Materials Today Communications 36 (2023) 106607

Contents lists available at ScienceDirect

Materials Today Communications

journal homepage: www.elsevier.com/locate/mtcomm

Materials characterisation and software tools as key enablers in Industry 5.0 and wider acceptance of new methods and products

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ARTICLE INFO

Keywords:
Characterisation
Manufacturing
Digitalisation
Artificial intelligence
Data management

ABSTRACT

Recently, the NMBP-35 Horizon 2020 projects - NanoMECommons, CHARISMA, and Easi-stress - organised a collaborative workshop to increase awareness of their contributions to the industry "commons" in terms of characterisation and digital transformation. They have established interoperability standards for knowledge management in characterisation and introduced new solutions for materials testing, aided by the standardisation of faster and more accurate assessment methods. The lessons learned from these projects and the discussions during the joint workshop emphasised the impact of recent developments and emerging needs in the field of characterisation. Specifically, the focus was on enhancing data quality through harmonisation and standardisation, as well as making advanced technologies and instruments accessible to a broader community with the goal of fostering increased trust in new products and a more skilled society. Experts also highlighted how characterisation and the corresponding experimental data can drive future innovation agendas towards technological breakthroughs. The focus of the discussion revolved around the characterisation and standardisation

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https://doi.org/10.1016/j.mtcomm.2023.106607
Received 16 May 2023; Received in revised form 28 June 2023; Accepted 4 July 2023
Available online 5 July 2023

processes, along with the collection of modelling and characterisation tools, as well as protocols for data exchange. The broader context of materials characterisation and modelling within the materials community was explored, drawing insights from the Materials 2030 Roadmap and the experiences gained from NMBP-35 projects. This whitepaper has the objective of addressing common challenges encountered by the materials community, illuminating emerging trends and evolving techniques, and presenting the industry's perspective on emerging requirements and past success stories. It accomplishes this by providing specific examples and highlighting how these experiences can create fresh opportunities and strategies for newcomers entering the market. These advancements are anticipated to facilitate a more efficient transition from Industry 4.0 to 5.0 during the industrial revolution.

1. Introduction

The materials community has confronted several challenges in EC-funded projects, which sometimes require collective engagement of experts to come up with harmonised solutions and realise a broader impact across markets. The *European Materials Characterisation Council* (EMCC) is essential to support collaborative European projects on adapting to new EC directives and to facilitate the wider impact of achievements regarding the strategic objectives and Industry 5.0 application needs in the characterisation field [1,2]. By aiding the scientific and technical excellence of novel characterisation tools and infrastructures with the support of strategic roadmaps, innovative outcomes are realised towards the digital transition and the increment of EU Industrial competitiveness worldwide [3–9]. This is a collective effort between the various platforms who are contributing to the wider landscape of materials markets, such as the *Energy Materials Industrial Research Initiative* (EMIRI), *European Materials Modelling Council* (EMMC), *European Technology Platform for Advanced Engineering Materials and Technologies* (EUMAT), and *Advanced Materials Initiative* (AMI2030) which recently published the Materials 2030 Roadmap [10]. These platforms are joining forces with stakeholders to develop and transfer to the society novel technologies and materials. Especially under the umbrella of AMI2030 initiative, such collaboration is envisioned to reshape EU industry, aiding policies and regulations towards a stakeholder-driven economy [11], and outcome-oriented roadmap to support the emerging innovation markets and their corresponding needs.

This work is the outcome of a joint workshop organised by the three H2020-NMBP-35 projects, where experts and stakeholders, cooperating under the umbrella of EC-funded projects and various platforms, were brought in a common table to discuss about emerging scientific and technological topics and share their knowledgeable insights. The views of 28 experts were collected, representing multiple sectors in the materials field and 10 different countries in Europe, UK, and Norway: 10 experts from universities, institutions, and Research and Technology Organisations (RTOs), 1 from a national standardisation body, 1 from a Small-Medium Enterprise (SME), 8 experts from the industry, and 9 representatives from European initiatives and platforms.

The main topics covered were characterisation and standardisation, the suites of modelling and characterisation tools, as well as data exchange procedures. The Materials 2030 Roadmap and the lessons-learnt from NMBP-35 projects thematic covered the broader landscape of today's materials characterisation and modelling community's concerns.

This work aims to provide the materials community with answers to common dilemmas, to shed light on new trends and evolving techniques, as well as to outline the industry views on emerging needs and success stories of the past with specific examples, which can create new opportunities and strategies for new entries to market derived as outcomes by high-level EC-funded projects.

2. European landscape on materials characterisation and modelling domains

2.1. Standardisation in fit-for-materials characterisation

Nowadays the creation of **standards fit for materials** is an emerging demand by materials markets. The characteristic example of magnetic measurements, in which the materials key properties may be totally different depending on the assessment method (i.e. most common wattmetric measuring method) and type/anisotropy of material [12]. Thus, there is a significant need for standardisation in characterisation, as highlighted by this example and considering the impact of fit-for-purpose materials standards across different domains. The use of improved and agreed standards is essential not only for activities related to commercialisation but also for science and innovation as such [13]. The evolution of standards can have a generalised impact as an enabler for easier data and information exchange. This is the **motivation of companies in getting involved in the standardisation system**, trying to change or improve existing standards since there is a constant demand for accuracy, consistency, and reliability, especially regarding analytical techniques and technological aspects. As an example, ELODIZ is working within CHARISMA project in the revision and improvement of the standardisation landscape of Raman spectroscopy [14]. It was underlined that the new challenges related to the green and digital transition, as well as data science must be addressed by implementing widely accepted industrial commons, confirming that the consistency of standards across different domains is critical for international collaboration and establishing an international, broadly implemented, and easily applicable standardisation system.

It is encouraging that **many European projects are engaged in standardisation processes**, because their consortia can allocate their technical expertise and power to help advance and implement the standards. The scientific community has identified the need and benefits of cooperating with Standardisation Committees to find ways to exploit the results of Research and Innovation (R&I) activities. Also, developing FAIR (Findable, Accessible, Interoperable, and Reusable) [15] databases and common strategies for storing and sharing data will contribute to dealing with some of the current challenges in research. However, a standardisation framework yet to be realised; ongoing work within IUPAC task groups and the Committee on Publications and Cheminformatics Data Standards is moving towards this direction, emphasising on FAIR data, data interoperability, and machine readability [16].

However, there still remains the challenge of engaging and motivating experts to participate in such standardisation activities. For instance, industries are profit-focused and outcome-oriented. Hence, they use predominantly in-house equipment and SOPs/methods for their products without the need to involve third parties. On the other hand, it takes time for academia to join standardisation work, which is considered a complicated task, often unnecessary for their research workflow and unjustified as extra cost. In the NMBP-35 joint workshop it was highlighted that the scientific community can identify the drivers for standardisation by answering the questions "why do we need standards?" and "what is the impact that will be created?". Contributing to standardisation by either improving existing standards with the findings of the project or developing a new standard based in their outcomes will enhance the impact of the project results and facilitate their market uptake.

Especially, in light of the climate and energy crisis, online and non-destructive characterisation tools can broaden the opportunities for minimising manufacturing footprint by advanced process control [2]. **Advanced process analytical tools** (PAT) can minimise manufacturing footprint. For instance, Raman spectroscopy is an interesting non-contact technique that essentially works with UV, visible and near infra-red (NIR) light, which is an attractive feature to analyse and assess glass quality [17]. This can be regarded as a symbiotic material-characterisation pair. Glass manufacturing requires tremendous amounts of energy for processing, as often remarkably high temperatures are employed, in the range of 1500 °C and sometimes also rare and expensive ingredients like lithium, which could be challenging to acquire. Raman opens the possibility to control and monitor the process online [17], which from the glass end-user perspective is important because it enables glass manufacturing to become resource efficient. Another benefit of glass characterisation by Raman spectroscopy is that it is a simple technique to investigate material properties even in liquid form, which cannot be achieved by classical optical methods, neither diffraction methods, which are difficult to be implemented, nor NMR methods, which may not be as accessible as Raman, due to the high cost of NMR technique. Standardisation for the glass manufacturing industry is difficult at the moment. However, much can be achieved with Raman methods development, since there are a lot of materials and process parameters under consideration that can be assessed, such as the manufacturing history and the impurities [18].

2.2. Characterisation and modelling suites

Harmonising Raman measurement and calibration procedures to achieve **reproducibility can open interesting perspectives for the numerical methods to complement the characterisation methods**. For instance, an existing gap was outlined in the organisation and accessibility of data on glass manufacturing and properties, which restricts the data exchange and exploitation of in-house research data [19], thus reducing the opportunity of AI capabilities expanding to the glass sector. There is a wide range of glass data, but the vision to exploit these data is currently missing. The only data that can be accessed and used are derived from personal research. Raman spectroscopy can be a potential suitor for acquiring material information from a high dimensional parameter space related to the material structure, which is starting from the order of the number of few atoms. On that basis, new data generation would be the key ingredient to bring machine learning into the spotlight, realising a wider impact in the exploration of the parameter space [20]. This includes the mining of relevant material parameters that are derived from Raman spectra in combination with glass thermal processing history, including thermal processing windows, cooling speed and temperatures, and with glass properties data. Thus, the correlation of the broadbands that represent superpositions of the complex arrangement modes can be linked to a prediction model for material properties that can be deployed to monitor very subtle changes of the material quality, which is of main industrial interest.

Another topic raised was **how physics-based models' exploitation can fit into the characterisation suites of the future**, and specifically electronic models for Raman spectra simulation or supporting the assignment of spectral features to materials features. NMBP-35 project CHARISMA is contributing to such objective under the framework of open science, developing models that will be accessible and open to public; for example, models related to reference materials for calibration. Ab-initio methods and DFT are used to build the physical models of the systems that are studied. There is planned effort to calculate their Raman spectra and identify the spectral features and validate calculations with experiment. The project will also support the acquisition of spectra without influence of the optical part or any other contribution by the environment, aiming to the pure material response. The spectra data generated will be made available in the NOMAD repository and all project outcomes will be open and accessible there.

On the digitalisation pillar, the **applications/graphical user interfaces (GUIs) that are being developed, can be integrated with AI** and lead to exciting applications in the use cases; however, it was argued that performance bottlenecks could appear, and then it would be challenging to address them and investigate whether it would be the data, the model, or both that would be the real problem. The limited interaction between theory and experiments, especially if someone considers that theory can be disrupted by an experiment, was identified as an obstacle in the past, and there is no clear consensus, still, on how to address this limitation [21]. This refers to the framework where data-driven and physics-based modelling is required, from developing and designing a new material to using the material or eventually the product. It is a mission for EMCC and EMMC to bring these topics together and to propose dedicated actions and task group exercises to address the common challenges that materials research communities are trying to solve at present, including data models and software, and consider how ML and AI integrated approaches in use cases can generate impact and value for industry [2].

The cooperation between modelling and characterisation communities was identified as a key feature to meet the needs for accelerated product development. VIPCOAT project, as well as other projects involved in similar topics to NMBP-35 projects, is working to implement an innovation platform which brings together industry, academia, government, standardisation, and other legal bodies, as well as society, by materialising the European Vision on Open Innovation Frameworks [22]. In connection to characterisation and the well-aimed landscaping of the actions needed for standardisation, **standardisation could be bringing the solution to the problem of the high-quality data demands for the development of modelling suites** to cover several aspects of materials development. In addition, the **importance of understanding what society needs** was highlighted, because society is the real end-user. Modelling and characterisation should eventually address society's requests by offering sustainable, circular, and ethically-bound solutions to the materials market. Moreover, it was emphasised that EMMC and EMCC can act as facilitators towards meeting the societal and industrial needs by bringing those communities to work together for such scope in a framework of cooperation, communication, and synergy.

2.3. AI and data exchange procedures

Process parameter optimisation is a big case study of AI exploitation, because even a slight percentage of improvement in the efficiency of a model can be a deal-breaker. In that case, after the user sets the target, machine learning algorithms can give useful output on necessary adjustments in order to achieve the objectives set in the design phase of the manufacturing process. Thus, since data access is a critical aspect for data science, **it is crucial to have suitable databases** where data integrity is protected and preserved. There is a gap on organised databases or datasets, as commented for the glass manufacturing sector, where there is potential for data exploitation opportunities utilising in-house produced data and data used by industry, but this also requires a framework with **open access** for exchange procedures and external management. Ansys, for example, is conducting a lot of work utilising artificial intelligence in exploiting small- to big-size data, and apart from the commercially available and very restricted data, it also works with open-access tools, such as PyAnsys, a rich open-access Python environment with multiple possibilities offered to the users. However, data exchanges between big industry players are difficult since IP issues can arise. The current strategy of EU industry is to exchange and share data only in the framework of collaborative projects; even there, companies and industry, in general, are eager to share their data.

Another cornerstone of the NMBP-35 joint workshop discussions was

the importance of AI and alternative methods to help with data exploitation since AI is a great interpolation system. Furthermore, while societal and geographical data are considered as big data and, thus, a big effort is needed for their processing, materials data, considered as small to medium sized and coming out from machine lines, are an excellent source of data to be used in AI. There, AI holds a key role, since the experiments from which data are derived are often expensive, difficult to reproduce or can be performed only on the boundary conditions. Thus, all the space in between can be filled with data from AI, and is a great place for AI to flourish in materials science field [23,24]. To that end, companies such as Ansys, offer open access data under commercial terms, and also work with open access tools (their own or third party) to build a technological ecosystem, such as PyAnsys.

In the future, AI is expected to offer the potential to reproduce the simulation of e.g. Raman spectroscopy, and generate spectra corresponding to material structural properties via the development of physics informed machine learning and explainable machine learning. Therefore, industry does not underestimate the power of basing some AI prediction on, for example, a Raman peak ratio. Physics informed and explainable machine learning can achieve high impact in the materials science landscape if there is integration with databases and access to vast amounts of annotated semantic data [25,26]. An interesting point is that AI can, in some cases, fill in data gaps, and thus, dataset completeness can be increased, which is crucial when indexing data in public repositories. In other cases, AI is going to be an ever-extending body of knowledge for an industrialist. At present, there are good examples of applications in additive manufacturing (AM), where a lot of data is generated for every build and product. It is claimed that there are about 140 parameters that could be utilised for optimising a specific product, and the level of complexity increases considering many machines across many products. In this direction, data analytic techniques like machine learning and artificial intelligence will play a key role in AM, thus having a disruptive character. **AI, however, can be misleading** in cases of industrial business transactions and of communications, and thus it is required to be able to transport information and to rationalise AI strategies beyond the black box model development step. Therefore, industry considers AI as a useful tool for data exploitation and processing, for example using it to base prediction on a Raman peak ratio. However, AI should be used with caution since it could lead to false data production at times.

So far, one main limitation of AI is identified as the scenario where the predictive modelling is genuinely derived from a statistics/probabilistic perspective, similar to the suggestion/recommendation systems that can suffer from unforeseen changes in the trend of data, including statistical/computational/human/systemic biases [27]. For example, AI and generated models were not effective in the beginning of the pandemic because the situation suddenly changed the context of the machine learning, and the new data in those sectors were not represented by the previous statistics. Implementing AI in combination with known norms and equations could bridge such gaps. Since it is going to be disruptive as a technology, what is needed is to work together with the best combination of equations representing the existing theory and background knowledge. In this direction, there have been new developments in physics informatics. Physics equations can be used to build the engine of solving complex tasks, i.e. in the calculation of unknown equation parameters via the utilisation of partial differential equations, in efficient manner and is expected to lead to fruitful and productive outcomes [28]. Simplicity provided by any means of AI or assessment methods is appealing and sometimes very powerful. **In science, as soon as physics is involved in the background calculations, one should expect efficient calculations, as well as disruptive impact of the predictions, overcoming the bottleneck of the black box effect.** Although, there is still scepticism from the research infrastructure side about AI and potential impacts, which might be overcome as soon as scalable, adaptive, and explainable machine learning paradigms rise utilising physics norms and improving societal skill-force and access to open AI tools [25,26,29]. In conclusion, AI in materials science applications remains a bright field of R&I since there are many open questions, still waiting for the scientists and the community to answer.

3. Materials 2030 Roadmap – characterisation and modelling as horizontal enablers

NMBP projects and EC strategic objectives escalated over the years from the level of materials improvement and innovation into more complex objectives of components and systems of components, with an increment in the level of accomplishment. In this process, Advanced Materials 2030 Initiative (AMI 2030) can play a key role to drive the research agenda into the right direction. The challenge to do that effectively depends on engaging **relevant and representative stakeholders** of the European landscape, considering the broadness of the defined Strategic Materials Innovation Markets [30], as well as from shaping their scope and strategic objectives in order to translate them into research and innovation methodologies.

The policies and vision for 2023–2030 will include dedicated actions for characterisation enablers that will be involved in the innovation paths for materials innovation markets, which requires close interaction with Safe and Sustainable by Design (SSbD) frameworks. Characterisation has a broad impact on materials markets since every evaluation of properties contains a characterisation enabler, and these are concomitant in every call for materials development. At present, the three NMBP-35 projects are harmonising characterisation methodologies using materials at high readiness level for exploiting standardised tools to industry, which is part of the ongoing Materials 2030 Roadmap [30]. Furthermore, the SSbD framework needs to introduce and work with new methods, and improve the existing ones. Thus, there is an exciting potential for characterisation, and practically, for all the markets that are seeking sustainable high-performance materials, i.e., sustainable textiles, sustainable packaging, sustainable agriculture, etc. for combining sustainability and safety in parallel, which are part of the digitalisation framework, aiming to ensure that new technologies will have the minimal (negative) impact on people and planet.

3.1. Digitalisation policy in Europe

At high level of policy, everything is driven towards green and digital in various technologies that are contributing with data and knowledge generation to this field. The first message, as brought from AMI 2030 initiative, is that an end-to-end approach is taken about generated materials data by both modelling and characterisation. Industries have already joined the Materials Digitalisation working group 1, contributing to setting the stakeholder-driven priorities towards the strategic outcomes in a stakeholder-driven EU economy.

Regarding the AMI 2030 Digitalisation working group [31], a starting point has been to investigate what data we have today, and what is the need to access and use that data. Then the second priority is the constantly generated new knowledge. Data generation is an ongoing and living process that certainly surpasses the access to huge data, where it is still unclear how to define robust pathways towards data openness and data management, as well as methods to analyse and process this data. The main problems are around the management and documentation of metadata, e.g., a common methodology for expanding domain ontology and representation of knowledge in i.e., knowledge graphs. An iterative process is required to perform-assess–improve the materials design phase, and throughout the product life cycle. It has been a challenge to identify the context of this iterative management and documentation process and the right path to address it collectively in the Materials 2030 Roadmap, which has been done via several horizontal strategic actions [10]. To achieve a good system for documentation and management of data, policymakers should be engaged, and support the developments in that direction, so that the widely accepted strategic research innovation agenda driven by AMI 2030 initiative can be translated into actions that are straightforward at the policy level. This is another big and emerging challenge, which requires collective effort.

AMI 2030 will be organised through a certain governance process. The digitalisation agenda is really driving the materials field via a system run by the community. Specifically, EMCC and EMMC will play a big role, because both represent the stakeholders and experts that are driving the innovation markets by helping industry to benefit from materials informatics and novel R&I methodologies and exemplifying their application across industrial sectors. To achieve AMI2030′s objectives, there is the need for its goals to be well-defined to deliver on what these innovation markets need and beyond, and ultimately to realise the benefits for the end-user that actually is the society. Since the priorities can only be a few, there is an ongoing effort to capture the current state of the art across different fields. The vision of the necessary developments integrates and homogenises the diversity of approaches indicated by experts in the new version of the Materials 2030 Roadmap, building on the previous accomplishments of EC FP and Horizon Europe programmes.

At more specific level of digitalisation, the semantics, ontology, EMMO, CHADA, and interoperability to modelling, AI, and characterisation could have a positive impact IoT in industry. The characterisation (meta)data structure (CHADA) is a unique result which has been standardised, and is used to extract the semantics for characterisation. NanoMECommons is taking specific use cases of characterisation to extract the specifications and links/interdependencies of methods according to end-user needs. There is an effort to simplify the completion process because currently completion includes free text, which can make it almost impossible to transform human readable forms into machine-readable language to represent the domain knowledge. Thus, one emerging need is to have a glossary that describes the characterisation and the background knowledge around it, so CHARISMA and NanoMECommons projects are documentating the terminologies used for each characterisation technique in a collaborative environment, i.e. Wikidata, which can be used for open collaboration between experts and research community. It is important to engage more experts in this effort of trying to determine widely accepted terms for describing the experiment of characterisation, and such great impact could be the outcome of a synergy between NMBP-35 and other characterisation projects, such as OntoTrans and Big Map projects, on characterisation semantics.

Another challenge that was highlighted during the NMBP-35 workshop was that there have been projects that performed tasks on ontology development before the CHADA standardisation, and it is needed to define the framework for the utilisation of ontologies already developed following different standards. EMCC as well as EMMC can be the platform to facilitate the coordination of those efforts in the digitalisation domain, and facilitate the reuse and expansion of ontologies by sectors. For example, TEESMAT project has established the terminology for energy sector and batteries, whereas in NanoMECommons it is amongst the objectives to expand the domain knowledge in the standardised methods for materials/product properties nanomechanical assessment. In that end, another key point is about the common vocabulary. Thus, a more efficient way to collaborate is created, as well as to generate and analyse the data, which is opening the road for multiple applications and the similar philosophy helps further integration of all these different characterisation techniques and CHADA. One recent outcome in this direction is the ontology based on CHADA *CHAMEO* [42], which is a machine readable version of CHADA and supports interoperability in the characterisation domain based on EMMO principles [43].

3.2. Industrial competitiveness and high-level innovation goals aided by collaboration framework and centralisation of knowledge

From an industrial point of view, **sustainability should be a major industrial driver**, as it is now, and will be in the future, for the automotive company Stellantis (former FIAT), for instance, which has a global approach to material engineering. At the first years of Stellantis, an industrial plan was published focusing on a complete decarbonisation of the products by 2050, with a 50 % reduction of CO_2 emissions by 2030. To meet this challenge, a deep intervention is needed not only on propulsion and energy storage systems. This process involves several different materials and sustainability approaches. Amongst the strategic objectives of Stellantis by 2030 are the increase of the green material content in metallic components to 50 %, and in polymer components to 35 % by weight [32,33]. The expected impact on the mobility sector is high, emphasising the vision of a half-tone vehicle instead of 1 tone. Regarding energy storage, not only the active material in the battery cell, but the whole battery pack needs to ensure specific performances, including thermal dissipation and automation, two major industrial challenges to overcome that will be big drivers in the immediate future.

Designing against failure is and will remain a technologically relevant priority in materials engineering. One critical need in materials development is to build the required knowledge to prevent failures and introduce defect tolerance [34,35], as well as to develop fast and accurate testing methods for materials assessment as a “Hardware Cloud”, including virtual prototyping (“Software Cloud concept”) [34]. It was noted that in most of the occasions car companies do not manufacture all their product’s parts themselves. Therefore, there is the need establish collaborations and partnerships to assess materials and ensure that their structure and properties comply with the specifications to enter the markets, and are safe and ready for responsible use. Still, the materials ultimate requirement is to be leading to affordable end-products.

Another topic was about the need for a framework for **sharing background knowledge and data**, which currently exists only in the form of collaborative projects. Synergies and coherent communication are lacking and are underexploited for characterisation and modelling communities to produce common suites or tools that are easy to understand. Furthermore, when industries and IPs are put in a collaborative and partnership context, technologies and data that are protected by background knowledge which cannot be shared. Therefore, community experts and end-users are sceptical about bringing in their background within common projects with other companies, due to competition. Although this question is often complex to address, there has been progress in regards to openness.

Stellantis, for example, started sharing material information almost 20 years ago with the IMDS system that was created by a car maker consortium to share the material components until the basic substances composition [36]; several years of discussion were needed in order to manage the level of disclosure that the supplier was comfortable with. Therefore, it has been a common case in collaborative projects, to enter in a direct communication channel with the material supplier and end-user, in order to ensure that royalties and ownership are properly disclosed regarding materials information, which are the competitiveness assets. Direct support from the end-user to the supply chain, and vice versa can facilitate and spur collaborative innovation [37]. The end-user will endorse the material provider to increase the TRL of research and innovation activity in the specific field, and in the end enable the product to have the adequate readiness level to enter the market. In any case, material information is owned by the supplier, so the whole supply chain needs to be involved in this discussion, and the activities related to production are managed by suppliers, not by end-users. Recently, EU automotive industries partnered together in an innovation network for knowledge sharing with a dedicated materials data space, *CATENA-X* [38], which aims to advance quality management, logistics, maintenance, supply chain management, productivity and sustainability, laying on the foundation of the European cloud data infrastructure *GAIA-X*.

Another topic raised was about the ongoing establishment of the digitalisation agenda, and the stakeholders needs regarding exploiting data produced in the past. Specifically, end-users store massive amounts of data generated by production, characterisation, and modelling. Focusing on the technical part of reusing data in a dynamic manner, a challenge to confront in the future, it was questioned whether end-users benefit from past data to design new materials or components, especially when data were produced 10 or more years before. It was concluded that data do not expire or age, even though it can be worth to reproduce specific data due to a low cost and improved value compared to previously generated data, and overall, it seems wise to keep the data stored.

Companies are outcome-driven, and this could imply that decision-making is aided by static designs based on the outcome of materials characterisation, and thus empiricism in validating that materials meet the specifications to reach the market. On the other hand, utilising previously generated data to identify modelling-aided process windows and optimising the operations based on evidence-driven implications for process design can be a more efficient strategy for both increasing the TRLs and for the final product design in entering the market faster and with success. Thus, a question was raised, from an end-user perspective, if data are used to exploit new products or industrial digitalisation objectives, which for example, come into characterisation and digitalisation strategies used for benchmarking new materials. There is a need to cultivate a data-rich way of thinking, which requires multiple levels of actions, starting with education of people and society [34], and multiple sources of information that bridge the physical to digital world.

It was noted that in-house data repositories of end-users are established about specific characterisation techniques, and the data generated by those techniques are exploited to produce material cards for materials modelling. This is an internal policy applied by Stellantis, and specifically two strategies are followed concerning materials. One regarding the evolution of a traditional material, where composition, as well as physical and chemical behaviour are employed in order to seek for new challenges, new boundaries, and performances driven by the market. In other cases, the approach to material engineering and design is more disruptive, seeking for important evolution of industrial products to meet new product requirements. In conclusion, as an outcome from these questions it was commented that data cannot be reproduced, expire or age, even though there can be specific data worth to be reproduced due to a lower cost and improved value compared to when data were generated, and overall, it is beneficial to keep all data stored.

Characterisation methods and improvement of materials and products is a symbiotic process. For the evolutive material, the characterisation and validation activities, as well as experience and data, are used in a disruptive approach in order to innovate, to build new know-how and knowledge. In the process, the characterisation methods must be defined and improved. Stellantis exploits its repositories in a collaborative environment with external institutions and universities, where a method is developed in deeper detail and with different instruments, which are not accessible in the internal facilities. This strategy has been employed to build common competencies and share knowledge on disruptive materials development, thus sharing a common background with clear ownership rights of the method for testing and the method for material development.

3.3. Success stories of centralised knowledge and data exploitation in the past

There are clear business cases for storing, sharing and reusing precious knowledge and data generated in the past. he first influencing example is the one of **Dow Corning Corporation** (glass manufacturer), with the end-user focusing on glass materials production with improved impact resistance for aerospace and defence sectors. That project was dropped before its accomplishment; however, the end-user stored the data and metadata, and then about 2007 was able to resurrect them when Steve Jobs was seeking for a glass to be indestructible on iPhones, benefitting with a huge commercial interest [39]. Granta Design Ltd. (acquired by Ansys Inc. in 2019) was involved in data management solutions for Dow Corning Corporation, and continues to be the industrial leader for materials information management software such as Ansys Granta MI. This is the foundation that end-users are laying today and with open innovation digital ecosystems within their companies and with a clear business case for reusing precious knowledge and data generated in the past.

The second story is about **Japan's paradigm**. Japan provided every company and industry with access to a centralised database created to build a common know-how in depth, which provided security and strategic advantage for the development of advanced research and technology in Japan back in 1980 s′ and till today [40]. The European Community was suggested to see the benefits in mimicking this and focus the efforts across a common research line, specifically on data saving and ensuring availability with adequate guidelines and clear ownership rights, and case specific management for stakeholders owning precious data. Following this paradigm can enable more companies to flourish like the Dow Corning success story and increase their market share by orders of magnitude.

3.4. Vision for sustainable partnership models in EU

Europe should steer to industry towards joining partnerships, European initiatives and innovation platforms can materialise the vision of creating a collaboration ecosystem between industry and research infrastructures, including academia. In Nanoscience Foundries and Fine Analysis (NFFA) project, partners are offer **access to both large infrastructures and laboratories for industry**, affording access to distributed research infrastructure from large synchrotrons to sophisticated laboratory methods, which often is considered as a limiting factor.

One issue is the intellectual property rights, which sometimes precludes the publication of results, which has to be strategically handled, finding formulas to satisfy both sides. Another aspect debated was about NFFA's role as an intermediary working between research infrastructures and industry, where a profit can be made by research infrastructures. Therefore, their strategic implementation agenda and plan can be included in EMCC Roadmap supporting the vision for required actions to be taken within the next 5 years.

In the view of a business/sustainability plan, it was discussed that both industry and research infrastructures can benefit throughout the process of materials development; in pre-competitive phase, industry is often very open to publish, because they use model systems, with limited use of confidential know-how. Confidentiality issues may arise when a product enters a phase of readiness, which is closer to the market or application. In this case, this is even an advantage because NFFA project members can use the access for precompetitive phase in order to work with industry to make them approve, accept and assume their methodology. Thus, when the product enters the stage where information is sensitive and confidential, then industry will be happy to pay for services, since they will have trust in the methods due to successful previous cooperation, and they will not have to pay for taking the risk, which means that industry will be willing to establish more collaborations.

Another discussion topic was the **motivation of industrial partners joining initiatives such as NFFA, EMCC or AMI 2030**. By participating and contributing to calls for roadmapping activities and working closely with experienced and skilled experts across industrial sectors, they contribute to bringing an organic process into innovation agenda and industrial revolution. This has been enabling in terms of engagement with emerging needs and problems faced by industries being recorded, thus making such exercise more efficient, and to shape a broader perspective on the requirements for the next developments.

Participation in collaborative projects and initiatives with strategic impact in material engineering enables the creation of collaborative frameworks, which allow stakeholders to share data more freely among themselves and with other industrial sectors, the extensive research and innovation activities needed to ensure product competitiveness motivate such collaboration. For instance, Stellantis participates in collaborative projects with other automotive industries with competing interests, sharing data with competitors [38]. Thus, industries rely on collaborative initiatives; this also has additional benefits, i.e., keeping technicians up to date with the current state of the art and being able to follow the materials evolution, especially considering that employees are oriented to follow a long-term career in the companies. Thus, the overall impact is keeping products up-to-date, meeting the society needs, and upskilling the personnel in disruptive sectors of materials and methods evolution, as well as keeping up with the testing instruments and standard materials, which are evolving as well.

4. Conclusions, takeaway messages, and outlook

Instrument suppliers are working towards dedicated and affordable solutions for end-users, which means that highest capabilities and resolution are not required in every application. When a new instrument with lower capabilities or resolution is going to be used, but more affordable, for a well-suited application, a trust concern becomes an issue. There is a need to develop methods to validate and perform the harmonisation and standardisation of these tools that are useful. Advanced and more reliable technology through harmonisation will open a wide range of application arenas. In the case of Raman spectroscopy, there are examples with Raman handheld devices applied to compounds detection. It would not be daring to consider that the future would bring Raman detection even in mobile phones. Standardisation differs from harmonisation, regulations, and certification/conformity assessment and is considered by the European Commission (EC) as one of the tools that can make the projects' results acceptable to the industrial sector and realise their uptake in the market. The importance of standardisation was outlined to facilitate the industrial transition and acceptance of such innovative methods and products developed within Research and Innovation (R&I) projects.

The critical challenge is developing new methodologies and technologies and harmonising and standardising them appropriately to achieve higher capacity. New tools, enabling faster data exchange and processing of many measurements, combined with automatisation, will contribute to the broader application of the NMBP-35 projects' results in the industrial sector. Regarding materials data uniqueness, stemming from different instrument suppliers and hardware features, an example was given by CHARISMA project on Raman spectroscopy development and standardisation. It was noted that through benchmarks of reference materials, algorithms, and protocols developed, accurate, and consistent data collection and handling is possible, regardless of the Raman equipment used.

The transforming society and the undergoing digitalisation activities are pushing for new solutions to cope with different forms of crisis, including the supply chain, energy, health, and environment (already confronted to some extent). It was shown that standard assessment methods can also have a role in social exploitation of new project-derived technologies. In a context of projects achievements and their corresponding new technologies, people can have in the future first-hand experience of the application of physical and chemical principles. These projects afford changes to the best interest of society. Delivering high-tech to non-technically educated users requires intuitive user-friendly devices and interfaces; for example, plug&play or single-button automated routines. This may be challenging to implement, but it will foster maximum society engagement. Such scope is where data science, artificial intelligence, common metrics, data analytics, and the implementation thereof in a robust software is critical. People having more access to validation process rather than trusting the given label or any other label, could see such technologies naturally entering the markets, just as they have seen barcode scanners in supermarket telling the product prices. Increasing societal awareness of technologies helping people's day-to-day life on food or any other application may, in turn, upskill the society. The harmonisation of technologies and data science all together will bring the technology to users who are not necessarily highly educated in the art. The only limit will be in the imagination and funding.

In addition, in terms of digitalisation efforts, there is a common interface for NMBP-35 projects, which has been transformed into an initiative via EMCC working groups for synergy on the terminology development for characterisation. This initiative facilitates sharing of the domain knowledge towards interoperability and wider impact. It is important to engage the community on common challenges like this, where the aim is to capture and organise the metadata of characterisation, because after that, AI will excel when accessing structured data. This could find application in the automation: automate procedures, analysis, or methodologies execution in smart manufacturing plants, and even implement and reproduce part of testing automatically with the support of robotics.

In order to envision the latter, i.e., the robotics reproducing experiments, the community has to define a strategy to (i) capture the thoughts of the scientist, (ii) conceptualise knowledge and (iii) assess correlative information to perform evidence-based decisions, and (iv) assure that the cognitive knowledge for the methods can be stored and reused in an interoperable manner (i.e., according to EMMO guidelines). This is much in relation with another European initiative, MAPs, coupled with a collaborative spirit from USA and Canada, and coming from the concept of autonomous or self-driving labs, articulated through the workshop report Materials Acceleration Platform [41].

Besides that, it should be noted that the community needs the structured data and terminology to be in machine-readable form and accessible to achieve IoT wireless connection, which is a mean of improving the application of the technologies; if you can connect a handheld Raman device to the network, the user can get instant comparison of your data utilising the power of databases, in order to automate and simplify the analysis task for the users. Machine readability of methods' outputs holds much promise for extracting fast and vast amount of data from any single measurement and analysing existing data silos.

Following the success stories of the past, the centralised data management was considered as a policy to build the momentum for European materials excellence in the next 40–50 years. Industries show interest in opening their data and sharing background knowledge under the right conditions and framework. Competition is a hurdle to consider; however, European policies of digitalisation, circularity, and SSbD foster an ongoing evolution of materials engineering in numerous innovation markets; this is the hallmark of a new era. The technologies are transitioning to achieve decarbonisation goals, so that evolutionary materials are currently in the precompetitive stage, where industries and suppliers are open to establishing collaborative schemes in order to build the required know-how to realise new entries in the market.

There is an opportunity for Europe to establish a centralised plan for data management in the digitalisation agenda, which can address the needs for exploiting materials data and standardised materials testing methods in an adequate framework. Materials data can be exploited in dynamic materials manufacturing windows, supporting innovation, safety, and sustainability by design, whereas it can be a thesaurus of knowledge to be used in future breakthroughs, including AI empowered exploitation, according to societal needs. In addition, standardised methods can be used by industries as a tool for producing ecolabels and materials cards which are representative of the material quality, commercial value, and added-value to society. To facilitate this vision, data exchange procedures should be enabled by the storage of organised data for testing methods that allow the stakeholders to seek for adequate and quantitative techniques that serve structure- and materials-specific testing, validation, and benchmarking. Beyond data organisation, it was highlighted that in order to exploit data we need models. On the NMBP 35 and other relevant projects, there is work in the making, with emphasis on the heart, on the soft art of the measurement methods. The touching base with the very specific applications of NMBP-35 projects is through the data treatment and analysis of information generated.

NFFA and EMCC are continuously developing their networks, bringing together stakeholders and experts from multiple disciplines to identify major challenges, new trends, and industry and societal needs. All this information is put together in a harmonised manner in strategic roadmaps, and the advantage of testing a Roadmap is that it is offering the capability of opening a large network of infrastructures to industry. Thus, the vision of the Roadmap can be broadened by actually the Roadmap going "live", and giving the feedback in a dynamic and organic manner with impactful directions to solve upcoming new and unforeseen industrial and societal challenges.

CRediT authorship contribution statement

All the authors contributed equally to this manuscript.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

No data was used for the research described in the article.

Acknowledgements

The Workshop was supported by EU H2020 project NanoMECommons, GA 952869, CHARISMA, GA 952921, EASI-STRESS, GA 953219, and EsSENCe COST ACTION CA19118. This article/publication is based upon work from COST Action *EsSENce COST ACTION CA19118*, supported by COST (European Cooperation in Science and Technology).

Miguel A. Bañares, Raquel Portela, Nina Jeliazkova, Enrique Lozano, Bastian Barton and Iván Moya have received financial support from the EU H2020 project CHARISMA, GA n. 952921, Bojan Boskovic, Ennio Capria, Costas Charitidis, Donna Dykeman, Spyros Diplas, Gerhard Goldbeck, Marco Sebastiani, Elias Koumoulos, Silvia Giovanna Avataneo, Miguel A. Bañares, Raquel Portela, Anastasia Alexandratou, Athanasios Katsavrias, Fotis Mystakopoulos have received financial support from the EU H2020 project NanoMECommons, GA n. 952869, Nikolaj Zangernberg and Ennio Capria have received financial support from the EU H2020 project EASI-STRESS, GA n. 953219, Natalia Konchakova has received financial support from the EU H2020 project VIPCOAT, GA n. 952903, Costas Charitidis, Elias Koumoulos, and Spyros Diplas have received financial support from the EsSENCe COST ACTION CA19118.

All authors would like to specially acknowledge Anastasia Alexandratou, Athanasios Katsavrias and Fotis Mystakopoulos for their support in NMBP-35 joint Workshop organisation and documentation, and Steffen Neumann for his insights during the NMBP-35 joint Workshop discussions.

Appendix. Example on use case that showcases the long-term horizon beyond the NMBP-35 project results on materials assessment methods and social benefits

There has been the paradigm of CHARISMA project with the Raman tools that are being developed, which can provide benefits to multiple sectors. An example in the food supply chain was introduced, where Raman would be applied to assess the state of packaged meat if the actual due date depends on the state and concentration of Raman active chemical substances related to the microorganisms inhibition that are employed by ENCAPSULAE active packaging. Meat has a foreseen expiry date based on expected shelf-life, and is discarded regardless of its status, but the useful life can be shortened or lengthened depending on the packaging and storage conditions. Raman spectroscopy would enable in-situ test and on-demand re-asses the shelf-life date on the labels of meat as soon as it remains compliant with the safety specifications for consumption. This is a very valuable social technological token EU citizens, who can envision the impact of applying physics with simplified plug-and-play tools for analysis directly in their lives.

In this case, an argument was presented to show the importance of standardised assessment methods versus AI and data-driven intelligence, when checking the state of the agent that is protecting the food by preventing bacteria growth. It is important to prove that these additives capacity is not depleted, rather than hoping that the food will be protected by assuming or making a predictive modelling estimate. For this specific example, standardised methods based on the level of protection are required for food market logistics, because one can assess what is changing with time and if an additive is efficient with any Raman instrument and provide feedback to management procedures. Thus, an end-user or supplier should then be able to prioritise delivery and distribution of the products with shorter lifetimes, saving the fully protected for later distribution. This apparently trivial approach is instrumental to minimise wasted out-of-date perishables. This concept can be applied in many formally equivalent cases.

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