Report on NMBP-35 Workshop:
"From Research to Industry: How Characterisation and Digitization Change the Game"

Costas Charitidis, NTUA (Greece)
NanoMECommons coordinator, EMCC and EMMC Organisational Management Board

Miguel A. Bañares, CSIC (Spain)
CHARISMA coordinator

Raquel Portela, CSIC (Spain)
CHARISMA coordinator

Georgios Konstantopoulos, NTUA (Greece)
NanoMECommons project manager and EMCC Associate Member

Savvas Orfanidis, NTUA (Greece)
NanoMECommons project manager and EMCC Associate Member

Theodoros Tsatsoulis, NTUA (Greece)
NanoMECommons project manager and EMCC Associate Member

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

Nikolaj Zangenberg, DTI (Denmark)
EASI-STRESS coordinator

Ennio Capria, ESRF, (France)
EMCC Organisational Management Board

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

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

Yanaris Ortega Garcia
EU Project Officer

17th January 2024

Contents

List of Figures

List of Tables

1 Background

Advancements in industrial products require progress in materials characterisation tools and computational modelling techniques. Integrating multi-scale characterisation and real-time data with cutting-edge modelling enables the discovery of complex functional materials, crucial for next-generation products. Material characterisation is central to understanding structure-property correlations, while predictive modelling offers opportunities for innovation and reduces reliance on extensive experimental testing. Integration of these processes into industrial R&D facilitates reliable materials and process designs, scaling up production, and quality control. Central access to tailored tools and models throughout the value chain is necessary, supported by user-driven Open Innovation Test Beds. Active contribution to European initiatives fosters collaboration and drives progress in materials science and industrial innovation.

The NMBP-35-2020 joint workshop titled "*From Research to Industry: How Characterisation & Digitization Changed the Game*" took place on January 17th, 2024, in Madrid at CSIC's premises. The event aimed to explore the transformative impact of experimental and theoretical characterisation and digitization in the materials sector. Organised by the NMBP-35-2020 projects NanoMECommons [1], CHARISMA [2], and EASI-STRESS [3], the workshop received support from the European Materials Modelling Council [4] (EMMC) and the European Materials Characterisation Council [5] (EMCC). It featured industry talks, insights into the European Materials Modelling and Characterisation Council's vision, and the latest research and exploitation results from European projects.

The workshop aimed to explore how characterisation and digitization are shaping this transformation. The event facilitated collaboration and knowledge exchange among diverse stakeholders including academic scientists, researchers, engineers, and industry representatives. Key discussions centred around:

- The role of characterisation and digitization in driving the transition to Industry 4.0 and 5.0, particularly focusing on achieving circular and safe manufacturing practices.
- The significance of high-quality, reliable, and openly accessible data for effective modelling and process optimisation.
- The necessity for collaboration and knowledge transfer among existing characterisation projects, testbeds, and European councils (EMMC and EMCC) to address the multidisciplinary nature of this field and drive innovation.
- Exploring the potential of standardisation and harmonisation to facilitate interoperability and broader adoption of advanced materials and manufacturing techniques.

This report encapsulates the key presentations and discussions from the workshop, shedding light on the potential of experimental and theoretical characterisation and digitization to shape a more resilient, sustainable, and digitally driven materials sector.

Following an opening session that set the stage with project coordinators and representatives from the European Commission, the day unfolded with industry leaders from Bosch, IRIS, and BASF sharing their expertise on digitization and advanced analytical techniques. The vision of the European Materials Modelling and Characterisation Councils was presented then, followed by an open discussion fostering collaboration between industry and research. The final session showcased current opportunities for industry, featuring presentations from the organising projects, a company born from an Innovation Action, and other relevant projects in the field. The day concluded with an interactive session, solidifying the connections forged throughout the event.

[1] https://www.nanomecommons.net/
[2] https://www.h2020charisma.eu/
[3] https://www.easi-stress.eu/
[4] https://emmc.eu/
[5] http://characterisation.eu/

2 Session: Industry Talks

2.1 DIGITAL TWIN in Metal Material manufacturing

In the first presentation of the session, Hermann Autenrieth (Bosch) gave insight into how Bosch had implemented digital production platforms on a pilot scale, which enabled them to extract in-line characterisation quality data and compare it to modelling results. Cases were presented based on the nitridation process and physical martensite transformation in steels.

Process modelling in combination with machine learning/AI-tools and data statistics, furthermore, should enable the company to reduce process time and perform quality assurance more efficiently. The pilot cases demonstrated the need for proper ontologies to enable the comparison between modelling and characterisation data.

2.2 Raman as a Process Analytical Technology (PAT) tool for industrial manufacturing

Secondly, Susana Gómez Sanza (IRIS) presented how the company had integrated quality tools and standardised procedures into their Raman spectroscopy products to enable direct integration into production lines. Iris have had an active strategy to engage in European projects to be in the frontline for introducing innovative technology to industry.

The presentation clearly showed the value from equipment manufacturers integrating standardisation to digitalisation of results into the measurement processes to enable real-time process adjustment.

2.3 Digital transformation of the analytical Labs in the Chemical Industry

Finally, Rui de Oliveira (BASF) introduced how a huge company with more than 100,000 employees is working to transform its material characterisation labs into a common digital platform. The aim was to improve data know-how and data management in the Life-Cycle Management of the core sustainable products, processes, and assets at the core of the company. This should also shorten time-to-market and leverage digital transformation to enable usage of multicriteria modelling and cognitive computing.

The transformation requires several different labs and measurement tools to be "retro-fitted" to, e.g., system upgrades, unified data formats, and operation procedures, which is a huge task. However, the successful unification would pave the way for advanced automation, e.g. cobots performing weighting and measurement operations, netbooks with access to BASF data and process simulation tools, and AR glasses to improve human-machine knowledge integration. The presentation also highlighted the need for developing joint semantics/ontologies within the characterisation and modelling communities across many industries and partners around Europe.

2.4 Conclusions

The insight from the industrial perspectives made it clear that the digitalisation of materials characterisation and modelling is becoming an essential strategy for the industrial front-runners. This transformation defines the additional requirement for R&D projects, that the results can be transferred to the digital platforms at the companies.

3 Session: European Materials Modelling and Characterisation Councils vision

This session brought together experts from the EMMC and the EMCC to discuss harmonising knowledge modelling across EU projects.

3.1 Harmonising Materials Knowledge Across EU Projects - EMMC

The need for new focus areas for EMMC was highlighted on top of the existing ones, i.e. model development, digitization & interoperability, software, impact in industry, and policy. This new focus areas may include advanced methodologies like AI and ML, guidance on ontologies and open innovation platforms. Collaboration between modelling and characterisation is crucial, with modelling explaining and complementing characterisation results. Digitalisation plays a key role in representing processes and outputs related to materials. The nanoMECommons project is developing harmonised protocols and data exchange procedures for nanomechanics, while efforts are underway to update existing frameworks like CHADA and MODA. The need for a diverse community to contribute to these efforts was emphasised, as current representations lack clarity and consistency. The use of a Business Process Model and Notation (BPMN) and a fundamental ontology like EMMO to address these issues was also proposed. Finally, EMMC's service offerings for projects was highlighted as well.

3.2 Advanced characterisation in the Digital era; vision, opportunities, and challenges - EMCC

A vision of EMCC to become the reference organisation for integrating materials characterisation into the digital world was outlined. Digitalisation is foreseen as the core engine for an efficient manufacturing-modelling-characterisation loop. Furthermore, the EMCC's role in the CHADA project and the development of an open CEN Workshop Agreement (CWA) definition was highlighted. Updating existing CWAs like CHADA (CWA 17815) and MODA (CWA 17284) remains a priority, which will be addressed through a new CWA supported by the nanoMECommons project. Once more, the reference ZENODO platform is highlighted, where CHADA is accessible [6]. This was indicated as a reference where ongoing projects can find examples and tutorials for the development of CHADA form. Combining modelling and characterisation is crucial, and stakeholder feedback emphasises the need for a clear regulatory framework, standard output data formats, comprehensive documentation, and integration with machine learning tools. The potential of machine-readable versions of CHADA and MODA, as well as the nanoMECommons project's use of BPMN and CHAMEO ontologies for automated data input was pointed out. Finally, the presentation concluded by stressing the importance of an open innovation environment for the user-driven development of taxonomies and ontologies. The final recommendation for ongoing projects on characterisation was to join the next CWA on MODA/CHADA integration, where all these issues will be discussed and made public.

3.3 Panel Discussion and Conclusions

The session concluded with a panel discussion of key points and challenges raised in the presentations. Actionable items and future directions were identified, emphasising collaboration, open standards, and digitalisation for efficient materials development. Main topics of the discussion included:

- How can mechanical characterisation contribute to advancing circular economy goals, and what measures are lacking to address uncertainties in the performance of recycled materials?

[6] `https://zenodo.org/communities/oyster`

- Strategies for enhancing the quality of data: What initiatives are essential to elevate the accuracy and reliability of data employed in research and industry?
- Enabling modelling schemes for industrial certification: What prerequisites are necessary to integrate modelling methodologies into established certification processes within the industry?
- Role of modelling services pre-certification: How can modelling services benefit industries in the preliminary stages before formal certification, and what value do they bring to the overall process?
- Integration of AI in industrial operations: At what juncture can Artificial Intelligence be seamlessly integrated into industrial processes, particularly considering its circular economy implications?
- Tribology and its role in the circular economy: How does tribology contribute to circular economy objectives, and what potential challenges or opportunities does it present?
- Spectroscopy's relevance to the circular economy: How is spectroscopy connected to circular economy principles, and in what ways can it contribute to sustainable material practices?

Firstly, the use of characterisation techniques throughout a material's lifecycle was discussed. Industry can benefit from a digital standardisation approach. The workflows for assessing domain specific materials qualifications can be a key element in ensuring consistent quality control of recycled materials properties. The reproducible and widely accepted methodologies can then facilitate the screening procedures since the main bottleneck for the industrial applicability of recycled materials is their performance variability. Thus, the digital documentation of assessment methods and the accessibility to their curated metadata can enable the generation of high-quality data by stakeholders. The CHADA and MODA, and their further development using machine readable technologies is an ongoing initiative among experts in EU to set the principles required to achieve industrial applicability of digitalising the workflows for materials lifecycle monitoring across the industrial supply chain. With such proposed action stakeholders can benefit from establishing common procedures for generating materials assessment data by increasing trust in recycled materials and their properties, enabling them to improve the management of the supply chain and qualify materials for reuse while supplementing the supply chain of secondary markets with greener materials that qualify the performance requirements.

On the other hand, a significant effort is made in the EU to develop digitalisation tools which cannot be overlooked. The scepticism of the industry in adopting modelling schemes in materials certification is a main risk surrounding this investment. To enable industrial applicability, the transparency to these workflows was one key element proposed since algorithms are particularly adapted to the physics and the chemistry of each material technology. Even though materials characterisation may not be completely substituted by modelling in materials certification, predictive modelling can accelerate operations and provide insights across various scales, where characterisation uncertainty is high or where characterisation is performed on highly anisotropic materials and larger components are required to be physically tested, and thus time savings can be realised. However, it is important to note that modelling can find application in the domain of materials and process design and prognostics, which can provide early insights for improving decision-making for enhancing the resources management, as well as the combination of materials performance, circularity, process adaptability, and provide alternative materials options. This is a critical step in ensuring the compliance to regulatory framework concerning key materials agendas in the EU, such as the Advanced Materials Initiative, the safe and sustainable by design framework, and the critical raw materials agenda.

In terms of artificial intelligence, the industrial insights exemplified the potential of its use in real world materials production, although two main problems concerned where about the specificity of this kind of predictive modelling and analytics on the industrial domain, which restricts the wider applicability, whereas the second concern raised was about the generative nature of such programming approaches from the scope that experts may adapt, improve or proceed to day-to-day changes in the algorithmic architecture to include more data, to reduce noise and biases, and other adaptations subject to technological advances (computational power, programming languages evolution, release of new libraries or discontinuation of the support to existing programming libraries).

Moreover, another topic which is critical to materials engineering was about the impact of the environment on material systems, for which automotive batteries were brought into consideration since it is a rapidly developing industrial domain. The i-Tribomat project employs the development of methodologies to predict material lifetimes in different operational settings, and exemplified how laboratory-scale testing and production can yield high-performance materials tailored to specific environments. In addition, the importance of materials characterisation and modelling in studying systems (materials and their application environments) is essential to generate data that represent their operational life-cycle, which is a domain where data accessibility is very restricted and can contribute to better performances by design to reduce the defects or other shortcomings of materials which reduce their resistance and usable service life. Finally, the generation of data that represent the material operation behaviour can assist the establishment of accurate modelling and artificial intelligence schemes and provide materials data analytics, especially considering the case when it is not feasible or comfortable to obtain such data from characterisation methods. This domain is expected to be an emerging technology since a growing trend is to establish sensors which are integrated to the internet-of-things and where vast amounts of data are generated, but interpretation may not be optimal.

Furthermore, the diverse benefits of spectroscopy for the industrial sector were discussed, especially in the context of circular economy challenges. Spectroscopy and monitoring are highlighted for their potential to minimise production waste and enhance material selection and quality control in recycling processes. The potential of combining spectroscopy and AI for efficient decision-making tools in the industrial sector was examined. While acknowledging the user-specific nature of such tools, the potential for customisable solutions based on Raman spectroscopy and AI was acknowledged. It was importantly noted that such non-destructive materials characterisation methods should be developed to benefit from direct insights without requirement of sampling or pausing the production, while obtaining valuable information on materials structure.

In summary, the panel discussion examined the outcomes of EU projects, and the insights of key EU initiatives and industry about efficient materials development, emphasising on domains where the need of open standards and digitalisation are emerging, as well as the potential direction of technological developments towards industrial innovation and sustainability.

4 Session: Current Opportunities for the Industry from Research Facilities & Projects

More than two hours were devoted to offering insights into cutting-edge research and its potential to revolutionise the materials sector through digital transformation and enhanced analytical capabilities. Each project participating in the workshop presented how its activities contribute to the advancement of material characterisation and digitization, highlighting the latest innovations and research outcomes in the field.

4.1 NMBP-35 projects

4.1.1 CHARISMA | Miguel A. Bañares

CHARISMA project (Characterisation and HARmonisation for Industrial Standardisation of Advanced Materials, GA 952921, 2020-2024) aims to harmonise Raman spectroscopy for characterising materials across their lifecycle and across various industrial domains, demonstrate the utility of harmonising Raman data, and standardise harmonisation protocols, thus making Raman spectroscopy an open and more efficient technique. CHARISMA focuses on reviewing existing standards and practises and open-source initiatives and proposing new developments and protocols, including a Raman data calibration protocol and samples, a Raman data format (based on NeXus), a Raman ontology, a Raman device twinning protocol, and a FAIR Raman data repository. The project involves the collaboration between academic and industrial partners to develop theoretical Raman data (in the NOMAD repository), tools for calibration and analysis, such as Altaxo and Oranchada, and application in real-world scenarios, with a demonstration in the fields of security (Raman-active nanomarkers), food active packaging (Raman-active additives), and synthesis of catalytic nanomaterials (real-time in situ Raman monitoring).

4.1.2 EASI-STRESS | Nikolaj Zangenberg, DTI & Manuel Sanchez Poncela, ArcelorMittal

The EASI-STRESS project presented a status on using standardisation and harmonised procedures as a tool for improving the industrial uptake of new measurement techniques. The work is in the final stages where experiences from initial simple benchmark samples are being employed on six industrial products from the partners. Part of the work also includes setting up a commercial measurement service inspired by the Open Innovation Test Beds which will enable companies to make use of the services either directly with large-scale research facilities, RTOs (such as DTI and CETIM), or as academic collaborations.

The progress was illustrated by Manuel Sanches Poncela form ArcelorMittal who introduced a special sample, the additive manufactured steel arch, which was used as a benchmark sample in EASI-STRESS. Results were shown for different measurement techniques, both advanced neutron and synchrotron diffraction techniques, electron microscopy results and different simulation tools, which, in general, showed good qualitative agreement.

4.1.3 NanoMECommons | Costas Charitidis

NanoMECommons project aims to establish a transnational and multidisciplinary research and innovation network to address the challenge of characterising nanomechanical materials across multiple industries.

The primary objective of nanoMECommons is to implement innovative nano-scale mechanical testing procedures within real industrial settings. This will be achieved by developing harmonised and widely accepted characterisation methods aimed at reducing measurement discrepancies and improving the interoperability and traceability of data.

To accomplish this objective, nanoMECommons will provide protocols for multi-technique, multi-scale characterisation of mechanical properties relevant to various industrial sectors. Additionally, it will offer novel tools for data sharing and broader applicability across the NMBP domain. These tools include reference materials, specific ontologies, and standardised data documentation.

4.2 From Project to Company: i-TRIBOMAT | Xavier Borras

i-TRIBOMAT [7] will provide the world's first open innovation test bed dedicated to validating and up-scaling new materials, thereby enabling intelligent tribological materials characterisation and fostering industrial innovation in the European manufacturing industry. For each tribological case, i-TRIBOMAT will find an individual, adapted solution (damage analysis, material development, property determination or simulation, etc.). The company is a story of the success of the Horizon 2020 programme of the European Commission, as it was created in the frame of the European project with the same name funded under the call DT-NMBP-07-2018 - Open Innovation Test Beds for Characterisation (IA).

4.3 Other relevant characterisation and modelling projects

4.3.1 AID4GREENEST | Ilchat Sabirov

The AID4GREENEST project [8] focuses on developing AI-powered tools for green steel technology. Launched on September 1, 2023, and set to conclude on August 31, 2026, it boasts a €4.94 million budget and involves ten partners from four countries. The project aims to deliver six main results, including AI-based models for steel microstructure characterisation, computational tools for process microstructure relationships, and methods for predicting and testing steel's creep life. AID4GREENEST emphasises sustainable innovation, life cycle assessment, and standardisation activities to improve efficiency and reduce environmental impact in the steel industry.

4.3.2 NanoBat | Ferry Kienberger

NanoBat [9] aims to develop a novel nanotechnology toolbox for quality testing of Li-ion and beyond Lithium batteries which will be faster and more accurate than existing methods. Like this, NanoBat will help to reduce the environmental footprint of battery production, support the evolving clean energy transition, and increase the competitiveness of the e-mobility battery sector in Europe.

4.3.3 DigiCell | Ferry Kienberger

DigiCell [10] aims to revolutionise the battery manufacturing and testing processes in response to the soaring global demand for batteries, driven by climate change mitigation efforts and the rapid expansion of the electric vehicle sector. With a focus on enhancing efficiency, reliability, and sustainability across the battery value chain, DigiCell utilises advanced modelling and machine learning techniques. Its multidisciplinary team is developing innovative measurement tools and digitally integrated battery models, leveraging artificial intelligence and machine learning to optimise both lithium-ion and beyond-lithium cell solutions. Backed by over €6 million in funding from the European Union's Horizon Europe programme and the Swiss State Secretariat for Education, Research, and Innovation (SERI), DigiCell aims to catalyse a significant impact on future battery cell technologies, aligning with the EU's objective of achieving climate neutrality by 2050 through the European Green Deal.

[7] https://i-tribomat.eu/
[8] https://aid4greenest.eu/
[9] https://www.nanobat.eu/
[10] https://www.digicell-project.eu/

4.3.4 CHALLENGES | Anacleto Proietti

The CHALLENGES project [11] aims to develop advanced nano-optical techniques and metrological protocols for real-time characterisation of materials using plasmonic-enhanced Raman, IR, and photoluminescence signals. With a budget of €4.69 million, it targets enhancing device performance, quality, and reliability across various industrial contexts including CMOS electronics, silicon photovoltaics, and 2D materials. The consortium comprises 15 partners from seven countries, focusing on non-destructive analysis, nanoscale precision, and integration into production lines.

4.3.5 iENTRANCE@ENL | Alfredo Picano

iENTRANCE [12] aims at advancing nanoscience and nanotechnology for energy transition and circular economy within the NextGenEU Program. Managed by CNR-IMM Bologna, iENTRANCE seeks to leverage nanotechnology research infrastructure for sustainable energy solutions. It involves a consortium of Italian research institutes and universities, focusing on catalysis, photovoltaics, and new material development for energy applications. The initiative emphasises open innovation, open science, and the FAIR data principles to foster collaboration and knowledge sharing across its network.

4.4 ACCORDS | Daniel Fernández Poulussen

ACCORDs project [13] is an effort to address the imperative need for safe and sustainable commercialisation of nano-, advanced, and smart materials, particularly focusing on 2D nanomaterials like graphene. Despite Europe's successful transition of graphene innovation into various commercial sectors, the lack of standardised characterisation and risk assessment methods poses challenges for further development and widespread adoption. The project seeks to develop a comprehensive characterisation framework that correlates material properties with toxicity, facilitating predictive strategies for safe and sustainable utilisation of graphene-containing products. By establishing reliable methods and guidelines, ACCORDs aims to support the continued commercial success of advanced materials while ensuring minimal environmental and human health risks.

4.4.1 GC-MAC | André Colliard Granero

GCMAC, the German-Canadian Materials Acceleration Centre [14], leverages world-leading expertise and facilities in Germany and Canada to provide an innovative and agile ecosystem in energy materials science. Its research capabilities include fundamental materials theory and modelling, interfacial electrochemistry, AI-enabled materials design, high-throughput computational and experimentation methods, design-to-device workflow, data science and analytics, and advanced characterisation tools. Aligned with the global shift towards a de-fossilised, decentralised, efficient, and economically viable energy infrastructure, GCMAC focuses on advancing robotic materials acceleration platforms (MAPs) to drive R&D strategies in this direction.

4.4.2 SITOLUB | Amaya Igartua

SiToLub aims to develop in silico tools that allow the design of safe and sustainable lubricants. The project follows the framework of safe-and-sustainable-by-design new chemicals, which is one of the keystones of a sustainable future, alongside reducing the overall use of chemicals and products in general and recycling.

[11] https://www.challenges2020.eu/
[12] https://www.ientrance.eu/
[13] https://accordsproject.com/
[14] https://gcmac.de/

4.5 Insight Talk: The use of analytical research infrastructures to support industrial innovation | Ennio Capria (ESRF)

The main point to retain about this presentation today is that Analytical Research Infrastructures (ARIs, (among which synchrotrons sources like the ESRF), may contribute and already contribute to industrial innovation, supporting R&D and QA activities of SMEs and LCs. They are supporting industry in new material development and in the optimisation of processes and products. This is indeed part of their mission and they have dedicated resources for this. Furthermore, they are often active at the core of dedicated ecosystems (like the one of Grenoble). This can allow them to make available a know-how that can go far beyond the simple deployment of our instrumentation.

If we think about the opportunities related with it, there is a quite low hanging fruit to be harvested in these large-scale research infrastructures, that today are also organised in the framework of ARIE [15] (Analytical Research Infrastructures of Europe). This is the deployment of streamlined routine services capable to run high throughput standardised experiments, where large lot of similar samples need to be characterised in an automatic fashion. These novel routine services need new pipelines to be consolidated going from the data acquisition to the data reduction, to the data analysis. These systems will be capable to produce huge datasets capable to feed AIs in a feedback loop between sample production, characterisation and modelling with the results to accelerate the discovery of new material and a more rational design of new products.

Unfortunately, today, when one thinks about ARIs supporting industry, often only considers their contribution to the scientific excellence pillar, where a lot can be done, for sure, in collaboration with industry, in the pre-competitive phase of the product development. Nonetheless, it already exists a proof of evidence that, by considering ARIs as potential business partners for industrial projects at higher TRL/MRL, could result in an incredible acceleration in material discovery and new product design. Nonetheless, this would need external stimulation, because this activity falls somehow beyond the core business of these facilities and industry would be a fast follower indeed, but would not take the initiative, due to a perceived lack of specific competences.

In conclusion, there is strong evidence that whatever strategy would be defined to support advanced material based industrial innovation, it would receive enormous benefits if these considerations will be taken on-board.

4.6 Conclusions

The presentations that different projects made in the third session of the workshop highlighted innovative approaches in materials characterisation and digitization. These projects collectively showcased advancements in digital twin technologies, analytical techniques, and their applications in improving industrial processes and product development.

5 Summary, Conclusions, and Outlook

The event encouraged collaboration and innovation, with sessions focusing on digital twin technology, Raman as a Process Analytical Technology, digital transformation in analytical labs, and opportunities for the industry from research facilities and projects. Key outcomes and follow-up actions can be identified as follows:

Event Outcomes:

- Both characterisation and modelling activities are fundamental to the Advanced Materials domain, and their contribution is essential in both science and policy (e.g., Green Deal, Digitization).
- There is a significant need for a robust and standardised data structure and semantics. This is a focal point for all projects in characterisation/modelling, but further efforts are required.

[15] https://arie-eu.org/

- Standards are the language of industry; we must translate more research outputs into standards. This will facilitate broader adoption and reduce costs.
- At the request of the EMCC, the EMMC is establishing a new focus area on Characterisation and Modelling.
- Digitization is necessary to optimise the manufacturing/modelling/characterisation triangle efficiently and effectively.
- EMCC initiated a survey roadmap, and preliminary results were presented.

Follow-up activities:

- Suggestion of a potential call topic IA or RIA in relation to the work performed in the funded characterisation calls to advance the TRL.
- Topic of a possible final NMBP-35 joint workshop in October organised in Paris (OCDE premises) or Brussels by CHARISMA together with the final project event.
- Participation in interlaboratory studies like the one that CHARISMA will launch this year to test the Raman calibration protocol.
- Collaboration in the development of the CEN workshop agreements (CWA) foreseen in the organising projects:
  - The CWA 17815 on “Materials characterisation - Terminology, metadata and classification” (2021) promoted by OYSTER project has been a first step in materials Characterisation Data (CHADA) standardisation. NanoMECommons is proposing a follow-up CWA on iCHADA.
  - Two CWAs on “Raman devices calibration, verification and twinning protocols” proposed by CHARISMA will have their kick-off meeting on February 28, 2024. They cover two topics:
    - CWA 1: Raman devices calibration and verification protocols
    - CWA 2: Raman devices twinning protocol

In conclusion, the event catalysed advancing collaboration, innovation, and standardisation within the Advanced Materials domain. It emphasised the critical role of both characterisation and modelling activities in shaping scientific advancements and informing policy decisions, such as those outlined in initiatives like the Green Deal and Digitization. The formation of a new focus area on Characterisation and Modelling by the EMMC, in response to the EMCC’s call, signals an effort toward establishing robust data structures and semantics, alongside the translation of research outputs into industry standards to drive broader adoption and reduce costs. Embracing digitization will further optimise the manufacturing/modelling/characterisation triangle, while ongoing initiatives such as interlaboratory studies and the development of CEN workshop agreements promise to enhance collaboration and standardisation within the field.

Acknowledgements

The Workshop was supported by EU H2020 projects NanoMECommons, CHARISMA, and EASISTRESS.

Figure 1: Workshop Group Photo: The photo was taken at the premises of CSIC where the workshop took place.

Table 1: Event Agenda.

09:30 - 10:00	**Opening**	
10:00 - 11:30	**1st Session: Industry Talks**	
	DIGITAL TWIN in Metal Material manufacturing	Hermann Autenrieth (Bosch)
	Raman as a Process Analytical Technology (PAT) tool for industrial manufacturing	Susana Gómez Sanza (IRIS)
	Digital transformation in the Chemical Industry	Rui de Oliveira (BASF)
11:30 - 12:00	**Break**	
12:00 - 13:30	**2nd Session: EMMC & EMCC vision**	
	Harmonizing Materials Knowledge Across EU Projects - EMMC	Alex Simperler (GCL)
	Advanced characterisation in the Digital era - EMCC	Marco Sebastiani (UniRoma3)
	Panel Discussion	Georgios Konstantopoulos (NTUA) Alex Simperler (GCL) Susana Gómez Sanza (IRIS) Amaya Igartua (AMI & i-TRIBOMAT) Raquel Portela (CSIC) Miguel A. Bañares (CSIC) Marco Sebastiani (UniRoma3)
13:40 - 14:30	**Break**	
14:30 - 16:30	**3rd Session: Current Opportunities for the Industry from Research Facilities & Projects**	
	CHARISMA	Raquel Portela & Miguel A. Bañares
	EASI-STRESS	Nikolaj Zangenberg
	NanoMECommons	Costas Charitidis
	From Project to Company: i-TRIBOMAT	Ilchat Sabirov
	AID4GREENEST	Coordination Team
	NanoBat	Ferry Kienberger
	DigiCell	Ferry Kienberger
	CHALLENGES	Anacleto Proietti
	iENTRANCE@ENL	Alfredo Picano
	ACCORDS	Daniel Fernández Poulussen
	GC-MAC	André Colliard Granero
	SITOLUB	Amaya Igartua
	Insight Talk: Analytical research infrastructures to support industrial innovation	Ennio Capria