CEN WORKSHOP AGREEMENT

CWA 17284

April 2018

ICS 01.040.35; 35.240.50

English version

Materials modelling - Terminology, classification and metadata

This CEN Workshop Agreement has been drafted and approved by a Workshop of representatives of interested parties, the constitution of which is indicated in the foreword of this Workshop Agreement.

The formal process followed by the Workshop in the development of this Workshop Agreement has been endorsed by the National Members of CEN but neither the National Members of CEN nor the CEN-CENELEC Management Centre can be held accountable for the technical content of this CEN Workshop Agreement or possible conflicts with standards or legislation.

This CEN Workshop Agreement can in no way be held as being an official standard developed by CEN and its Members.

This CEN Workshop Agreement is publicly available as a reference document from the CEN Members National Standard Bodies.

CEN members are the national standards bodies of Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Former Yugoslav Republic of Macedonia, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and United Kingdom.

EUROPEAN COMMITTEE FOR STANDARDIZATION
COMITÉ EUROPÉEN DE NORMALISATION
EUROPÄISCHES KOMITEE FÜR NORMUNG

CEN-CENELEC Management Centre: Rue de la Science 23, B-1040 Brussels

Ref. No.:CWA 17284:2018 E

Contents

Page

European foreword

This CEN Workshop Agreement (CWA 17284:2018) has been drafted and approved by a Workshop of representatives of interested parties on 2017-12-11, the constitution of which was supported by CEN following the public call for participation on 2016-12-16.

A list of the individuals and organizations which supported the technical consensus represented by the CEN Workshop Agreement is available to purchasers from the CEN-CENELEC Management Centre. These organizations were drawn from the following economic sectors: Advanced Technology, Chemical Engineering, Research & Development, and Materials Modelling.

The formal process followed by the Workshop in the development of the CEN Workshop Agreement has been endorsed by the National Members of CEN but neither the National Members of CEN nor the CEN-CENELEC Management Centre can be held accountable for the technical content of the CEN Workshop Agreement or possible conflict with standards or legislation. This CEN Workshop Agreement can in no way be held as being an official standard developed by CEN and its members.

The final review/endorsement round for this CWA was started on 2017-10-03 and was successfully closed on 2017-12-03. The final text of this CWA was submitted to CEN for publication on 2018-01-04.

Below is a list of companies/institutions that endorsed this CWA:

— **Access e. V. (Dr. Georg J. Schmitz);**

— **Consiglio Nazionale delle Ricerche (Dr. Vincenzo Carravetta);**

— **Eidgenössische Technische Hochschule Zürich (Dr. Mathieu Luisier)**

— **Fraunhofer IWM - Institut für Werkstoffmechanik (Dr. Adham Hashibon)**

— **Goldbeck Consulting (Dr. Gerhard Goldbeck)**

— **Helmholtz-Zentrum für Material- und Küstenforschung GmbH (Dr. Natalia Konchakova)**

— **Imperial College London (Dr. Liliang Wang)**

— **Karlsruher Institut für Technologie (Dr. Wolfgang Wenzel)**

— **Nanolayers - Research Computing (Dr. David Gao)**

— **Norwegian University of Science and Technology (Dr. Heinz A. Preisig)**

— **Politecnico di Torino (Dr. Pietro Asinari)**

— **SINTEF - The Foundation for Scientific and Industrial Research (Dr. Jesper Friis)**

— **Technische Universität Wien (Dr. Jesús Carrete Montaña)**

— **Tyndall National Institute (Dr. Eoin O'Reilly)**

— **Università di Bologna (Dr. Emanuele Ghedini)**

— **Université de Picardie Jules Verne (Dr. Alejandro A. Franco)**

— **Université de Mons (Dr. David Beljonne, Dr. Jérôme Cornil)**

— **University of Warwick (Dr. Dhammika Widanalage)**

This CEN Workshop Agreement is publicly available as a reference document from the National Members of CEN: Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Former Yugoslav Republic of Macedonia, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and United Kingdom. Comments or suggestions from the users of the CEN Workshop Agreement are welcome and should be addressed to the CEN-CENELEC Management Centre.

Introduction

It has been demonstrated in many individual cases that materials modelling 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 modelling field consists of a number of communities. These communities have established different terminologies which typically focus on specific application domains and on particular types of models. As a result, a wide range of domain specific software codes have evolved. However, applications to industrial problems in advanced materials and nanotechnology require a strong interdisciplinary approach among these fields and communities. There is therefore a need to establish a common terminology (definition of concepts and vocabulary) in materials modelling.

A standardized terminology will improve future exchanges among experts in the entire area of materials modelling, facilitate the exchange with industrial end-users and experimentalists and reduce the barrier utilizing materials modelling. The common language is expected to foster dialogue and mutual understanding between industrial end-users, software developers, scientists and theoreticians. Standardization of terminology and classification has been identified as critical to collaboration in and dissemination of European research projects. In particular, standards will facilitate interoperability between models 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 simulation.

The classification helps translators by translating industrial problems into problems that can be simulated with materials models. It assists workflow development where several models can interoperate in addressing a specific end-user question.

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

1 Scope

This CWA includes definitions of fundamental terms for the field of materials modelling and simulation. Computational materials models in this CWA are understood to be physics-based models. This CWA does not include data-based models.

The definitions enable a classification of materials models. Using the entity and physics equation concepts, leads to a relatively small number of distinct materials models replacing the current situation of opacity of materials models and simulations that make the field hard to access for outsiders.

This CWA also provides a systematic description and documentation of simulations including the user case, model, solver and post-processor: the “materials MOdelling DAta” (MODA). This document seeks to organize the information so that even complex simulation workflows can be conveyed more easily and key data about the models, solvers and post-processors and their implementation can be captured. A template MODA for physics-based models is described in order to guide users towards a complete documentation of material and process simulations.

The CWA is based on the Review of Materials Modelling (RoMM) [1]. A MODA for data-based models can be found in the RoMM [1].

2 Normative references

There are no normative references in this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

3.1
Entity
self-contained, internally frozen, structure-less representational unit of a material

Note 1: The modeller chooses to describe the material at a certain level of granularity and does this in terms of the behaviour of a set of entities.

Note 2: There are four types of entity, one for each of the four levels of granularity:

1) electron entity: a representation of an electron [SOURCE: IEV 113-05-18]

2) atom entity: a representation of an atom [SOURCE: IEV 113-05-20]

3) mesoscopic entity: a representation of a set of bounded atoms (e.g. group of atoms, molecule, bead, cluster of atoms, nanoparticle, grain)

4) continuum volume entity: a representation of the material bounded in a region of space within which the material is considered by the modeller to be described by the same set of properties

Note 3: Electron entities, atom entities and mesoscopic entities are chosen for discrete representations of the material. Continuum volume entities represent the material as a continuum.

Note 4: Any material can be described by any of the entity types.

EXAMPLE: The internal structure of a material can be described as an arrangement of electrons or atoms interacting with each other. Alternatively, the modeller may identify discrete grains as mesoscopic entities and model the behaviour (e.g. magnetism) of the material based on internal and external forces on grains. The detail of a granular structure can also be captured by partitioning the grain into different continuum volumes.