EMMC and EMCC communication on Digital Integration of Horizontal Enablers in Materials Ecosystems

Introduction

The digital transformation of technologies and services provides the basis of the Industry 5.0, which complements the existing Industry 4.0 paradigm by highlighting research and innovation as drivers for a transition to a sustainable, human-centric and resilient industry.

The materials and manufacturing industry is becoming more and more reliant upon a digital ecosystem in which stakeholders are connected, comprising aspects such as data and knowledge, technologies, human resources, applications, and operations. Digital market-places are being built that connect manufacturers, suppliers, distributors, and their consumers so that they can share resources to create what are essentially virtual organisations. Today, digital industry ecosystems are evolving rapidly, driven by powerful economic forces, and they will have a lasting impact on how manufacturers interact with materials suppliers and their customers.

Materials discovery and life cycle management requires the involvement of skills and capabilities from many disparate communities ranging from chemistry, materials science, physics, engineering, information technologies and data science. Key advanced technologies and tools from these fields include materials synthesis, robotics, characterisation and modelling, ML/AI and ontologies. A Common Digital Ecosystem needs to warrant interoperability between all such “horizontal enabler” technologies and to capitalise on commonalities between them. Their integration will be a cornerstone in the digital transformation of the manufacturing industry.

Improving resilience and sustainability as well as ensuring safety of materials in all products throughout the life cycle requires a wide and complex range of trusted information on materials and process behaviour, along the entire lifecycle of the product and its associated material, reaching far beyond the quality and quantity of data sets currently available to industry.

Recent advances in “horizontal enabler” technologies including materials simulation, characterisation and materials informatics demonstrates that digital integration would enable closed-loop research that can design, perform and interpret simulations and experiments in an ecosystem of companies collaborating cross-borders.

In this short communication, we address the challenge to go beyond the ordinary multidisciplinary research approach. We envisage a **common, digitally integrated materials ecosystem** incorporating ontologies for different materials technologies and domains providing full interoperability. Such a system will enable companies to collaborate on more intelligent materials analysis, use and re-use of data, supported by advanced data science tools (including machine learning and artificial intelligence).

Such an industrial ecosystem will support materials and product manufacturing companies, in meeting their strategic objectives regarding resilience and sustainability, leading to more targeted design and development of safe and sustainable materials and processes, faster upscaling and effective quality control.

The European Materials Modelling and Characterisation Councils (EMMC[1] and EMCC[2]) are associations with a broad network of industrial stakeholders, focussing on horizontal enablers and who together address the cross-domain issues that arise during the ongoing digital industrial revolution and with this document we put forward our views for the future.

State of the Art of Materials Development Integration

Due to the advances in modelling, high-throughput experimentation and characterisation, it has become possible to rapidly generate data and propose new materials, formulations, and products. So far, the progress in materials-oriented research has showcased modelling activities being validated by characterisation and modelling has provided continuously improved understanding of mechanisms measured. Novel integrated protocols include multi-scale characterisation (from atomic scale to macroscopic) combined with respective multi-scale modelling to understand scaling relationships in the behaviour of advanced materials and these protocols have often brought unforeseen causal effects to light that were hidden in scarce data.

The **rich and rapidly growing amount of data** on materials and their property, synthesis, characterisation and behaviour during manufacturing remain largely un-curated, unintegrated, and unexplored due to the compartmentalisation and lack of consistent documentation of this information, e.g., such data remain in the primary research lab in various forms and shapes. The full potential of the effective exploitation of both textual data and published chemical data often still needs to be harvested.

Typical of material science is that it employs different perspectives simultaneously (a material can be seen to consist of electrons, atoms, particles or continuum). Initial steps in terminology, classification and data documentation for multi-perspective materials and characterisation workflows have been done, establishing the now widely accepted data structures MODA[3] and CHADA[4], respectively. Due to the lack of ontologies based on physics the EMMC continued the data documentation work, supporting a physics, semiotics and mereotopology based top level ontology for applied sciences called EMMO[5] (Elementary Multiperspective Material Ontology). Ontologies for horizontal enablers like simulation and characterisation have been incorporated as domain ontologies. The EMMC and EMCC are furthermore driving the EU

[1] https://emmc.eu/
[2] http://characterisation.eu/
[3] https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/RI/cwa17284_2018.pdf
[4] https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/ICT/cwa17815.pdf
[5] https://github.com/emmo-repo/EMMO

funded collaborative projects "Industry Commons" (ONTOCOMMONS[6] and DOME 4.0[7]) to develop a widely agreed digital representation environment called the OntoCommons EcoSystem (OCES) linking existing ontologies for both the materials and manufacturing domains and to build a data sharing market-place connecting existing market-places.

Drivers to digitally transform the Materials Ecosystem

Although initial steps are taken towards digital integration, the current level of integration does not yet translate into increased speed at which required materials are developed, implemented, and tested, and a considerable gap towards upscaling remains. Also, it is way behind the integration level of manufacturing data, which has been the main focus of the industry 4.0 transformation for obvious reasons. **A key issue is that the understanding and interpretation of data is currently not sufficiently effective**. This hinders the fast development of new and more sustainable materials and manufacturing processes that take into account product and their materials.

A lot of integrational work still needs to be done to move beyond this initial phase of development and to incorporate full life-cycle considerations. The materials and manufacturing community is in need of inverse design technologies, bridging length and time-scales, which require the access to well organised and standardised data. The integrated methodologies should aim to help invert the design paradigm by starting with the target performance and searching for an ideal material that fulfils the specifications. This **requires an efficient cross-sector materials design ecosystem** where tools developed and serving the needs in one discipline or geographical region and across materials domains and applications are easily understood and integrated with another.

Most importantly, there is the need to develop human aspects of the ecosystem and address education to raise and upskill experts with materials and engineering domain expertise as well as data science and semantic technologies expertise. Terminologies, standardisation, certification and LCA tools naturally require common agreement between the human experts in the involved fields to reach widespread adoption.

Collaborative actions are needed to further develop a common materials ontologies system and to link it to manufacturing ontologies. It is important to continue the large work on the EMMO and OCES and as a next step, to promote fundamental activities that identify conceptualisations in the different applied science domains and convert them into agreed interoperable concepts to link the network of different ecosystems. There is a need for standardised interfaces based on the OCES between all horizontal enablers like simulation, characterisation, synthesis and materials informatics to be used by materials, manufacturing and environmental ecosystems. There is a need for heterogeneous data processing tools and focused methods to curate, integrate, and transform the data into new, experimentally testable hypotheses. This will allow the ecosystems to create sophisticated data infrastructure and interchange platforms that can be linked and exploited, enabling efficient and informed

[6] https://ontocommons.eu/
[7] https://dome40.eu/

material design. There is a need for technologies that combine machine-readable descriptions of the experimental and simulation plans that could help suggest new directions for materials development. There is a need for improved data interchange that will improve interoperability of instruments between vendors and techniques, accelerating the material characterisation and thus their discovery. Finally, increasing the amount and quality of data available will assist and make more reliable machine learning and AI approaches which are instrumental for the material-by-design concept.

The digital integration of the materials horizontal enablers is key to fully achieve the industrial digital transformation and the safe and sustainable by design framework currently being developed under the Green Deal pack of actions.

Activities proposed to create and support a Materials Ecosystem

The EMMC and EMCC suggest that the above needs could be met by activities with the following characteristics.

Digital Transformation of the Materials Ecosystem

- Build and agree common vocabularies, taxonomies, ontologies, and open data standards and formats. Establish across the entire materials science field meaningful descriptors (conceptualisation) to derive insights from abundant data. Develop a common ontology enlarging the Industry Commons OCES to enable digitalisation of the advanced materials discovery cycle through closed-loop integration of data, metadata, and materials from all parts of the discovery cycle including high-throughput experimentation and high-performance computing.

- Coordinate actions towards integration and standardisation of multi-scale computational modelling, materials synthesis and characterisation methods and autonomous robotised synthesis that is steered by predictive knowledge-based approaches combined with AI-based theory to arrive at new or improved sustainable materials with desired properties. This will maximise the potential and value of data, and contribute to a European-wide semantic knowledge base started in the Industry Commons.

- Coordinate the development of education and training of experts with semantic and domain knowledge. Develop the role of benefit advisors who will enable a broader community of non-experts to participate in the materials discovery process.

- Assist companies to participate in this emerging ecosystem via the materials data marketplace, and bring their internal systems fully up to date with forward-looking technology platforms that are open and connected.

- Reach agreement on benchmarking for methodologies, data valorisation, standards, certification and LCA methods.

- Improve data dissemination in an international data ecosystem.

Support for the Materials Ecosystem

- Develop standardised ways of interoperability between horizontal enabling materials science methodologies and experimental data collection and data analytics to support the digital transformation.

- Develop digital data-based interfacing and integration of Materials, Manufacturing and Environmental Sustainability domains to address the Digital and Green transformations.

- Development of green "machine driven" materials development processes where materials modelling, characterisation, knowledge systems and artificial intelligence are utilised to perform high-throughput screening, interpolate and extrapolate correlations to ensure complete coverage of conditions and materials properties. Develop new knowledge-based and machine learning algorithms that generate candidate materials and develop decision modules, the corner stones of an environment where targeted design and development of materials and processes is accelerated.

- Develop innovative digital twin strategies, to support efficiently the mining of materials information during service life, that combine novel characterisation and modelling to support the establishment of efficient management strategies.

Expected Benefits of a Materials Ecosystem

- An integration uniting digital and materials horizontal capabilities building a common knowledge base in the materials ecosystem.

- Digital knowledge and automation tools incorporating materials modelling, characterisation and data documentation, ontology and robotisation of synthesis, leading to accelerated understanding and design of novel, high-performance and sustainable materials.

- Centrally linked data infrastructures would increase reproducibility and traceability of new results. Finding relevant information about techniques, applications, and tools would become less time-intensive. Trusted data would be provided based on benchmarking.

- Agreement on horizontal enablers like standards, certification and LCA methods.

- Materials discovery would exploit the “feedback” from and guide new characterisation experiments or simulations routes to arrive at new synthesis routes and materials, enabling greater productivity, less repetition of failed experiments or calculations, rapid identification of new areas of "design space", and better-informed research decisions and necessary adjustments made possible by tightly tied together operation that will optimise design and development.

- Sustainability achieved through automated and decentralised decision-making towards materials-by-design with an extended materials and product service lifecycle in the manufacturing sector.

- Democratisation of materials discovery via education, training and support via benefits advisors, enabling a broader community of non-experts to participate in the innovation and discovery process.