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MICROSTRUCTURE MODELING IN ICME SETTINGS

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Abstract

The importance of microstructure simulations in ICME settings is discussed with respect to their added value provided to macroscopic process simulations and their contribution to the prediction of materials properties. Their role in integrating the scales from component/process scale down to atomistic scales and also in integrating the experimental and virtual worlds will be highlighted. Practical implications for coupling a heterogeneous variety of codes and tools to microstructure simulations will be discussed using the example of the commercial multi-phase-field software MICRESS®. The paper concludes with some conceptual thoughts about a future standardized format for the description of digital microstructures.

Introduction

"Microstructure" - a term not uniquely defined and understood differently by varying communities. Typical perceptions are e.g. "what you see under the microscope", "the grain size distribution" or "all defects in a material". At the state of current knowledge, a possible and meaningful definition would read: "All internal structural features in a Representative Volume Element (RVE) affecting the properties of the material". In other words: Microstructure is a spatial distribution of elements/atoms and defects in a given volume. Nature helps to reduce this very general description by the "self-assembly" of regular structures (crystals/ phases/ grains/ molecules) allowing treating thousands or even millions of atoms as a single "object" or constituent. Microstructure thus becomes an "arrangement of objects in an RVE". These objects may be 1D, 2D or 3D e.g. phases, grains, precipitates, defects, dislocations, nano-precipitates, atoms and much more. This definition of a microstructure at least comprises following objects and phenomena: phases and phase boundaries (phase transformations), grains and grain boundaries (recrystallization, grain growth), precipitates, point defects, vacancies (diffusion, phase transformations), dislocations (crystal plasticity, recovery), crystal structure of the phases (defect properties), crystal orientation (anisotropy, texture), elemental distribution (chemical composition, segregation) and probably much more.

It is important to note that the microstructure – besides the overall chemical composition of the material - determines the material properties. There are no "processing – property – relationships" but only "processing – microstructure" and "microstructure – property" – relationships [1]. The basis for the description of a microstructure is given by the RVE which defines the volume of material under consideration. The RVE can be a 2D approximation, but in many cases a 3 D representation is necessary. The microstructure can then be described at different levels of detail: the RVE scale, the object scale, and eventually the continuous scale between or within the objects located in the RVE.

RVE scale: If properties/structures do not vary over the RVE, the average, homogeneous property is equal to the local property at each point. Such a description holds for liquids, gases and amorphous structures. As soon as crystallinity comes into play anisotropy becomes important. The homogeneous RVE then corresponds to a single crystal but now revealing full crystalline anisotropy. As soon as multiple phases are present in the microstructure a first approach is to consider the fractions of these phases in the RVE without knowing their spatial distribution. Such phase fractions can nowadays be easily determined/estimated by thermodynamic software tools for given conditions of temperature, pressure and overall chemical composition of the RVE. Knowledge about the phase fractions already allows for a first estimate of effective properties of the RVE by using volume averaging concepts. Next refinements of the microstructure description are distribution functions for the different objects like grain size distributions, precipitate size distributions, orientation distribution functions etc. A number of current microstructure models refer to the calculation of such distribution functions and their evolution during processing.

Object scale: Sizes, aspect ratios, positions, orientations and mutual arrangement of all individual objects in the microstructure, i.e. the topology, are described. In a first approximation these objects each have homogeneous properties (e.g. same concentration of alloy elements anywhere in the object) which may however change from object to object.

Continuum: In a further refinement down to full spatial resolution (e.g. down to a single voxel in a numerical representation) local variations inside the objects are taken into account. The highest level of detail comprises data for each point in space (i.e. each voxel in a numerical representation), which themselves have been simulated/calculated considering the single voxel itself again as an RVE, but at a much smaller scale. Examples for the latter are size distributions of nano-precipitates within a grain.

Microstructures – along with the properties of the phases constituting the microstructure - eventually determine the properties of technical, multiphase and polycrystalline materials and components. A harmonized methodology to describe, characterize, model and analyze microstructures is thus most important. The following sections will shortly highlight some major topics in experimental characterization and numerical modeling of microstructures before eventually discussing a possible approach towards a unified digital description.

Experimental Microstructure Characterization

Significant progress has been made in the last decade both in the area of 3D characterization and observation of microstructures and their evolution in time (“4D”). 3D microstructures provide the full information depth with respect to the anisotropy of the effective properties of the materials and also with respect to their processing and evolution under operational conditions.

3D experimental microstructure characterization may proceed either post mortem or in-situ. It may be static or follow the dynamics of evolution. *Post mortem* methods comprise e.g. light microscopy (e.g. grain size/grain topology), EDX (segregation), EBSD (crystallography /texture) and indentation experiments (plasticity, dislocation densities). 3D extensions of these 2D methods can be realized by serial-sectioning metallography, computer tomography or combined focused ion beam with EBSD/EDX methods for example.

In the case of metals and alloys *in-situ measurements* in general require high luminosity x-ray or synchrotron sources. In solidification research thus transparent organic analogue systems are used to study the dynamics of evolving microstructures.

An experimentally challenging task is the integration of information being obtained by different techniques e.g. in aligning the characterized area when changing from one method to the next. Future developments are expected with respect to integrating experimental observations with virtual data allowing for knowledge based evaluation and assessment. An example is the assessment of phases observed in a LOM measurement with the help of thermodynamic calculations [2].

A big step towards a 3D digital representation of experimental microstructures (EBSD type data) has recently been published and is based on Dream3D [3]. Dream3D is an open source code, and the data format being used in Dream3D is based on HDF5 [4]. This approach and the HDF5 format seem to be easily extendable beyond EBSD type data and also to simulated microstructures.

Microstructure Models

A large number of models and simulation tools for microstructure evolution exist for the different levels of detail. Prominent models for 2D/3D/4D description/prediction of microstructure topology and its evolution are especially Cellular Automata type models, phase-field and multi-phase-field models, phase-field crystal models and crystal plasticity models.

Modeling of 3D microstructures evolving in time using such tools is performed at all scales and for different processes like solidification, grain growth, recrystallization (dynamic/static), solid-state-transformations, precipitation, plastic deformation and others. The models may further include fluid flow, electrostatic/electromagnetic fields and other phenomena.

Modeling of Microstructures in ICME Settings

Microstructures and respective models for their evolution are at the borderline between continuum scale process models and electronic/atomistic/mesoscopic models and thus provide a natural bridge between these different length scales. The role and needs of microstructure modeling in an ICME environment will thus be discussed in more detail for the example of a multi-component, multi-phase field model [5]. In combination with thermodynamic and kinetic databases [6] this model allows for simulation of microstructure evolution during solidification and solid state transformations in technical alloy systems [7].

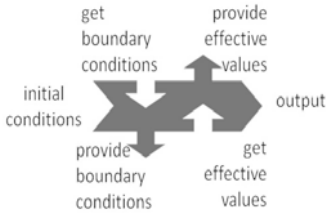

Fig. 1:
Basic topology of a software tool in an ICME setting. This topology allows assembling respective “puzzle parts” along the time/history (from initial conditions to output/final conditions) and across the scales via exchange of boundary conditions and effective values [8]

The first step in simulating the evolution of a microstructure is the specification of an initial microstructure, which may be achieved in various ways, fig. 2. A sound way to define this initial condition is to start simulations from a homogeneous, isotropic and stress free melt. The result of such simulations may then be taken to form the initial microstructure. Often details about all preceding process steps, however, are not available, and the initial microstructure may need to be defined on the basis of *experimental data* which may be available as *digital* or analogue *experimental data.* Sometimes neither images (analogue data) nor digitized experimental data (e.g. CT scans, EDX mappings,…) may be accessible, but only statistical information e.g. the grain size distribution. In such cases, *synthetic microstructures* become interesting and important. Once a common format to describe digital microstructures is established, retrieval of digitized microstructures from *microstructure databases* [9] may become increasingly important.

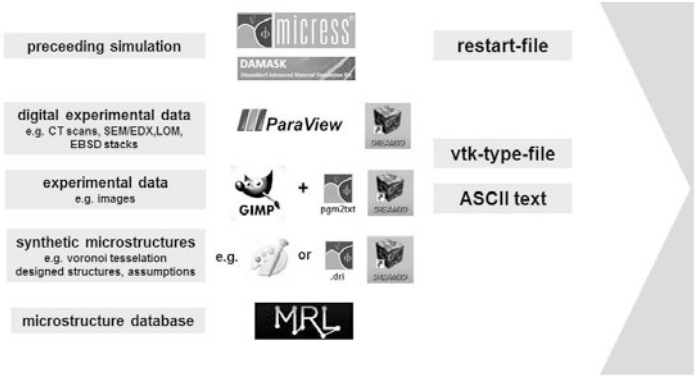

Fig 2: The "initial conditions" entering a microstructure simulation as initial microstructure may originate from a variety of sources (see text)

Synthetic microstructures may either be artificial, idealized structures (to test the different models for well-defined conditions) or artificial but realistic microstructures matching experiments to a large extent. They may be generated by Voronoi tessellation, by 3D extrapolations from 2D microstructure data, by combinations of microstructures (experimental/experimental, experimental/virtual, virtual/virtual) and/or by many other options.

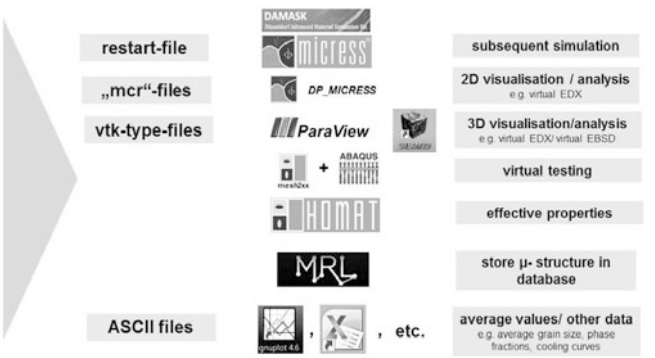

Fig.3:
The "output" of a microstructure simulation may become subject to a large variety of further operations (see text)

The "*output*" of a microstructure simulation may serve as input for a *subsequent simulation* or even establish an entire simulation chain. Examples are the simulation of laser welding [10] or simulation of plastic deformation and recrystallization by a combination of multi-phase-field and crystal plasticity models [11].

Besides a mere *visualization* in 2D and 3D by open source post processors e.g. paraview [12], a quantitative analysis similar to experimental methods becomes possible by "*virtual EDX*" and "*virtual EBSD*" type tools. In view of the digital nature of the simulation results, all information can be quantitatively evaluated in a straight forward manner.

Most interesting is the determination of the *effective properties* of the RVE from 3D microstructures. This evaluation may proceed via *virtual testing* using FEM codes like Abaqus [13] or by methods of *mathematical homogenization* [14].

Most current data from CT, EBSD or multiphase field methods are based on voxelized structured grids as numerical representations. Their conversion into grids/meshes being suitable for further FEM analysis is a frequently faced task and challenge. The development of fast, reliable and easy to operate algorithms for digitizing meshing/remeshing experimental and/or simulated microstructures will become increasingly important.

Linking and Coupling across the length scales – corresponding to the upward and downward arrows in fig 1 – are not addressed in detail here. Some of the challenges when applying microstructure information to the larger scale relate to self-consistency between the solutions for the different scales [15], to interpolation schemes which allow mapping the effective properties of a number of RVEs to an entire component, and others. Coupling microstructure simulations to the smaller, electronic/atomistic/mesoscopic scales essentially relates to data entering microstructure simulations, e.g. interfacial properties, kinetic data, properties of the pure phases and others.

Towards a Future Digital Description of Microstructures

There is a large and heterogeneous variety of different methods and numerical tools for the description and characterization of microstructures and their evolution. Only few of them have been depicted above. A future common standard for the digital description of 3D (4D) microstructures will largely facilitate future information and knowledge exchange, interoperability between virtual and real worlds as well as assist in integration of data obtained by different methods and models in each of these fields, for example:

- storage and retrieval of experimental microstructures in digital form (2D,3D,4D)
- integration of different metallographic results (LOM,SEM/EDX, EBSD,..) into a single file
- reconstruction of 3D microstructures e.g. from serial sectioning
- import of experimental data into microstructure simulations
- knowledge based, simulation supported evaluation of experimental results
- analysis of simulation data with same tools as used for experimental data
- daisy chaining of a heterogeneous variety of models with different functionalities
- …and many more…

The major question is on how to reach a commonly accepted de-facto standard. Before further specifying a digital description for a microstructure, it seems wise to reflect on some general considerations for such a standard:

- free and powerful software tools should be available to inspect the digital microstructures
- the numerical representation should be easy and intuitive in view of educational aspects
- in spite of being easy and intuitive it must be sufficiently flexible and versatile for more complex tasks
- should make use of existing de-facto standards
- 2D representation should be a limiting case of a generic 3D representation
- should reflect the multi-scale nature of microstructure data
- …more…

A common standard for the visualization of 3D data is based on the VTK format library [16] which is the basis for the free and powerful visualization tool paraview [12]. VTK allows for the representation of scalars, vectors and other entities and provides different numerical representations e.g. structured or un-structured meshes and a large number of import/export filters. Especially voxel type structured vtk grids provide an easy an intuitive approach to the numerical representation of the data and also match the voxel type structure of several data sources for digital microstructure data (CT, phase field simulations, etc..). VTK does not consider any domain specific notations for the nomenclature of individual entities.

VTK voxel data form part of a more comprehensive, "Hierarchical Data Format" (HDF5). This data format has already been applied to numerous fields, but does not provide any specific standardized nomenclature for the different data. However, HDF5 has been "customized" for the microstructure community e.g. in the frame of the free and open source Dream3D software data structure [3], which will be discussed in the following. The resulting format is called ".dream3d" and provides a nomenclature for a number of microstructure features. It is fully compatible with HDF5. The hierarchical data structure of HDF5 matches perfectly with the needs of a hierarchical description of microstructures as depicted in the introduction. The HDF5 format as used in Dream3D thus may serve as a guideline for the formulation of a standardized microstructure description. The essential feature of HDF5 is its hierarchical structure based on cell data, field data and ensemble data, fig 4. :

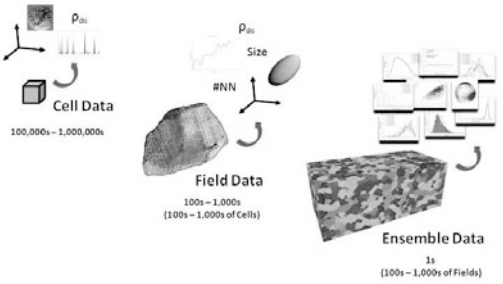

Fig. 4:
Basic structure of HDF5 comprising "cell data", "field data" and "ensemble data". For explanations see text. The figure has been taken from the Dream3D manual [3]

Cell data represent the smallest bit of information and are especially used to describe properties "continuously" varying in space (called fields in mathematics): In the future e.g. concentration fields, orientation fields, temperature fields, dislocation fields and others could be described by

cell data. Also GrainIDs varying from object to object, but not within the object itself, are specified as cell data and are required to specify different objects/grains in the RVE.

Field Data – not to be confused with the mathematical fields above **–** describe properties which are identical for a given grain which is defined as a "field of voxels" belonging to the same object/grain and being specified by the same GrainID. Examples of present and future field data are the phase of a grain, the average concentration(s) of alloy elements in a grain, the orientation of a grain, the average dislocation density in a grain and many others. In many cases „Field Data" may be considered as averages, which can be computed from Cell Data. This corresponds to a homogenization step at the scale of the objects/grains in the microstructure. In many cases, Field Data also provide an approach to synthetic microstructures by specifying an average concentration per grain instead of specifying a concentration value for each cell.

Ensemble data describe properties which are common to a number of objects like a number of grains all belonging to the same phase. Ensemble data may in the future characterize the thermodynamic data of the individual phases, the crystallography and the physical properties of the individual phases, the size distributions for the individual objects of a phase, the properties of interfaces and much more.

A special type of **ensemble data –** not currently explicitly specified in Dream3D - would be **RVE data.** RVE data correspond to the **ensemble data of all objects** in the RVE and describe properties of the entire RVE. Examples are the RVE geometry, the specification of the material in the RVE (chemical elements, phases, composition,..), the effective physical properties of the RVE, statistics of the RVE e.g. phase fractions, the boundary conditions on the RVE, and many others.

HDF5 further provides a data structure for other digital representations. These numerical aspects of HDF5 in the near future will allow exporting HDF5 data into meshes suitable for further FEM analysis using e.g. Abaqus [13]. The benefits of HDF5 with respect to ICME operations seem obvious and manifold. Linking to the larger scale can be easily realized via exchanging only the RVE-Ensemble data. Data from smaller scales can enter the per-phase ensemble data. Evolution of microstructures can be tracked by Field data and Cell data, homogenization or determination would correspond to the generation of RVE ensemble data from cell data and field data. The integration between the real world of material characterization/observation and the virtual world of microstructure simulations seems straightforward. The further exploitation of microstructures being stored in HDF5 by subsequent FEM analysis seems possible in the near future.

The current functionalities of Dream3D are essentially related to reconstruction and statistical evaluation of LOM and EBSD type data, where LOM (light optical microcopy) relates to geometries of grains and neighborhood relations and EBSD type data relate to crystallography and texture type data. Another important functionality of the present Dream3D is the generation of synthetic microstructures from statistical information. An important future extension of Dream3D would be the inclusion of EDX type data like concentration mappings of the alloy elements into the cell data, the inclusion of indentation experiment data e.g. local dislocation densities into the cell data, or information about the individual slip-systems into the per-phase ensemble data and many more.

Summary

This article has described the role of experimental and virtual microstructures in ICME settings. It has highlighted the strong need for and benefits of interoperability between the large and heterogeneous variety of modeling tools. One path towards interoperability is the specification of a common data format. HDF5 and VTK (as a part of HDF5) have a strong potential to evolve into such a standard. Synthetic microstructures being generated with Dream3D could already – without major effort - be further processed with MICRESS®. The reverse path has still to be exploited, but no major obstacles are anticipated. One of the key actions towards standardization will be the specification of a list of metadata keywords defining the nomenclature for all entities relevant for the description of a microstructure. A respective activity is currently ongoing in the ICMEg [17] project and is harmonized with 5 other European projects on modeling platforms.

Acknowledgement

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