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Fostering research and innovation in materials manufacturing for Industry 5.0: The key role of domain intertwining between materials characterization, modelling and data science

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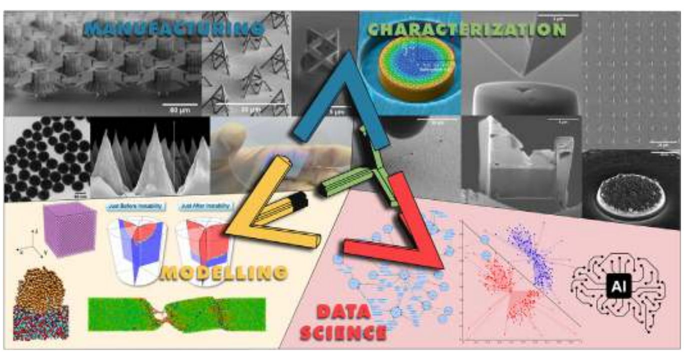
GRAPHICAL ABSTRACT



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ABSTRACT

Recent advances in materials modelling, characterization and materials informatics suggest that deep integration of such methods can be a crucial aspect of the Industry 5.0 revolution, where the fourth industrial revolution paradigms are combined with the concepts of transition to a sustainable, human-centric and resilient industry. We pose a specific deep integration challenge beyond the ordinary multi-disciplinary modelling/characterization research approach in this short communication with research and innovation as drivers for scientific excellence. Full integration can be achieved by developing common ontologies across different domains, enabling meaningful computational and experimental data integration and interoperability. On this basis, fine-tuning of adaptive materials modelling/characterization protocols can be achieved and facilitate computational and experimental efforts. Such interoperable and meaningful data combined with advanced data science tools (including machine learning and artificial intelligence) become a powerful asset for materials scientists to extract complex information from the large amount of data generated by last generation characterization techniques. To achieve this ambitious goal, significant collaborative actions are needed to develop common, usable, and sharable digital tools that allow for effective and efficient twinning of data and workflows across the different materials modelling and characterization domains.

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1. Introduction

The manufacturing industries in advanced economies increasingly rely on experimental data and models that can provide information on the entire value chain and life cycle, from material conception to end-of-life. More recently, there has been an emerging need to develop innovative routes for improving the circular economy of materials, strengthening the production of safe and sustainable materials, and driving the green and digital transitions needed for societies and economies worldwide, which lies at the basis of **Industry 5.0** [1].

In recent years, enormous progress has been made in materials characterization, modelling and informatics toward **Materials 4.0 and virtual metrology** [2]. Novel **integrated protocols** include multi-technique and multi-scale characterization combined with respective modelling methods to understand scaling relationships in the behaviour of advanced materials. For instance, (nano)materials modelling and artificial intelligence are utilized to perform high-throughput screening and interpolate correlations to ensure complete coverage of conditions and (nano)materials properties for improved reverse engineering [3,4]. However, such developments do not translate into the increased speed at which required manufacturing/processing is developed, implemented, and tested, thus, a considerable gap in upscaling remains.

In-situ, operando and real-time nano-scale characterization are additional areas of rapid growth, where the use of advanced data science tools can be of paramount importance to gain comprehensive knowledge and immediate assessment of the structure–property correlations of nano-enabled materials and devices, which are often unforeseen or hidden due to the *Big Data* analysis challenges [5–7].

> *"A key problem is that the understanding and interpretation of data is currently not effective, hindering fast development of new and more sustainable materials and manufacturing processes that takes all life cycle dimensions into account."*

To face this issue, the European Materials Characterisation and Modelling councils (EMCC and EMMC) [8,9] have established an open network with stakeholders to identify the Industry's emerging needs in a continuous process, which currently are not covered by European initiatives. This includes the need for dedicated and **balanced modelling/characterization** working groups to openly support the manufacturing needs for materials in more sophisticated applications (i.e. micro-electronics, green and competitive steel and other materials industries) and in everyday structural applications (need for structural systems/engineering tools), and service life considerations which can be tackled by design during the manufacturing stage.

In **Additive Manufacturing**, finite element predictive models and machine learning methods have been emerging to characterize internal defects thickness and length and by thermal distribution profiles monitoring. This non-destructive evaluation method has been complemented with statistical confidence by predictive modelling to realize innovative inspection models [10]. Applications can benefit from the establishment of process-structure linkages, especially regarding the locally resolved thermal histories which affect the performance.

Battery factories are facing 30–60 % variation for new manufacturing systems. This challenge can be addressed by utilizing transparent data in real-time to describe and support decision-making based on the integrated dynamics of manufacturing [11].

From these examples, the main challenge for materials development is related to the **integration, not just the combination, of materials informatics, high-throughput characterization, and multi-scale models**, leading to the development of "knowledge-integration-based" materials development processes.

To face this challenge, the need for the development of **digital representation environments** is introduced. Materials science experts and data scientists need to collaborate to build common **vocabularies**, **taxonomies, ontologies,** publicly accessible data-translation tools, and modern and open API-based infrastructures to accommodate all types of materials, processes and methodologies of investigation. The definition of the interactive levels is of particular interest to keep characterization and modelling utilising the evolution of the web to the semantics *Web 3.0* [12,13].

The realisation of **digitalisation of materials** development is key to achieving the green transition. It builds on a fully integrated and **digitally interoperable** approach for defining the optimal (i.e., cost, time and resource-effective) process for developing novel (nano-)enabled products.

It is essential to promote fundamental activities to identify interrelations between different data sets obtained from multiple characterization methods and modelling tools. Common data structures for documenting characterization and modelling have been developed and widely agreed upon in CEN Workshop Agreements ***CHADA*** [14] and ***MODA*** [15]. These form the basis for common ontologies across different domains. A key advance has been the development of standard representational framework, the ***EMMO*** [16], which can represent the multi-scale and multi-perspective nature of materials knowledge. Such a **common information framework** across different domains, with full interoperability between computational and experimental data, is necessary to manage and reuse the current knowledge. Also, wider adoption of both *CHADA* and *MODA* could be a leading tool to facilitate scientific excellence and the validation of the quality of adopted characterisation and modelling methods in publications.

In summary, the critical sectors in which fundamental and intertwined collaborative research actions are needed are:

1. Industry driven benchmarks for materials modelling, supported by new characterization standards ensuring that industry can benefit from advances with a high degree of repeatability and confidence.
2. Advanced characterization and materials informatics: development of "machine-driven" characterization and data analysis tools.
3. Model-based definitions: a dynamic response character is required for component design changes, which should be established on digital specifications that link microstructure and evolution mechanisms, geometric features, and location-specific properties with manufacturing process paths.

The EMMC and EMCC are working in this direction by promoting a series of actions to develop industrial-oriented digital representation environments and related knowledge generation methodologies. In particular, the digital environments should be combined with an **adaptive use of modelling and characterization** as a source of data and knowledge, building a benchmarked suite of capabilities. The result will be **FAIR data based on methodologies** able to deal with critical manufacturing and application fields, such as facilitate more efficient design space exploration, reducing physical testing and improving quality and speed.

In conclusion, to support both industry and application needs, modelling and characterization services must be digitalized, interoperable and connected seamlessly into manufacturing and enterprise data and establish decision-making systems via common conceptualization and ontologies. This will inspire the reverse and dynamic design using a currently underestimated knowledge sector of the use phase of materials and components. Such an *outcome-led* approach will address innovation challenges by-design, facilitate automation, aid sustainability and target an extended 'service life – lifecycle' in the manufacturing sector of advanced materials.

Data availability

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

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.

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