MATERIALS 4.0

TOWARDS MATERIALS 4.0:
WHAT IS HOLDING BACK THE NEXT MATERIALS AGE?

EXECUTIVE SUMMARY FOR:

- Standards for digital storage of materials related data
- Trust in data exchange for Materials 4.0
- The use of automation and robotics to improve innovation efficiency
- The storage of data and key requirements of data repositories and indexing systems

This report is commissioned by the Henry Royce Institute for advanced materials as part of its role around convening and supporting the UK advanced materials community to help promote and develop new research activity.

The overriding objective is to bring together the advanced materials community to discuss, analyse and assimilate opportunities for emerging materials research for economic and societal benefit. Such research is ultimately linked to both national and global drivers, namely Transition to Zero Carbon, Sustainable Manufacture, Digital & Communications, Circular Economy as well as Health & Wellbeing.

HENRY ROYCE INSTITUTE

Impact Data Metrics

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MATERIALS INNOVATION FACTORY

CATAPULT Digital

Ferroday Ltd

UKRI Engineering and Physical Sciences Research Council

Executive Summary

The Henry Royce Institute, together with the broader materials community, has supported the development of an idea for the Engineering and Physical Sciences Research Council (EPSRC) "Big Ideas Programme" which aims to collect exciting ideas from the research community.

The Materials 4.0 "Big Idea" was accepted by the EPSRC in 2020 and subsequently placed into its "Ideas Bank" which forms a pipeline of potentially transformative ideas which will be used in the development of a research strategy. The main outcome of the Materials 4.0 Big Idea process, was the identification of several barriers to the development of Materials 4.0: digital security and trust, digital standards, lab automation, and image storage and sharing.

This Big Idea makes a series of recommendations in order to enable Materials 4.0. This new suite of landscape reports details specific actions that would contribute to the delivery of the "digital-first" approach to materials science.

The core recommendation, which should be the primary action from this study, is the establishment of a **National Steering Group for Digital Materials & Manufacturing** which would examine the current state of digital materials science and explore the materials community's needs in areas such as education and training as well as in its engagement with the broader materials community, with other key strategic national programmes, and with government. It would also support the establishment of special interest groups that support the Materials 4.0 agenda and would assess the future needs of the community to achieve the transition to digital materials.

Introduction - What is Materials 4.0?

Developing new materials remains a slow, risky, and expensive process requiring validation at the lab-scale prior to any form of process scale-up or application related test programme. It means that a 20-year development cycle is not uncommon for safety-critical applications.

Given the considerable lifetime of many high-value technologies, infrastructures, and engineered products – from aircraft and vehicles through to buildings and industrial processes – we need to bring net-zero technologies into service within the next five years, if we are to meet our 2050 net-zero commitment. Some of these new technologies require materials that we do not yet have at our disposal, so a step-change in development time is needed to maintain and further grow market share for these critical sectors of the UK economy.

Materials 4.0 is a digital materials revolution which will accelerate the discovery, innovation, and validation of new materials. It will maximise the value of materials data and link the digital and physical via cyber-physical systems for prediction, classification, and control of material performance. It will provide capability and know-how to enable the UK to respond quickly in the cross-sector adoption of a materials informatics framework, combining capabilities from risk management, materials modelling, AI/machine learning, manufacturing informatics, and life-cycle simulation.

During the summer and autumn of 2020, workshops were conducted to support the development of the Big Idea proposal for the EPSRC[1] involving representatives from academia, industry, and the High Value Manufacturing Catapult (HVMC) centres. The proposal made the following four core recommendations:

- The need for the development of integrated tools, protocols, and methods to accelerate materials discovery, testing, and characterisation to dramatically reduce the time of materials development.
- Creation of infrastructure to meet the challenge, accelerating the pace of innovation.
- Developing demonstrators and accelerators enabling the acceleration of materials innovation across Technology Readiness Levels (TRLs).
- The need to engage, train, and develop researchers and research leaders at the interface of science, engineering, and big data to provide the skills and training needed to drive this interdisciplinary transformation.

Overcoming challenges and barriers to digitalisation – what is holding us back?

As part of the development process it became clear that some of the barriers to progress identified had also been highlighted, but not overcome, in previous materials-focussed initiatives around the world, namely:

- A workshop on Artificial Intelligence Applied to Materials Discovery and Design - Office of Energy Efficiency & Renewable Energy[2]
- A workshop on Artificial Intelligence Applied to Materials Discovery and Design, Advanced Manufacturing Office, Office of U.S. Department of Energy[3]
- A Materials Innovation Platform co-led by the Mexican Ministry of Energy (SENER) and the U.S. Department of Energy[4]

These activities, all related to materials, identify main barriers for the materials and manufacturing sector. These key barriers are not unique to materials and manufacturing; they have been identified in every sector where digitalisation has, or is, happening thus far:

- AI Roadmap - UK AI Council[5]
- Transforming R&D - MIT Technology Review[6]
- Review of Data Intensive Bioscience - Biotechnology and Biological Science[7]

All of these studies, including going right back to the original Industry 4.0 manifesto[8], highlight these same barriers.

[1] https://epsrc.ukri.org/research/ourportfolio/epsrcbigideas/
[2] https://tinyurl.com/pyxxdbsv
[3] https://tinyurl.com/2czywns4
[4] https://tinyurl.com/2rpy652f
[5] https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/949539/AI_Council_AI_Roadmap
[6] https://resources.perkinelmer.com/lab-solutions/resources/docs/ATR-TransformingRD.pdf
[7] https://www.ukri.org/wp-content/uploads/2020/11/BBSRC-201120-ReviewOfDataIntensiveBioscience.pdf
[8] https://tinyurl.com/4r2bdr6f

Henry Royce Institute reports

It is clear that these challenges and barriers are not limited to the materials manufacturing community, but overcoming them requires an understanding of what the materials science and materials intensive manufacturing sectors have in place already, and also understanding the range of solutions that are available.

As mentioned above, to explore these barriers more fully, the Henry Royce Institute commissioned four new reports to explore these common digitalisation barriers within the context of enabling discussions and progress towards Materials 4.0.

1. **Materials 4.0 - A Role for Standards:** In collaboration with Ferroday we examined the standards that are currently available for digital storage of materials related data and considered the reasons that these have not been widely adopted to date.
2. **Enabling trust in data exchange for Materials 4.0:** In collaboration with Digital Catapult we considered the issues relating to data-sharing and examined methods for sharing data between competing organisations for mutual benefit.
3. **Lab Automation for Innovation in Materials Chemistry:** In collaboration with the Materials Innovation Factory at the University of Liverpool, we reviewed the use of automation and robotics to improve innovation efficiency.
4. **Materials Microstructure Image and Data Repository Scoping Report:** In collaboration with Impact Data Metrics we examined a use case for the storage of data and identified key requirements of data repositories and indexing systems.

These reports examine in detail a range of opportunities where development of digital-first tools can lead to accelerated materials development. They also identify a range of challenges that require addressing, such as the proprietary nature of materials data and data interoperability.

Next Steps – recommendations for action

On the basis of these reports and the outcomes of the workshops, we propose the **establishment of a National Steering Group for Digital Materials & Manufacturing** to examine the key barriers to the development of Materials 4.0 and the strategy for overcoming them. The forum should look to lead this agenda, stimulating action in:

a. **Identification and delivery of education and training to close skill gaps** - understanding the current separation of material science and information science, and contributing to the establishment of recognisable career pathways for digital materials engineers that combine both disciplines.
b. **Landscaping** - advising UK government on the current state of the transition to a digital-first materials ecosystem, including establishing relationships with regulators to accelerate the integration of emerging technologies and applications, and supporting new or revised legal and contractual requirements for these technologies.
c. **Engagement** - there are a number of actions this forum could take to coordinate engagement in digital materials research within academia,

industry, and the HVMC network. This would also encourage significant integration with national data strategies and with the National Digital Twin Programme at the Centre for Digital Built Britain[9].

The United Kingdom is well placed to capitalise on world leading research in materials and manufacturing and significant investment in digital technologies. We are aiming to encourage a transition towards a digital-first approach to materials R&D in order to accelerate the solving of major societal challenges. We hope this landscaping report will act as a catalyst for the materials community to have a unified voice to achieve this transition.

[9] https://www.cdbb.cam.ac.uk/what-we-do/national-digital-twin-programme

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