Speaking the language of microstructures
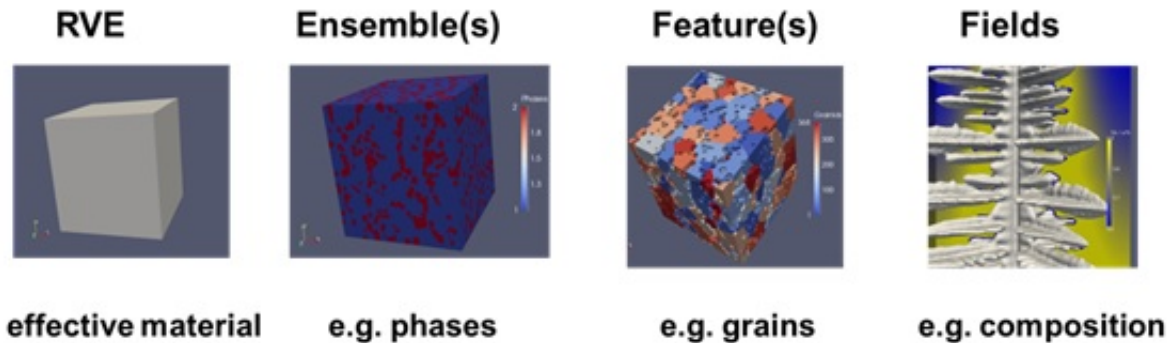
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Figure : Hierarchical structure of materials. Credit: 2016 Georg J. Schmitz, et al.

Researchers are developing a common language that can be used by computer software tools to describe materials at their smallest scale, with the ultimate aim of designing faster and better materials for our everyday lives.

Designing materials for use in the large variety of gadgets and structures that support our everyday lives involves understanding them at their atomic, electronic and macroscopic scales. Integrated computational materials engineering is a field of science that develops computational models so scientists can understand materials at these various scales, allowing them to tailor and optimize custom-designed microstructures with the necessary properties for the functions they are destined for. Several software tools are already available for this purpose. However, the "languages" they use to describe materials vary. This makes it

difficult for materials scientists to interchangeably use data from these tools.

A team of researchers at Access, a research centre associated with the Technical University of Aachen in Germany, has developed a "common language" for modelling and simulation tools used in studying the microstructures of materials. "Such a common language will allow for a seamless communication between different commercial and/or academic tools," says Access senior scientist Georg Schmitz. "Such communication is necessary, as most of the current problems can't be solved by a single tool alone, but need the interactions of different tools that also need to interact with experimental data," he says.

The microstructures of materials undergo changes as they are processed and as materials operate. Their description must thus be able to cover all the various changes that occur in materials over the course of their lifetime.

The team, which provides software tools for microstructure simulations, identified the needs and benefits of seamless communication with a variety of computational tools. They developed a set of "metadata descriptors" to describe the three-dimensional microstructure of any generic material. Their method was published in the journal *Science and Technology of Advanced Materials*.

Metadata are data about data. They provide information that enables the categorization, classification and structuring of data. In materials modelling, metadata play an important role in defining the properties, functions and eventually the performance of any component.

The common language, or set of descriptors, developed by the team can only describe the microstructure of a material at a given instant in time. Future research will need to consider the addition of descriptors that

cover dynamic and kinetic changes that happen in materials over time.

"Similar to the jpeg (joint photographers expert group) format [for exchanging digital pictures], the group looked for a data scheme allowing the future exchange of complex simulation data as easily as digital pictures are exchanged nowadays," explains Schmitz. "This provides a flavour of what can become possible in the area of materials science and engineering: faster developments of new processes and new materials, of processes and materials having a smaller ecological footprint, and of new materials with new functionalities for new or better products," he says.

More information: Georg J. Schmitz et al. Towards a metadata scheme for the description of materials – the description of microstructures, *Science and Technology of Advanced Materials* (2016). DOI: 10.1080/14686996.2016.1194166

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