and participants presented several project ideas and networking was promoted between participants.

Malgorzata Celuch proceeded with the second part of the presentation on behalf of EMMC. The problems which are still existing were presented, which are related with terminology and classification and standardised documentation. Some examples from projects were shown, and what is considered as a cornerstone was summarised. In MODA concept, this is the distinction of the different levels of abstraction or representation, where first a user case is identified, which is something that exists and based on knowledge and experience of what is needed, specific physics are assigned to the model to be developed. The results are obtained without any further post processing, and often a graphical representation is used for visualisation. All user case models, raw output and processed output are documented. The computational representation is hidden, since it is implicit; there is a simulation or a solver involved between them, although obtaining its output. The question now will be in how the development of both models and colours representations can be achieved and on how models and

³¹ The slides presented are available via <https://doi.org/10.5281/zenodo.5784379>

colours could be unified, as well as what kind of opportunities and challenges will be confronted.

Also, a different perspective was given, not as an official standpoint, but in the framework of sharing some ideas and thoughts about MODA and CHADA, which are not only consistent but also complementary. By looking at MODA and CHADA diagrams, the same colours are used, and a similar flow is adopted, so that compatibility between MODAs and CHADAs could be expected; one inconsistency has been identified since confusion could be caused focusing on the data or state of various operation or process. So, in a place where in a MODA we have a model that is an entity, in the CHADA we have an experiment which means a process that is going on. Similarly, MODA focuses on processed output, which means that data being the result of the modelling activity while CHADA focuses on the action of post processing. One possible suggestion would be to try and unify is to follow the graphic representation in a flow chart where we would use rectangles for data or state Versus diamonds for operation and process. An ideal combination could enable the data structures to be related on a “one to one” basis, so that each tangible element of a characterisation process has a corresponding dataset on a computer, which means an element of a model. And similarly, it could be enabled to have each physical process that goes on in an experiment to be emulated by an executable computer algorithm. So, if we could focus on this way of looking, both communities could improve the common language to exchange the ideas and go on further developments.

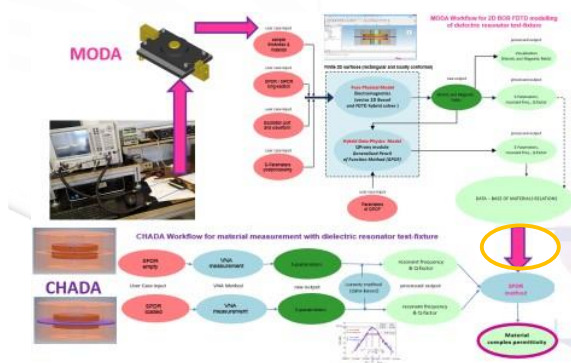
The twinning of MODA and CHADA has already been demonstrated and several examples of application in industry were presented. An example is about a set up for both modelling and characterisation, and more specifically electrical characterisation of materials in a gigahertz frequency range, which corresponds to the range used for phones and microwave ovens. The range of microwave tomography in medicine is important on several domains. A presented paradigm demonstrated a set up consisting of computer running the modelling, an apparatus which is running an experiment, which is driven by a computer application. This setup has been recognised as the European Horizon 2020 innovation beta, so this is a straight paradigm of having successfully twinned MODA and CHADA. A few suggestions for the community to consider were proposed. First, further efforts on development and unification; CHADAs are often a set of CHADAs, parallel, sequential, or linked, and distinguishing these elementary CHADAs may also help to reflect them by modelling. The second point is about when it is needed to go from this combination of the two experiments into the actual material data, where modelling is involved and this is always done, and most users believe that this is a kind of data conversion that is taking place in the apparatus is not fundamental, but actually is. Especially, these kinds of models are actually focusing on this essential test fixture on this environment where the experiment is taking place and the model will actually emulate the CHADA on a computer. As for the next step, that is about the raw data and post process data. So now in both MODA and CHADA all the raw data could be dark green and processed data could be light green. Moreover, the processing of the raw data is also the modelling, and this is shown in MODA.

Another benefit of twinning of the MODAs and CHADAs enhances the physical understanding of a case study for the researcher. This is the main point of the whole exercise, that knowing what kind of modelling corresponds to the specific characterisation, and vice versa, and helps the researchers understand what processes are going on in a material or in the apparatus using this material. Looking now at the objective opportunities and challenges of the two councils, it is a common will to enhance research, collaboration and the strong point is that standardised data can assist this process. The challenge is to adopt working systems, best practices, and standard operating procedures instead of the pre-established working habits. The ultimate target is to encourage industry to use these results. What is needed is to improve visualisation of the data structures, to devote a vast amount in training activities and develop this way of documentation. In the end, it is intended to enhance the European excellence through efficient and effective information flow, shorter time to market, but we have a lot of accumulated data in different formats, which is needed to deal with. Moreover, there is the need

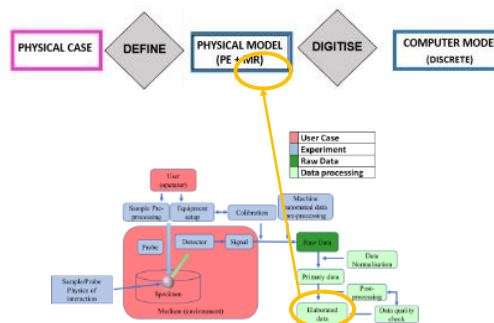
to simplify, unify, automate, disseminate, communicate, and teach.

Generalised relations between MODA & CHADA

1. CHADA needs input from MODA



2. MODA needs input from CHADA



3. a chain (network) of MODAs & CHADAs solves the User Case

Figure 3. Generalised relations between MODA & CHADA.

Possible directions to realise these objectives is to split the modelling in terms of MODA into two parts. The first is distinguishing the physical model and the second is digitising this model to have it on a computer. When we deal with data-based modelling, the first part becomes irrelevant. That leads to a low level result, since a part of data is used, and another model is utilised to obtain another set of results. In this way a recurrent scheme of modelling and data is acquired. The second point is about CHADA, which always needs input from a MODA, but a MODA also needs input from CHADA. In a presented graph it was shown a model graph where there are material relations and material parameters which will typically come from an experiment. A plain or a network of models and products is typically, what the user needs to solve the full problem.

Again, there are different problems to highlight, such as variability in the interpretation. It is also time consuming to fill the two tools and some experts say that there is not enough detail in MODAs and CHADAs, while others say they are too complicated. What is needed is to go for standardisation activities, integration, and establish foundations for machine interoperable data. In this direction, Workshops like this 1st co-creation Workshop organised by NanoMECommons, improve communication and collaboration. Another way could be to establish MODA and CHADA courses, including academic courses and teach standards at universities. Going beyond the materials research community, as there are many other physics and chemistries of interest in the industry, assemble success stories to show that it is worth going this way. A similar case is when there is a consulting process implemented, where documentation of results is this way to show the industry that an approach like this is useful. Possibly, a first enabling step could be the inclusion of MODA and CHADA as data supporting the publications quality and completeness. In this framework it may be worth having another workshop dedicated to combining MODA and CHADA.

3.4 Discussion - MODA and CHADA; challenges and opportunities for integration and exploitation to industrial stakeholders beyond EU projects

The discussion focused on the importance to unify MODA and CHADA as a next step. A current concern is that there are many running projects that aim at developing their own data structures and standards, and how these activities could be unified so that all the projects are developing CWAs which are harmonised and are in line with MODA and CHADA. One possibility could be to deploy common CWAs via synergies between the projects, which probably might be driven by project officers. Possibly it could be a preferable idea to go for one big CWA and standardisation activity rather than opting for separate CWAs. EMMC and EMCC aim is to integrate a pool of projects and stakeholders, not only European projects, but also Industrial stakeholders, other stakeholders, and to work together on one single CWA. Another concern is that standardisation activities are specific to a single technique or one material property, and it seems that this integration is not an easy task. Maybe if the approach is reversed to a top-down approach and what the community needs to have among data formats, taxonomies, libraries and afterwards go down to specific technologies could be enabling.

The interaction via Workshops can help to establish a common direction to proceed, but there are no ideal solutions and not on the short timescale of the projects. Examples of points for discussion, alignment and clarification include the color schemes of MODA and CHADA, and how they represent for example data and different types of processes. It was concluded that it is very relevant not only to have one common thing, but to facilitate the input from the users.

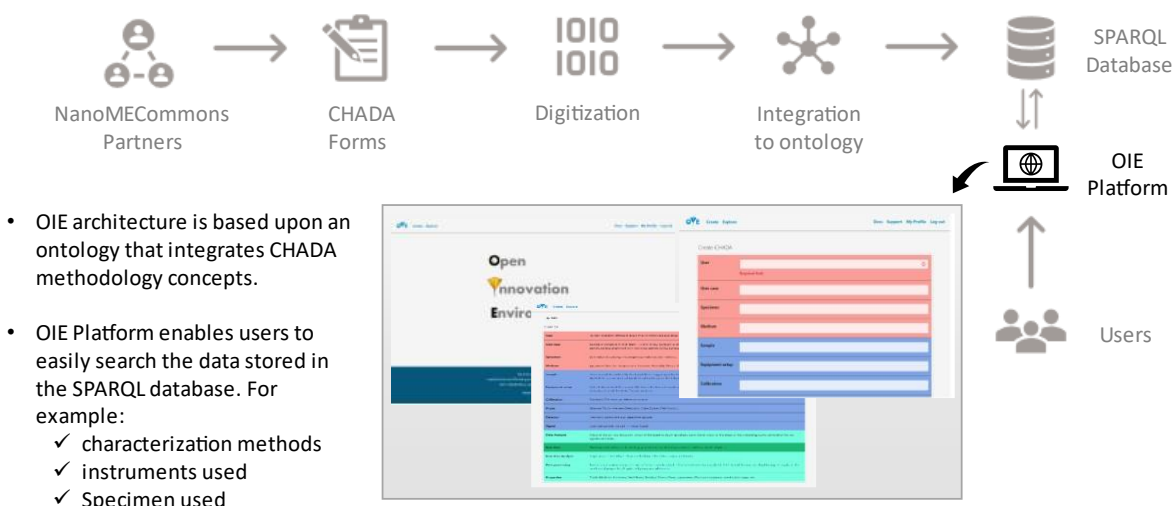
3.5 Discovery of new knowledge by aiding interoperability and integration in an Open Innovation Environment

The presentation focused on the developments achieved within NanoMECommons projects. The first part of the presentation was presented by Paris Varytis about the development of CHADA and ensuring interoperability via the integration of ontologies under the name of i-CHADA. The interconnected CHADA through the ontology and the findability and accessibility through the open innovation environment. A scheme of the whole process has been established within the NanoMECommons project. Regarding the CHADA forms, there are standard CHADA questionnaire forms were provided in PPT and DOC type files format and the current forms were filled in by NanoMECommons partners according to the specific characterisation methods that have been used. Regarding the ontologies that were developed based on NanoMECommons partners CHADA forms and their respective characterisation methods that are used in the project. i-CHADAs are explicitly defined, standardised, interoperable and machine readable. Regarding the open innovation environment, the architecture is based upon an ontology that integrates CHADA methodology concepts. And the platform enables users to easily search the data stored in the SparQL database and characterisation, including characterisation methods, the instruments, and the specimens that they have been used.

Gerhard Goldbeck proceeded to more insights in the work performed. Ontologies have been used widely for database integration, and to connect heterogeneous data sources to discover new trends. For example, they make database querying easier as they can organise the knowledge more around the domain expert rather than the IT system. With ontologies it is possible to write scripts for querying and they have already been used widely in a large international project funded by the pharmaceutical industry to integrate analytical processes, analytical labs, and equipment, which is called Allotrope. As a first step, when we go to i-CHADA we move to electronic forms rather than just PowerPoints and so on. With ontologies it is possible to enhance i-CHADA to machine readable interoperable systems and systems that enable users to retrieve information more easily and carry out a wide range of queries across all the information captured. For example, if a user wants to know which kind of materials have

been tested, what sample preparations were applied, which method has been used for data analytics and which reference materials were used. An important part of the development of the ontology that supports these systems are to capture these types of questions, called competency questions. These are what is required for a system to be able to answer hence meeting the user needs.

From CHADA to iCHADA



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Figure 4. Steps from CHADA to i-CHADA.

As a framework for characterisation ontology development, the EMMO top level ontology is being adopted. Ontology means having a certain domain or the world of characterisation interconnected and conceptualise on that basis. CHADA in terms of semantic representation provides already terms but is not yet machine readable and in interoperable format. The arrow of semantic knowledge organisation is to go to higher levels of formality and of definitions and this is basically the trajectory on which the project is moving. In NanoMECommons project, the objective is to map each colour entity to ontology classes, and the interrelations between them.

The EMMO ontology is the top level that gives sort of a reference frame and one of the things about EMMO is that it lets to describe things in different ways and different from the core perspectives. One of the perspectives is called persistence which emphasizes looking at the world as either and objects or processes (or states and actions), which provides a good link to MODA and CHADA concepts.

The community should look at the characterisation or the modelling now and as well in the future as a series of objects or entities or states and then processes, instruments (object) and measurement (process). But each of those can also have properties, so a certain measurement process can have properties taking place in certain environmental conditions. Obviously, materials and so on have properties, so these are the three kinds of fundamental concepts. In addition, these objects and processes can be described at different levels of detail (or granularity) i.e., by having certain parts in place, spatial parts of a machine, such as the detector for example, or processes having finer grained representations, such as a stage and operation, or an action. The latter also provides a connection to another standard, ISA 88³² process model.

Moreover, in terms of the properties the so-called symbiotic triangle is used. This connects the characterisation process that has a certain observer or instrument, the output data for the

³² <https://www.isa.org/standards-and-publications/isa-standards/isa-standards-committees/isa88>

measurement, and the material/sample, which is assigned a property as a result. That gives all the details which are required to fully describe a property and how it is being determined. So, a lot of time and effort is spent going through each of the entities and assigning them to the different types like properties, processes, and objects and so on, and connecting them to higher levels in the EMMO ontology. In the end, a diagram has been generated with all the connections between the entities and to give a little bit of a detail; the stages of the process from sample preparation, by calibration data analysis and measurement normalisation, data filtering and also in the measurement of the properties that is applied at that stage. The result is a characterisation methodology domain ontology, so this is a generic translation of the CHADA into a machine-readable ontology format.

For all these objects and for specific methods the implementation to make it really applicable the ontology work is realised in NanoMECommons. The advantage is that a more widely agreed description at the application level, so that a user can focus more on the specific experiment, data, and other applicable information. Regarding the open innovation environment, the user can then interact with the CHADA for example. But also, now doing queries across these domains when they are implemented by ontologies, and what was done by using the EMMO top and middle level ontologies is being developing applications then will allow connection of specific cases which can be stored in external data sources.

After the core presentation, a demonstration of the Open Innovation Environment followed from Fraunhofer and Yoav Naphson, including registration, browsing, and exploration of the documented testing methods and registered materials. The OIE presented is part of work related to OYSTER and NanoMECommons projects.

3.6 Discussion – Concepts/Objectives for Interoperability of characterisation and integration to an Open Innovation Environment for discovering new knowledge

Through the presentation it was shown how ontology works and how all these characterisation processes are interconnected. The short discussion part focused on what is needed to be clarified and how we can use this ontology to work on the process of the related procedures and go beyond the knowledge base that is available and discover new knowledge. It is clear how ontology works, for example, for the management of knowledge. But the question is how we can go a step further. For example, is it relevant or enabling to integrate artificial intelligence to go beyond?

There are different ways that ontology functions, i.e., it helps the human to explore existing knowledge. Actually, this is kind not new knowledge. On the other hand, this is also the Internet is appealing, and the “famous” Google search is performed, because using the ontology-based web in the end the community can come up with new ideas based on existing knowledge and by exploring this complex web of existing knowledge and without the ability to really do a very relatively easy exploration. It is also harder to come up with new ideas, an ontology does support the process of idea creation, and beyond that there are capabilities or ontologies to do logical reasoning and then a user can ask and find the relations.

Ontologies are currently limited in their applicability regarding the AI part, which is important because, where the ontology helps is to ensure that the data in the end belong to the right type of concepts. So, AI is kind of limited by factor of data organisation. And if data are not very well organised, then AI can be misleading or can take longer to converge, and the procedure will require more kind of post processing of the information of what is given as an output. Consequently, more well-organised information greatly supports the power and impact of using machine learning.

4. Session: Industrial Insights

4.1 Industrial perspectives on the utility of CHADA and MODA

In the first part of the presentation Rui de Oliveira represented BASF Chemical Industry, and more specifically the Division of Advanced Material and Systems Research, where over 3000 people are working on developing new sustainable materials, climate neutral processes and new chemicals. BASF chemicals are present in many everyday sectors including automotive, where major changes occur to move towards a sustainable and circular economy. The European chemical industry has the ambition to become climate neutral by 2050 and is seeking to contribute achieving the challenging targets of the European Green Deal. This revolution requires to have smart processes to serve materials evolution. BASF is involved in developing new systems, new materials for electrical vehicles such as battery materials, coating systems and many different plastics to serve the needs for lightweight components for automotive. Two specific technologies will be demonstrated in NanoMECommons, including coatings and plastics for additive manufacturing.

The focus in Industry nowadays is to realise digital innovations to shorten the time required for developments to achieve shortcuts for time to market. Exchange of data is an important sector since it is directly related to increasing confidence of customers and throughout the entire value chain. What is needed as a future orientation is to be able to get information, for example from customers and directly from the application environment of automotive coatings. For instance, it is important getting direct information about the quality of the painting and if any changes are observed during the painting process, where adaptation should occur in a short time to ensure targeted properties. In this direction new painting and optimisation solutions are required to serve the customers' needs.

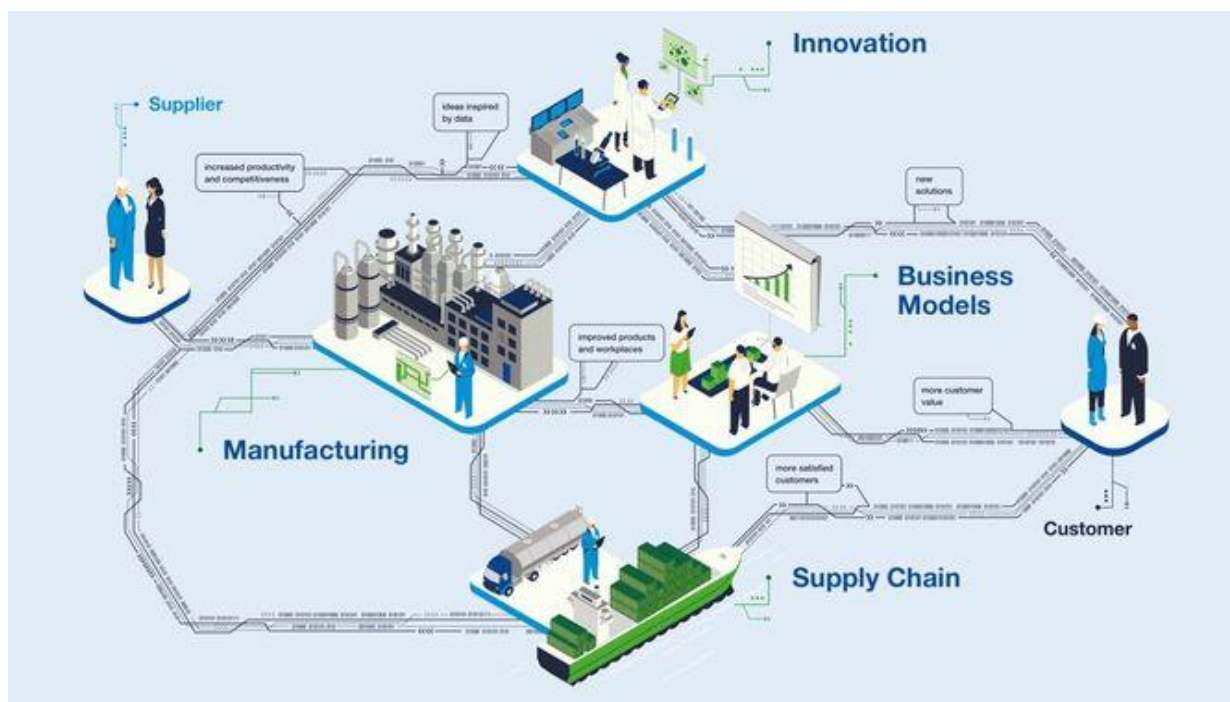


Figure 5. Smart Innovations and technologies (source: BASF)

Digitalisation is a must in the new era and what is needed is to get the best from this whole data that will be going through the entire value chain. In the future it is expected to use all this data and by integrating digital technologies to enable faster research and development process by using data science and modelling to develop better products and faster. Regarding data and developments of new materials, modelling is implemented nowadays at different scales, starting from quantum

chemistry chemistry up to predicting the microstructure and the final performance of materials. Different tools and modelling platforms are used to model the material at the different scales at BASF.

Also, multiple characterisation tools are required to cover the entire scale and value chain. The experimental data need also to represent the material at different scales. In the case of modelling some assumptions are made that do not always correspond to the conditions used in experimental characterization. Models' accuracy relies on data quality, and the link between characterization data and modelling at the different scale needs to be improved. CHADA and MODA could contribute to improve that link. There is a future need to have a better fitting in between experimental and modelling data. In previous session of the Workshop, several possibilities to act towards this direction were already presented to align experimental data and correct mutation, which is not limited only at one level in multiple scales. For that reason, the need to have well documented data and the adoption of commonly agreed structures is enabling to trace data throughout the entire chain. Relevant work is already being implemented for chemometrics in Industry to faster gain knowledge about materials chemistry. In this direction different chemical analysis, methods, and data provided from different methods are utilised, to get the fast learnings about the materials and chemicals and identify optimisation pathways for new applications. Another challenge is about collecting data from all over the world from BASF analytical labs, and from production sites. The challenge regards data collection and curation that are coming from these different testing facilities into a platform. Harmonisation of testing procedures is necessary for Industry, since high quality of data should be uploaded via a common platform that can be used afterwards for statistical analysis.

A video demonstration followed the first part of the presentation to show one example of what BASF is today starting to initiate in their R&D platform to support digital transition, specifically in the automotive coating sector. BASF's new Digital Material Profiling Lab incorporates two workstreams: a fully automated formulation, application, and testing procedure, and an integrated data ecosystem that provides BASF's R&D experts global access to testing data. Ultimately, this means more choice and better products for their customers. Different resins for automotive coating are formulated, applied, and cured in a high throughput process. Experimental data from i.e., contact angle, nanoindentation and nano scratch are generated and stored into a digitally connected data management ecosystem, which facilitates immediate accessibility to all of BASF colleagues globally and is enabling for finding faster solutions for customers. One quite challenging aspect is about how to synchronise those data.

In the second part of the presentation, Ferry Kienberger representing Keysight Technologies (over 13,000 employees worldwide) provided an overview of how it would be preferred by Industry to apply data structures, models, and interoperability for a new kind of application that is trending and has a high impact in the current revolution in industry. Several insights were presented about battery materials and devices, as well as for battery characterisation, and how the interoperability is important in a large ecosystem of measurement techniques. The presentation contained part of the work implemented currently in the EU project NanoBAT³³, and the NanoMECommons project respectively. Battery gigafactories are currently established in many countries around the world, there are already ten in Europe, while every month there is an announcement of a large automotive or battery manufacturer to either participate in a gigafactory, or to make their own gigafactory. This uprising trend for battery production facilities is nurtured by the emerging need of technology transition to electrification in the automotive industry.

The emerging needs also contain the simultaneous charge requirements at a certain time, which risk the energy grid going down, so there is a need to have a good balance. Those large disruptive technologies converge actually, and they are related to each other. Keysight currently works on

³³ <https://www.nanobat.eu/>

hardware test solutions, but also on software to serve and to measure all connected devices from an inverter to a machine emulator, or to test the charge-discharge properties of essential energy grid components. The energy grid is a large ecosystem, comprising automotive and charging stations, including home battery backup systems and gigafactories, and to bring this together requires a lot of interoperability, which is a current issue.

In NanoBat, an open innovation environment (OIE) has been created, where quite complex combined CHADAs and MODAs on battery materials test methods and modelling are used to get into interoperability. The data files used in the OIE ecosystem are in line with the goals of the Materials Characterisation Council (EMCC) and the Modelling Council (EMMC), which were also adopted from a pre-normative CEN workshop agreement (CWA).

The characterisation tools are based on nanoscale imaging combined with the electrical characterisation using broadband frequency methods, as well as impedance spectroscopy on battery cells or their components. The CHADAs for the characterisation methods were presented, as well as the MODA documentation for the used models for battery testing. The calibration is part of the interoperability to ensure accurate measurements. In this direction Keysight is active in the data management and calibration procedures to enable comparison with other testing data. The MODA was also presented related to the modelling part for an electrical experiment. The electrical characterisation using impedance spectroscopy ranges from 100 kHz down to low frequencies of mHz to characterise all physical, electrochemical, and electrical properties of a battery cell. Subsequent plots of the imaginary part versus the real part are fit by applying an equivalent electric circuit model. The model depicts all those electrochemical processes, while also nanomechanical properties (like the Young's modulus of an electrode or separator membrane material) or other relevant materials properties on the nanoscale can be included. For instance, the surface roughness, the pore size distribution, or emerging dendrites, particles, or other impurities during charging-discharging cycles, can be included in those models. In the end, an FEM model and simulation complement the state-of-the-art characterisation procedures to model electrical properties of batteries, combined with temperature modelling for instance. In the end, this is combined into simple models that can for instance be run on the firmware of test hardware in real time in a pilot line. By bringing together the CHADAs and MODAs, fast determination and prediction of materials properties is guaranteed, and this is a basis for establishing digital twin representations. All this helps to understand the physical basics of the battery efficiency and charge-discharge behaviour, but also safety like thermal runaway can be modelled with this approach. Regarding data file format and interoperability – which is a state-of-the-art and competitive topic – Keysight is using the HDF5 file format for lab data files as a common data model that allows then to integrate and interoperate.

4.2 Focused Automotive needs for new advanced materials and characterisation

Nello Li Pira proceeded with a presentation on the vision for the automotive sector paying attention to the emerging technological changes and the evolution of the materials used in future vehicles and components. CRF is in charge for innovation as and for Stellantis Group which represents 14 global car brands. CRF focuses on the development and the transfer of technical competences to the company and to external suppliers. CRF works closely with international consortia to achieve main targets in electro-mobility, standardisation, new methodologies, and component assessment. Nello Li Pira works in the Material Sustainability Engineering (MSE), the department that focuses on the material design and development, including the characterisation and the validation. The objective is to assure a global vision on materials and the updating of methodologies, which are required to implement materials and components as well.

Currently, the main drivers for new materials in automotive are focused around three main trends for the future e-mobility. The first one is the revolution in the vehicles due to the connectivity and

onboard intelligence with the final aim to realise autonomous driving in which the vehicles can communicate each other's and are automatically driven by solely using own intelligence. Then sharing mobility is a different approach to the e-mobility that needs, obviously a revolution in terms of connectivity, but also in terms of power supply to support the complete electrification and traction of vehicles. This ambition also means that energy storage systems will completely change. Energy storage and supply is the second main automotive trend. Another aspect is the personification. The performance equation means that especially for luxury segments, the people want a car that is unique, and dedicated design would be required to individualize the own style. Finally, sustainability is third main pillar; the target of the recycling materials in automotive is 30% by 2030 and this trend will change the today materials. There are a plenty of applications on the vehicle for sustainable materials: these could include different door panels, lens for the lighting and display, tires, dashboard, roof panels, bumpers, or metal body. R&D efforts are targeting today on the recycling and bio renewable material solutions, leaving low priority to recyclable materials in short-to-medium term. Briefly, the green materials are targeted to recycling materials coming from post-industrial or post-consumer processes, or from bio-substances originally by living organisms. Additionally industrial R&D activities focus on the extraction of raw materials from industrial production scrap (as foods) or from vegetable production.

The evolution of materials will move from current raw materials with only structural function to intrinsically multi-functional materials. Additionally, because the material will become more intelligent the improvement will include enabling technologies for sensing, display, connectivity, and electronics. The integration of new electronics functionality and intelligent onboard involve the concept of connectivity and autonomous driving. CRF is supporting the development of new materials for augmented reality, HMI systems and display as well as the evolution of monitoring sensors directly embedded in the dashboard for the driving assistance. Especially the new display, that are expected larger with higher resolution and quality including flexibility, will need fusion of plastics/ glasses and electronics with active surfaces, as hard coatings, low reflection layers or embedded switches which allow to easily disappear in switch-off mode. This revolution should be supported with new enabling materials and characterisation technologies since the level of complexity of devices is continuously growing.

New technology integration implies that the new electrical vehicle goes beyond the vehicle itself, but also energy sector and infrastructures should develop innovative solutions. A representative example is the connectivity of the vehicles with to other vehicles (V2V), pedestrians (V2P) and infrastructures (V2I). The emerging needs of the digital technologies are going to integrate 5G, RADAR and LIDAR technologies, and enable the augmented reality aspect of intelligence, which is expected to receive increased attention in the next 10 years. An interesting point of view is the utilisation of all these sensors to cover all the different detections and classifications of objects. The challenge is the fusion of the integration and the possibility to merge with the new emerging materials. To assess and to validate these materials, new methodologies are required to be developed and new standards needed for the characterisation.

Furthermore, new kind of approaches on standardisation is required, especially for the material assessment, which is part of the work involved in different European Projects, as for instance, in NanoMECommons. In this project the main goals are the development of new methodologies for electronics and multi layered structures, fundamental for the electro-mobility because the needs for increasing electronic contents and the electronic materials. In addition, the development of methodologies includes protective coatings, like new aesthetical finishing and the measurement of specific properties by standard mechanical assessment.

Some insights about materials for energy storage, such as new materials for batteries were presented. The interest of CRF focuses in the field on electrical/ thermal modelling of materials used within the new housing batteries packs that are aluminum or metal based one. Future developments are expected to be on the fields of fast charging, safety and improved vehicles autonomy. In this framework, CRF is working on the development of chemical, physical approaches to investigate current and innovative material for fuels cells and li-ion cells.

In conclusion, the need for a collaborative approach in the product development is the key message. Joining efforts among the whole supply chain is crucial to exploit the new materials, since products are increasing in complexity. Additionally, the larger adoption of innovative materials, the increase of sustainability and the enhancement of autonomy and intelligent require the definition of new requirements and standards, as well as new testing procedures to guarantee the reliability, performance, and safety of the new products.

4.3 Discussion - Evolution of materials in future vehicles: a new paradigm for the automotive components

In the presentation a lot of insights were provided on the automobile and connection to the Internet of Things, as well as the use of the machine intelligence. The discussion focused on the characterisation pillar and the possible interest of automotive industry to integrate a digital health monitoring system about characterizing a components state during the use phase. Possible realisation of these systems could be in the form of health monitoring, anomaly detection of a component which could give an output or alert when repair or replacement is required based on baseline specifications.

Nello Li Pira stated that CRF is working to integrate new sensor-based systems in the car in order to control and monitor the activity of the components, and then to collect all the data and send them to the main company in order to track, for instance, the maintenance or suspect and plan the substitution of the specific components. In this direction, there are several challenges to overcome which are not only technical; for example, just the sensor that collects the data and the required organisation procedures are demanding in order to ensure usability. Moreover, a legal aspect has come up, since there is the need for legal protection to overcome possible legal issues that are connected to the privacy of information, which needs a specific treatment to give that information to the companies or the different network. But from technical point of view the trend is moving towards this direction.

Some remarks focused on several synergies that can occur among European projects, since new assessment technologies are required. A new approach to characterise automotive components, and for monitoring these components is required to be developed both online and offline. Incorporation of digital platforms with modelling tools could be also enabling for automotive industry.

4.4 Digital Infrastructures

The presentation from Donna Dykeman from ANSYS presented insights in digital infrastructures that facilitate data exchange procedures. Information management impact was shown by using the development of Gorilla glass success story, which is an old paradigm regarding shatterproof glass development which is used in billions of phones and iPads or even other devices, which require the presence of a resistive and transparent protective surface for displays. This development would not have been possible if these data were not stored, as well as their metadata, which was not installed in the businesses of the past, as well as several other digitalisation aspects. ANSYS and GRANTA have been working on the digitalisation field for about 25 years, and especially on software and information management systems, and ANSYS specifically in engineering simulation and cloud platforms that enable Multiphysics simulations, which is being expanding into almost any Multiphysics challenge. The digitalisation aspect can have an overall aspect for a business to properly control their costs, since it

is required to ensure that high quality and organised data are accessible for reliable simulations, and even to be able to screen quickly for equivalent materials. In the materials science research and innovation activities, a digital infrastructure can boost efforts for developing lightweight and emerging new materials, which can support the electrification of vehicles and transformation in automotive, as it has been discussed in NanoMECommons Workshop. However, there are a lot of risks that is needed to mitigate. For instance, it is not only about looking at the carbon fibre footprint, but also ensuring that substances are not going to be obsolete to the restricted substances that they contain. This is indicative of the importance to know the very detailed chemistries and substances all the way up through your materials and enabling traceability all the way through to the product and its lifecycle is required.

The key message was that storage and management of data is the basis for a new business to realise financial development. Several surveys contacted by ANSYS have shown that engineers and scientists spend about 30 minutes a week searching for data on materials and especially for large organisations, literally hundreds of thousands of resources are spent every year looking for data. Moreover, companies declare that they duplicate about 20% of their data every year, due to inaccessibility/existing data or the data being non-usable. In addition, only about half of the data is being stored and recognised. In fact, the digitalisation work that was presented by BASF is a key reason of excelling in the market, since capturing all that process data is really challenging and some of the EC-funded projects where ANSYS is involved are about the process industry and pilot lines, where data often were stored in hand-written records. Digital revolution is emerging for the industrial sector.

The other dimension to information management, which was explained as well in the past two presentations (batteries and automotive) is that materials information is being collected through various stages of the product life cycle. Design through manufacturing and product management informatics is also important to declare that a product is safe throughout its lifecycle, which should also include the collection of information process throughout its lifecycle as well. ANSYS has specifically worked on relevant tasks, including the curation of these data, and in terms of the product lines, where it is needed to bring into products and materials the data for simulation. This functionality has been enabled by the development of a digital tool, which focuses on getting data in the right formats to be usable throughout the digital thread for modelling and simulation software. Moreover, the GRANTA selector tool is focused on designers and provides a very lightweight tool, which brings together extensive information, and the key feature is that you can compare the same attributes across thousands of materials and processes, and the conventional implementation requires technical cost and performance. Grand Semi Pro is another tool which appeals to users new to digitalisation and provides a fixed schema, something to set up and get running with very quickly store their data, providing the users also with the connections to modelling and simulation. The Granta MI Enterprise is the software tool which is used in European projects most of the time to develop a schema in cooperation with the end-user requirements. This tool is used also to curate data and create datasets for wider distribution, which includes a lot of collaborative work and connecting with data analytics, modelling software and digital workflows. Underpinning all these capabilities is the functionality to bring on reference data, and so this is always an important part of the projects that ANSYS is participating. In addition, ANSYS has already established strategic partnerships with testing houses or qualification bodies, which is indicative of the extend and impact of the digitalisation work in the field. Regarding the innovation, ecosystems and how these processes get started in collaborative R&D projects is that a FAIR data management for materials and processes is ensured. Bringing together a flexible schema is important, and even more important to bringing together the software that makes it FAIR. Collaborative data management between partners can find a web presence with ANSYS software, which is cloud hosted now as well. This is something that gives the partnership a lot of ownership and different access controls are usually provided, which allow to work privately before publishing something to the collaboration or the user can just work completely openly together on

developing that schema or that dataset. ANSYS has been also developing the software and tools to curate data for screening selection.

These digital tools can provide a vision for where that data can go and having a life beyond the project. Integration and digital workflows for modelling and simulation environments have been realised via CAD, CA and PLM environments that are representing either scientific or engineering workflows and processes that are embedded in organisations. Also, ANSYS is open and connecting with the software that users are developing i.e., in their projects, whether this is intended to be an open-source software code. This could be a route to establish partnership models that are available to pull things through to market and that is something that is a big takeaway for project ongoing partnerships to realise wider and successful exploitation of achievements, whether it is an OIE or a marketplace or research data.

ANSYS field to expand research is on emerging digital technologies, which include computational material science and materials for resource efficiency, while several developments have been realised in the last years, especially on additive manufacturing, and in the framework of digitalisation/Industry 4.0. Several tools have been created for data analytics for screening of materials for doing streamlined LCA. Another main and strong point are the activities for integrating the research into the engineering and scientific workflows and organisations. Recently, projects acted towards an open innovation environment with the vision of continuations and bringing the communities together and represent Europe on a specific material or manufacturing domain.

ANSYS is familiar and encourages the adoption of CHADA and MODA concepts, and as soon as the right tools are defined in a project working for gaining insights in product lifecycle, ANSYS establishes a highly interoperable System, which includes storing and flow of batch information through to an end point where data are being used, and so that is another level of granulation in terms of the digital thread that is needed. And finally, all these aspects are put into what can be used as a flexible and updatable scheme which underpins the management software and can handle many types of data formats. This procedure often requires six months to be completed, but sometimes it might take longer in terms of getting to a point at 18 months where the platform is released for use and validation during the project. It is also possible to connect equipment in the scheme, which could continue to evolve even after the life of the project. These systems are validated and creating a substance can be taken forward and identifying the protocol going forward and so finally there is a workflow element that can be implemented as well.

Regarding the ecosystems going forward, a special mention was about three topics, a) additive manufacturing, b) meeting sustainability in supply chain and c) computational materials engineering, which brings together the characterisation work, as well as materials modelling all the way up through engineering simulation. Regarding the additive manufacturing for us as a company, ANSYS was part of Amaze³⁴ project which was a huge 20-million-euro project and many partners, where the first scheme was realised in this field, where ANSYS was part of the dialogue on process parameter optimisation, and new tools are coming out in short term on using machine learning. In UK Drama project ANSYS is part of an ongoing demonstration. This is a project using an ongoing pilot line demonstration on which ANSYS tools are a part, while involvement includes Roadmapping as well, while the Sam project is bringing together the next generation needs for upskilling for additive manufacturing industry.

In another case, working on flight ease in a Clean Sky 2 project, the aim was the integration of a methodology for quick selection and quick screening into engineering workflows. This effort was continued on with Eco Bulk project and looking at how these ideas can be implemented in more public facing platforms and how it is continuing today with a couple of open innovation testbeds for building environment and biobased product development. Amongst other activities, ANSYS has built its own

³⁴ <https://cordis.europa.eu/project/id/313781>

consortium called the Emett Consortium, which is focused on the challenges of sustainability of products and advising on how to move things forward.

Regarding the integrated computational materials engineering, involvement of ANSYS in the very beginning was about the establishment of an accelerated methodology, in a high throughput materials modelling project looking at alloy development. The related activities continued through MSU related projects for integrating materials modelling in business decisions and creating interoperable platform development and it continues today, through the Musicode project, which is a project looking at organic electronics specifically and developing an open innovation platform and ANSYS is part of that interoperable workflow. And the other aspect to this is the characterisation data which can feed the models for verification, validation, calibration, and uncertainty quantification workflow.

ANSYS has collaborated with NASA, EMMC and some of the platforms that are either established or are emerging, like Nanohub and marketplace. Also, the ICMA work is relevant to the presentation topic, since it is important to recognise that really the Materials Information Management has two sides nowadays. It is not just the physical data that are needed to have the corresponding metadata, it is also the virtual data, and ANSYS has been working on expanding the schema to cover both sides. Not only obviously connecting to equipment, but connecting to modelling codes and HPC, and adjusting the environments. The visual environments that people use to interact with as well, because there are many different user needs.

One useful tool that is implemented through ANSYS environment is called opti-slang and is the connection of commercial software to materials modelling codes. This is a simulation workflow tool which can connect any type of modelling tool to its framework, and it can also run different types of analysis whether it's Geo ES 4, Tivity, robustness or connecting it with other programmes which will run those documents for the users.

So just in conclusion, the three main points that I wanted to bring to the table today was, you know, the business case for materials. Information management is well established. A long time ago Industry decided to harmonise their efforts, and not necessarily always be repeating and developing their own systems inside. There is a resurgence in the research environment to go out into their own systems. But for sustainability it is a bit of a cultural change that is needed. It is critical to harmonise the metadata, especially as was pointed out in the previous presentations, there are going to be new functionalities. There are going to be new ways of working with materials and even developing materials that are going to have an ongoing need for new harmonisation of the metadata, with no problem. When it comes to the software, it would be a good choice to work with the systems that the community has today to continue to mature them into new environments and realise sustainable ecosystems. Collecting the metadata was the key presentation message, while it was noted that innovation environments should constantly adapt to stakeholders needs to ensure the realisation of win-win scenarios. CHADA and MODA have taken already the direction to collect the metadata generated by the community and it is a need to use the systems that are going to integrate and connect with end users. Moreover, it was encouraged to continue to establish workshops in engineering and science processes that go beyond the research phase in development qualification, since dialogues are making it easier and faster.

4.5 Discussion – Building an industry-driven “innovation ecosystem” through the establishment of platforms for characterisation

The discussion was about the experience of ANSYS by the involvement in these projects, and the thoughts on digital innovation ecosystems. It was stated that digital innovation ecosystems help to minimise the effort, for example for characterisation or the effort spent in manufacturing. If this is not

the case, which actions should the community take to actually address this concern and take advantage of this benefit to have access to data in order to minimise the effort spent.

It was mentioned that this is a broad topic for discussion, but shortly it was discussed that the dialogue in the ecosystem has to be a continuously ongoing effort. It is not possible to ever stop having that ecosystem or dialogue and apparently this need has become more emphasised, and in some ways some efforts, even outside Europe, are trying to recreate what has already been established. This was the case in a similar Co-creation workshop organised on the other side of the ocean virtually this week, which was almost like it was trying to establish for the first time again the categories and the rules for Digitalisation of information. In some ways, the world has moved on from the basic conversation, but huge efforts and jumps are being made forward. What is important is that the community do pick up the tools that are available today because they have been in a way harmonised by industry, which can be regarded quite like what the characterisation community is doing with standards.

5. Brainstorming - Round Table session

The open discussion session was opened and moderated by Bojan Boskovic. The discussion started with a few basic points similarly to a roadmapping process. First it was established the direction on which we wanted to move, including some key points about the needs of different participants of the workshop with different backgrounds and disciplines, why and how they would like to go to certain destination. In the framework of Christmas spirit, the discussion moved around by identifying one Christmas wish obviously related to characterisation data and modelling, especially what participants would like to find as a solution if world was ideal.

A general discussion was kicked-off by Alex Simperler, who focused on something about which there is a lot as a discussion in the community before and during the workshop, specifically about the need for standardisation. Many projects have foreseen activities to standardise because they confronted similar challenges by looking into characterisation methods that is overarching a project and that needs to be communicated. Some good examples were presented, and a possible direction would be to avoid generating just another standard, because then there would be many related and complementary standards. A project should focus on the common stance as it investigates ontologies for example, since they are existing already, and it would not be something new. The aim should focus to coordinate what is already there and it has to be advised. An adequate strategy could be to go beyond another CWA and try to explore other efforts out of the project and join forces. One identified need is to build an organisation that would coordinate these efforts rather than diminish each other's efforts in the characterisation area for example.

Nello Li Pira underlined the automotive topics and his presentation key message about the revolution in car industry, which requires a lot of new methodologies for characterizing new materials to increase the competence. Also, what is needed is to increase the sharing of the competence within our partnership regarding the power supply or a resource institute, just because we see that the challenges for the future will be many in a couple of sectors, i.e., the batteries, intelligence, safety, which means that we have to share the competence and skills, just to overcome these potential issues and we can do it together. So, the need to collaborate was emphasised, because we cannot go by ourselves very far, so this was the key message.

Bojan Boskovic emphasised on the powerful message from automotive and the last presentation about the discussion of open innovation as well as the plurality of the approaches in the field, which highlight the need for information to be open and collaborations to be reinforced.

Costas Charitidis commented on the industrial needs which include enabling characterisation approaches to gain insights into material service life. Also, some perspectives in the incorporation of modelling are needed to make useful predictions for the materials service life and currently there are many ways of characterising the ageing of a material. This includes the different duration of exposure to ageing or mechanical loading, creep, especially when it is about polymers of course, and afterwards there are differentiations in respect to environment, which may lead to stress cracking and UV ageing.

Rui de Oliveira commented that another relevant point of interest for industry besides the long-term properties of polymers could be the evaluation/characterisation of possible release of microplastic from wear/abrasion (mentioning also i-Tribomat Project). There is an industrial interest to obtain more information on the impact of ageing especially considering that the objective is to increase the duration of use of materials for a more circular economy. This can be tackled by modelling, but models should be adapted for industrial purposes. We can use the synergy between characterisation and existing models and get actually kind of a hybrid modelling approach, where you can combine experimental data, data science & modelling for fast prediction of long term properties.

Donna Dykeman from ANSYS added some insightful comments on the discussion of BASF and NTUA. Previous experiences indicate that there are some models which you can apply to predict stress relaxation and increase type of data to try and predict. The challenge is how to get that long term data. This becomes an issue of collecting data for tracing, while there is also the financial aspect of the procedure to continue to collect them and establish a historic digital management infrastructure, which requires adequate maintenance. One possible approach is to multiply data analytics techniques and adopt machine learning techniques in the future to try to extrapolate where the materials condition during service life, but a possible bottleneck is the challenge confronted when the discussion is about the possible ways to calibrate a model if data are not already in place. By having long term test programmes implemented, it could be a key initiative. This is something that Japan has been doing well for a very long time. This is an interesting field, which could be considered for investigation and to bring together those forefront players. Possibly, we need to establish those programmes so everyone can benefit in terms of what does European industry needs. This field includes a vast amount of data management and data analytics procedures and could be an opportunity to get deeper into this field to be able to use not only for the selection and design activities, but also to calibrate and validate the next generation of models. Certainly, this dialogue would be welcomed and the chance for ANSYS to be a part of that dialogue.

One thing that is very clear less than speaking openly about it, is that for the selection of bio-based materials there's very little data, while there is documented a lot of information on PLA basic metrics. But still, there are very little data that can be used for designing similar biobased materials, which is another identified gap which is directly connected to the revolution of automotive industry and the emerging need for new materials, especially considering sustainability and this is something we are working on with projects.

Bojan Boskovic summarised that especially from ANSYS angle of the historical maintenance of data, it is actually an existing issue and in parallel it is necessary to have in the prospect of data, ageing and the long-term programmes, something that definitely the community should look into and make a note from this discussion, due to its enabling character. Some of the comments could be possible suggestions to Commission for future steps because they are where the data would make the key difference, but it is something that needs to be committed in the long term through various institutions and infrastructures.

Gerhard Goldbeck added a comment regarding obtaining access to the right amount of data. To ensure a smooth and fruitful progress in the field, a robust strategy to organise the data is required, which is something which is being conducted successfully in many projects. On his behalf, the Christmas wish is about establishing a better way of sharing and ensuring the openness about the way in which data are organised. This is being realised with the ontologies is one way, but in the end, there is also the need to know the way each initiative uses to standardise and make interoperable data, in order to make easier the accessibility. Another risk is not organizing data and ending up with unstructured and unusable information.

Emphasis was put on the point that we need to organise data, but it is difficult to access to and gain insights in the work and approaches from different projects or key players who organised data differently. It would be ideal to have a common i.e., reference book with commonly accepted pathways to unify the way of organizing data amongst organisations, instead of having to somehow learn how to integrate with different organisation approaches, which is a very difficult task. Also, there are some other specific issues related to the variety of instruments in regard to software and hardware, and the numerous existing standards on different fields, and eventually there is a need on defining a lot of things, which is demanding and time-consuming, but absolutely needed in order to manage and organise information properly.

Another remark from Bojan Boskovic was about the big data and if artificial intelligence is something that can solve on its own the organisation of massive amounts of data or if we do still need the organisation of the data with other currently established methods.

Gerhard Goldbeck responded that there is the need to organise data using methods that currently include ontologies. Specific reference was made on some interviews with MIT and about a review on the application of artificial intelligence to cope with data. The resume conclusions were that AI cannot handle this task and the reason is kind of understandable when having to deal with lots of data. In addition, because everything was very fast, not a lot of data organisation was put in place. This is a good example that showed that there is very limited use of artificial intelligence on the organisation of data till now.

Malgorzata Celuch added some comments regarding her background in the field of electromagnetic characterisation, where data definition is more straightforward, and we tend to understand what is meant by specific material parameters. But since the field is well established, there are a lot of data which are not consistent and the question is at which time we make progress from organizing data to comparing data, which are validated or mutually validated data. In this field there is not a need that these data are included in data structures from the very beginning. The main issue in this field is that there are data obtained from many providers, and it is needed to control the data from one data provider to another. Especially, when you have to launch a project and compare the results, there is an emerging need to control data, so that it is preferred not to generate too much data without knowing how to relate one source to another. The Christmas Wish in this case is about obtaining a magic answer regarding the solution to this issue. Currently, there are so many data with very little standardisation and validation, and any efforts are solely dependent to the individuals or there is the need to learn how to launch the data from a similar project, and even in some cases there is the need to regenerate data to compare the results. This is also the case in an ongoing project, where there is a process of repeating the same measurements, so the main issue in that case is not about if you document data. The counter example is that since you have documented data, but data have not been validated previously, then there is the need to run from the very start the experiments and overduplicate the required effort.

Alex Simperler shared a positive experience ahead on a very low scale regarding modelling using the crystallographic database. When it comes to a database which incorporates validation and curation of data, these kinds of issues are eliminated. Also, the factor for the X-ray characterisation is that even if it is something in very small scale, the ability of having an overview of data is possible, because the data visualisation provides a direct estimate of what is going on. These kinds of data offer the ability to test and compare your data. Curation of data is the message in this case, to be usable and give the ability to apply with i.e., machine learning calculations or to be usable in other models.

Bojan Boskovic highlighted the fact that data can be trusted from different sources since data are curated and this is an identified gap today. Thus, the concept of curation is currently missing, which can prove important in the future of the market of trusted data.

In the approach presented from Malgorzata Celuch and relevant experience, data can be considered trusted if someone uses three different methods around a couple of laboratories, when data are derived by the circulation of the same samples. Since repeatable results are acquired, then the data are considered as trusted, with a variation not exceeding 5%.

Rui de Oliveira added from an industrial perspective, where there are other kind of concerns. For global companies with numerous testing facilities spread all over the world, a concern is to ensure that the data quality does not depend on the testing facility, namely Reliability and Repeatability must

be guaranteed. It is not possible, regarding resources and time, to afford double checking constantly across the entire development process. Another comment was about data and long-term data documentation. It is true that when we look back in characterization track records, an improvement in documentation and data storage has been realised across the years. One concern is that historical data derived from some characterisations that were done 20 years ago on similar materials are not always available anymore for comparison either due to a change on software, database, or LIMS system. Indeed, one aspect to think about is the long-term storage of this kind of data, and to avoid always to have to recharacterise the same material if there is availability from previous work. This permits more efficiency in R&D processes, avoiding spending money in repeating and rather dedicate this budget for new developments, which are needed to achieve more sustainable solutions.

Regarding the Christmas Wish from BASF and Fiat (CRF) beyond data, reliability, and repeatability, is to realise actual time shortcuts in product development and faster characterisation, i.e., to evaluate the homogeneity of a fabricated film, especially when dealing with multiphase and multi-layered systems. Support is needed to realise adaptive manufacturing and the ability to detect online defects and to compensate this kind of effect directly during the process, which is also relevant to the discussion of ageing since cracks or defects that may be developed during the process could accelerate the degradation process and result in materials failure. These points summarize what the automotive industry needs to think about in the future of characterisation, which will be enabling and will allow to make a fast decision at the end.

Malgorzata Celuch also added that another wish would be Industry to work closer with Institutions and RTOs, so that there is interaction and research on samples and relevant commercial requests to make such measurements. This will give the opportunity to collect and document more data. This is not the case for everyone, since it is possible someone is not interested to organise data or either to open or share their data, due to competencies in the field.

Alan Ryder referred to characterisation projects that work to harmonise tools for Industry, but what was missing from the presented approaches about developing standards is the engagement with ASTM or ISO. It was suggested that standard methods of analysis and testing should be communicated with the standardisation organisations from the very beginning of the projects and ensure that the risk to reinvent the wheel is avoided by using the expertise in those agencies. This is also an exploitation method to ensure longevity of project results, which ensures the usability from industry beyond the duration of a project. Currently, the procedure of using CEN Workshops leads to pre-standards rather than standards, which comparatively are well-established by ASTM and ISO. In research projects, the Consortia may be consisted of a lot of companies or actors but may not be able to fund the development of a standardised approach; for instance, standardisation activities for suspension characterisation, which is enabling for particle size reporting. It was suggested that these organisations should be invited into projects, the project should establish ways of communication, which will enable a continuous overview of project objectives, possible via technical meetings, regarding standardisation and ensure that there is the experts' guidance and consultancy to move into the right direction. Also, synergies with Joint Research Centers may be enabling towards these objectives.

George Konstantopoulos from NTUA made an addition as a closing remark in the framework of brainstorming. Since a lot of data are generated in all projects and what is trending right now is many metaverse projects, it was remarked whether all these models and data could be usable to establish digital representations in a metamaterial or even establish testing meta-labs in a virtual metaverse. This could be a business model for the future to attract more businesses. In this direction it seems that there is a recognised trend right now, since many metaverse projects came into life.

Gerhard Goldbeck added that the open innovation platforms and the different platforms could be a paradigm. It is needed to gain more experience on the ways to better coordinate OIEs and report into an overarching system and the community has to work towards convergence.

This discussion and the last remarks closed the Workshop event, with the participation of over 60 experts around the Europe.

6. Conclusion and Outlook

The Workshop enabled communication amongst RTOs, SMEs, Industry, and European Councils EMMC and EMCC, and the experts provided useful and up-to-date insights, which facilitated the discussions and the identification of the next steps for our community. This event can be regarded as a follow-up event to EuroNanoForum 2021 Satellite event on “Advanced materials modelling and characterisation: strategies for integration and interoperability”, which was powered by European Materials Modelling Council – EMMC ASBL, and the European Materials Characterisation Council – EMCC. In the ENF event, several topics that should be addressed by both EMMC and EMCC were identified. The NanoMECommons Workshop provided updates and insights in the work performed towards this direction, and identified some key and enabling activities for the future.

Table 1. EuroNanoForum concluding remarks, and insights gained by NanoMECommons Workshop.

Make MODA and CHADA interoperable and machine-readable

In the framework of NanoMECommons 1st co-creation Workshop, many remarks were made about CHADA developments, since the main focus was about the characterisation centered activities. More specifically, CHADA development by the incorporation of ontologies is the step beyond, which is performed currently in NanoMECommons. This is what will make CHADA interoperable, and more specifically the domain ontology which was developed is enabling the integration of CHADA in an Open Innovation Environment, since the developments in CHADA have set the basis to make it machine readable. Another feature is that efforts on the i-CHADA development focus also on simplifying the completion process, which is enabling towards a wider adoption.

Both MODA and CHADA should be introduced more to industrial stakeholders so they go beyond EU projects and become a standard to report on modelling and characterisation, respectively.

Already, there are many paradigms of MODA and CHADA adoption in EC funded project, and use cases especially in NanoBAT, where the CHADA is used to feed FEM models with the required data by Keysight, which is an Industry focused on energy sector. Apart from the end-users participating in NanoBAT, Oyster, NanoMECommons, Cornet, RealNano, Charisma, and other projects affiliated to EMMC and EMCC, further steps are required though to realise that MODA and CHADA become a standard and go beyond the EU project activities.

Can our communities find ways to compare “materials” so one could confidently say, when two specimens are identical?

In Pat4Nano, Charisma, and Easi-stress, there are multiple efforts on establishing standardised procedures, including reference materials, sample handling, and testing procedures. The

communication channels established with instrument manufacturers to get deeper into the software and firmware and gain insights about factors that may affect a measurement, and realise relevant improvements, which could be achieved by harmonizing the output from the applications developed by different manufacturers for the different available instrument. Another communication channel has enabled the interaction with standardisation bodies, so that it can be realised an actual methodology to say if two specimens are identical. Harmonisation efforts for materials characterisation is performed also in NanoMECommons project, where standardisation activities are foreseen for nanomechanical characterisation and further development of the interoperable CHADA, but in the framework of workshop, not many details were presented.

Do our communities consider meso and nano materials in-depth?

Some insights were presented in the work of NanoPAT and Pat4Nano, where characterisation methods focus on spectroscopic process analytical technologies, which are used for characterisation of dispersions and suspensions in solvents from micro to nanoscale. In NanoPAT a digital platform is used to support digital manufacturing and adaptation using data-driven AI technologies, while in Pat4Nano modelling and simulation activities are complementing characterisation, since the technology transfer and support to regulatory bodies can be better realised.

Interoperability and Open Innovation are not about sharing propriety data – they share concepts, ideas, better understanding of the underlying physics, ways of finding knowledge, etc.

One case which is under development in NanoMECommons project is the deployment of the interoperable CHADA structure in the Open Innovation Environment. In that case the competency questions could be utilised by users to find answers in characterisation problems. An example to be demonstrated within the project is to ask a question about what nanomechanical protocol to adapt in order to characterise the retained austenite in automotive metal-based coatings. By establishing the online knowledge base, which will correspond to characterisation workflows documented in CHADA from the characterisation of many different materials (metal, polymer, ceramics, thin films, devices, MEMs, and so on), the knowledge base will be used under the functionality of a domain ontology, and will give answers about the characterisation protocol, the nanoindentation tip, the nanoindentation depth as an enabling mechanism for sharing and finding knowledge related to characterisation protocols.

Make industry more confident in both our communities' efforts by working to high standards and demonstrate the benefits of novel tools and concepts

Relevant work was presented by i-Tribomat project, while there are and other open innovation testbeds offering services open for industry and optimizing tribology standards. What has been

already achieved is the establishment of harmonised tribology protocols, well-supported by a well-documented database and a digital modelling and simulation platform. This platform is enabling by offering interactive services for collaboration and guidance to industry. In this manner the communication is facilitated, and industry can address a current problem, and over 250 experts are available to discuss and offer services based on the industrial needs. Thus, characterisation or modelling services will be targeted to confront the industry needs rather than performing a black box characterisation. In addition, dedicated work to serve the testing needs under intensive application environment to adequately describe materials behavior have been realised by i-Tribomat OITB.

The Workshop organisation and related activities have been considered as an adequate communication tool to bring together academic and experts communities, SMEs, stakeholders, and European councils. The Workshop made a step further to provide the community a structured consultation process by identifying orientations and emerging needs, where enabling technologies are required to realise actual progress.

An emerging need is the adaptation of current technologies in the new era of characterisation, as it is essential to think green and digital to conform with new needs of our community:

1. We should prioritise standardisation of characterisation to harmonise the efforts in European level and address the need for a common characterisation data structure to support characterisation protocols development; one action coordinated by the EMCC is the development of Universal CHADA
2. Efforts to link characterisation data with modelling of materials properties is a commonly accepted direction, which will be coordinated by the synergy of European Materials Modelling and Characterisation Councils.
3. From a strategic point of view, we need to focus on high-throughput materials characterisation facilities and relevant models as we know for fact that we enter a new era where the digital coin is called "data". Data will feed the data-driven representations of materials and processes by validated predictive modelling and AI. Thus, the need for development of high-speed, 4D standardised characterisation methods is crucial to contribute to the successful evolution of the Industry.
4. Interoperability promotion by domain ontologies and data curation can be enabling for knowledge management and technology transfer, in order to enable continuation of proceedings within EC-funded projects and beyond their ending and realise industrial exploitation of results and new tools which have been developed.

The vision for materials characterisation includes:

- Linking process to product, which can be enabled by characterisation and high-throughput instrumentation; use twin digital(-virtual) representations for a more circular economy and establish common ontologies and data documentation standards and strategies
- Monitor the materials service life and ageing profile throughout the life cycle;

characterisation of a broad spectrum of the ageing behaviour upon exposure to intensive and extensive environmental stress is required. These efforts can flourish with the combination of modelling, and data management, including organisation, curation, and storage.

- Support the 3Rs (reduce, reuse, recycle) and Green Deal in manufacturing by-design and reduce technological risks; novel automated tools (plug-and-play), interoperable standards, and digital infrastructures, which are being and will be used to tackle and reduce the production of e-waste and real waste including the identification of efficient end-of-life handling strategies.

Of course, on this journey it is important for us to give back to the community added value in several dimensions:

- Prioritise ethical and human values
- Be conscious about safety and environmental health
- Improve skillset of EU citizens on ontology-based digital manufacturing
- Reinforce the made in EU trademark and improve the societal impact of manufactured materials, including end-of-life handling with a digital certificate
- Embrace integration of a wide range of stakeholder communities and support industry transition and technological changes

and support the activities towards our goals of:

- Smart and adaptive manufacturing
- The development of smart and eco-friendlier materials
- Support regulation and policy by establishing and integrating tools which will offer to Industry an accelerated time-to-market, and mitigating the risk to enter the market late or even at a time when needs or trends have changed
- Develop tools for supporting manufacturing processes and improve materials for enabling the quality assurance, to support decision-making for improving energy and resource management in Industry

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APPENDIX 1: Event Agenda

Online, 13th December 2021

Time	Subject	Presenter
10.00 – 10:15	Welcome, Introductory words, Opening of the Workshop agenda	Costas Charitidis Coordination Team NTUA (NanoMECommons, EMCC)
10:15 - 11:55	Session: Interoperability - Standardisation - Harmonisation	
10:15 - 10:40	Can our communities find ways to compare “materials” so one could confidently say, when two specimens are identical?	Nikolaj Zangenberg, Miguel Banares DTI, CSIC (Easi-stress, CHARISMA)
10:40 - 11:05	Do our communities consider meso and nano materials in-depth?	Alan G. Ryder, Ioannis Kakogiannos NUIG, IRIS (Pat4Nano, NanoPAT)
11:05 - 11:30	Directions in modern (4D) characterisation to support emerging manufacturing challenges in Industry	Stergios Logothetidis, Argiris Laskarakis AUTH (Cornet, RealNano)

11:30-11:55	Make industry more confident; demonstration of the benefits of novel tools and concepts.	Ivana Toth, Xavier Borrás, Dirk Spaltmann, Mirco Kröll AC2T, BAM (i-TRIBOMAT)
11:55 - 12:20	Break	
12:20 - 13:40	Session: Think Digital - entry to a new era	
12:20 – 12:50	Bringing digitalisation of characterisation closer to Industry needs - Make CHADA interoperable and machine readable	Marco Sebastiani, Costas Charitidis UNIROMA3, NTUA (EMCC, OYSTER, NanoMECommons)
12:50 – 13:15	MODA and CHADA; challenges and opportunities for integration and exploitation to industrial stakeholders beyond EU projects.	Gerhard Goldbeck, Nadja Adamovic, Malgorzata Celuch GCL, TU Wien, MTT-S (EMMC, Ontocommons)
13:15 – 13:40	Concepts/Objectives for Interoperability of characterisation and integration to an Open Innovation Environment for discovering new knowledge	Gerhard Goldbeck, Pierluigi del Nostro, Yoav Naphson, Elias Koumoulos, Paris Varytis (IRES, FRAU, GCL)
13:40-14:30	Lunch Break	
14:30 - 15:45	Session: Industrial Insights	

14:30 - 14:55	Industrial perspectives: challenges that are addressed with iCHADA, CHADA-MODA integration	Rui de Oliveira, Ferry Kienberger BASF, KEYS (NanoMECommons, NanoBAT)
14:55-15:20	Evolution of materials in future vehicles: a new paradigm for the automotive components	Nello Li Pira CRF
15:20-15:45	Building an industry-driven “innovation ecosystem” through the establishment of platforms for characterisation	Donna Dykeman ANSYS
15:45-16:00	Break	
16:00 - 17:00	Session: Roundtable	
16:00 - 17:00	Open Discussion - Brainstorming	Moderated by: Bojan Boskovic
17.00	Closing of the Workshop	Coordination Team

APPENDIX 2: Event Pictures

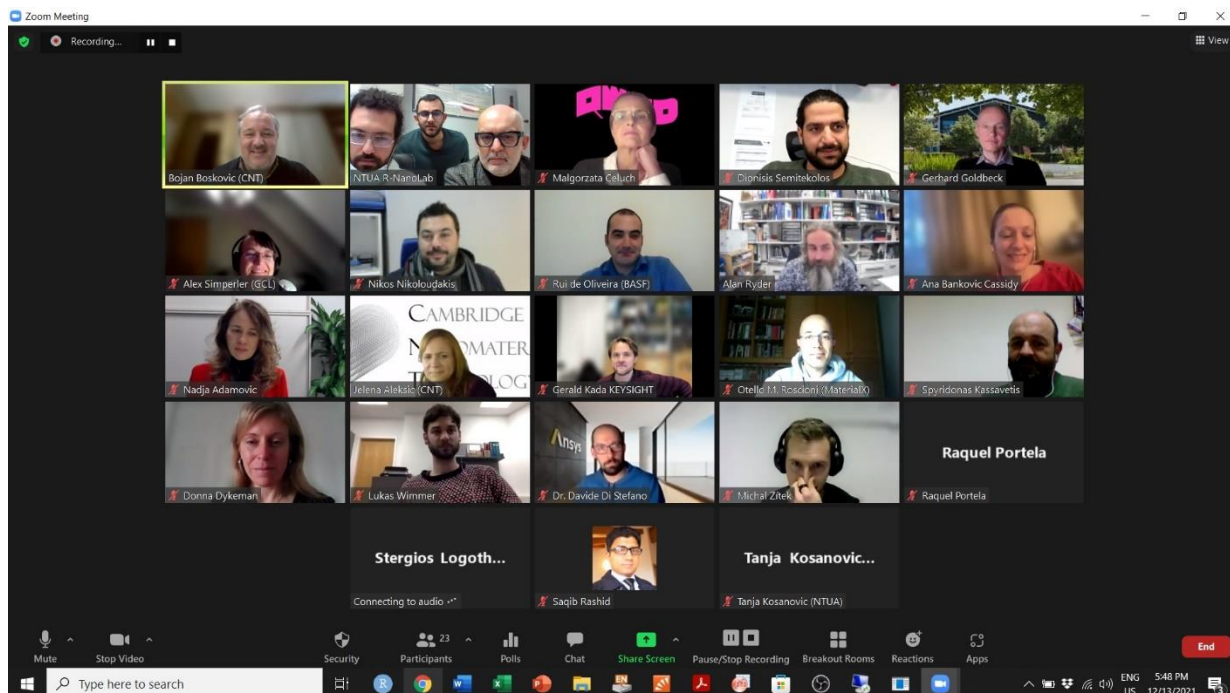


Figure 6. Presence of experts, stakeholders, NanoMECommons, EMMC and EMCC team members in the NanoMECommons Workshop.