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Materials characterisation - Terminology, metadata and classification

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Ref. No.:CWA 17815:2021 E

Contents

Page

European foreword

This CEN Workshop Agreement (CWA 17815:2021) has been developed in accordance with the CEN-CENELEC Guide 29 “CEN/CENELEC Workshop Agreements – A rapid prototyping to standardization” and with the relevant provisions of CEN/CENELEC Internal Regulations - Part 2. It was approved by a Workshop of representatives of interested parties on 2021-10-01, the constitution of which was supported by CEN following the public call for participation made on 2020-11-05. However, this CEN Workshop Agreement does not necessarily include all relevant stakeholders.

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Introduction

Materials characterisation involves the identification and measurement of properties that are either intrinsic or manifest in a material. These properties identify the type, manufacturing/process history, and the state of the material. Characterisation allows us to handle, transport, process, engineer and use the material in the intended application. Characterisation methods can be divided into two broad categories; a) those used to identify the nature (structure, chemistry, microstructure, etc) of the material and b) those evaluating material behaviour and/or performance. [1]

The production of materials presents many challenges, particularly in the industrial environment. Real time monitoring of materials during synthesis and processing is desired for obtaining e.g., high precision, small specialty batches, processing monitoring of nucleation/growth at different scales (lab, pilot, production) and potential for feedback loops (adapt T, pH, etcetera). Such latest developments have widened the application domains for materials characterisation and increased its potential impacts to economy and society.

Specific recent domains for advanced characterisation include:

(a) Off-line characterisation of nanostructures/nanoparticles, where the focus is on detailed analyses of nanostructure/nanoparticle properties that can influence a wide range of material behaviour.

(b) Real-time material characterisation, where the focus is on obtaining real-time information on (nano)materials properties, delivering multiple benefits (e.g., better process knowledge, and control; reduced development time and waste) in materials manufacturing processes by providing real-time information.

(c) In-line material characterisation, where the characterisation is performed in the production line, and the focus can be for example on:

- detailed analyses of (nano) particle properties directly in the flowing media and/or process flows

- analysis of the optical, electronic, structural properties and/or thickness of vacuum deposited or printed nanolayers, for long timescales and/or for large sample areas.

(d) Multi-technique and/or multimodal characterisation, where multiple advanced methods are combined to achieve complex information on material's behaviour and performance.

(e) Operando characterisation, where characterisation of the material is performed during its operation, and its performance is simultaneously evaluated.

As a consequence, communication becomes critical of the characterization tool to the process control of the material fabrication equipment, to enable improved process control and defect detection.

It has been demonstrated in many individual cases that materials characterisation is a key enabler of research & development efficiency and innovation and that the use of this technology can generate a huge economic impact.

Due to the huge variety and complexity of materials and the wide range of applications, the materials characterisation field consists of many communities. These communities have established different terminologies, which typically focus on specific application domains and on types of characterisation methods. As a result, a wide range of domain specific characterisation methods have evolved. However, applications to industrial problems in advanced materials and nanotechnology require a strong interdisciplinary approach among these fields and communities, especially when profound interaction

[1] From 2017 EMCC roadmap, www.characterisation.eu

with material modelling is needed. There is therefore a need to establish a common terminology (definition of concepts and vocabulary) in materials characterisation, to arrive at a common structure of materials characterisation metadata.

A standardised terminology will improve future exchanges among experts in the entire area of materials characterisation, facilitate the exchange with industrial end-users, experimentalists, as well as computational modellers, and reduce the barrier utilising advanced materials characterisation. The common language is expected to foster dialogue and mutual understanding between industrial end-users, equipment manufacturers, scientists, and theoreticians. Standardization of terminology and classification has been identified as critical to collaboration and dissemination of European research projects. In particular, standards will facilitate interoperability between methods and databases. The standardization is relevant for an integrated technological development and brings benefits for industrial end-users due to simplified and much more efficient communication in the field of materials characterisation.

The terminology, metadata and standardised documentation helps data interpreters by translating industrial problems into problems that can be analysed with characterisation methods. It assists workflow development where several methods can interoperate in addressing a specific end-user question.

In the future, this standardized terminology and metadata classification can be formalised into a taxonomy and an ontology of materials characterisation. Such an ontology will form the basis for formal metadata development with which methods and databases can be linked. These developments will further support efficient solutions for materials characterisation and the communication, dissemination, storage, retrieval, and mining of data about materials characterisation and increases the interoperability.

1 Scope

The main purpose of this CWA is to propose a widely agreed and common basic architecture for materials characterization data (CHADA), which can be used as a building block for the most complex characterization case studies, also comprising interactions with modelling[2] and process workflows.

The materials characterization field consists of a merge combination of process from multiple scientific communities, which have established different terminologies that focus on various application domains and types of characterization methods.

In addition to that, characterisation is an integral part of materials and product development, processing, and application. It involves stakeholders from:

- Industrial end-users of characterisation from processing and manufacturing industry.
- Scientists in both academia and industry developing new materials, properties, and applications;
- Technology integrators providing materials testing, multiscale analysis, characterisation, and consultancy services.
- Scientists from Academia, Research Institutes and instrument manufacturers who develop characterisation methods and methodologies.
- Manufacturers and developers of analytical instruments from both academia and industry.
- Standardisation Bodies and Metrology institutes.

For such reasons, the development of a common terminology for materials characterisation is mandatory and should include (a) Standardization of terminology and method classification, and (b) a guideline to translate industrial problems into problems that can be analysed with characterization methods.

On this basis, standardized terminology metadata and classification will be formalized into taxonomies and ontologies of materials characterization.

This CWA includes definitions of fundamental terms for the field of materials characterisation, followed by a detailed description of a new concept for data documentation in materials characterization (CHADA).

The definitions also enable a classification of materials characterisation methods.

Using the concepts of "user case" (which includes the sampling process, specimen, testing environment and characteristic length scale), "experiment" (which include the details of the measurement chain), "raw data" and "data processing", we propose a more straightforward classification of materials characterisation methods, replacing the current situation of opacity that makes the field hard to access for industry and outsiders.

This CWA also provides a systematic description and documentation of methods including the user case, method, raw data generation and analysis and post-processing of data: the "materials CHAracterisation DAta" (CHADA). This document seeks to organize the information so that even complex characterisation workflows can be conveyed more easily and key data about the methods, raw data generation and analysis, and post-processing of data and their implementation can be captured. A template CHADA for the methods is described to guide users towards a complete documentation of material characterisation.

2 Normative references

There are no normative references in this document.

[2] www.emmc.eu, MODA