Towards a Metadata Keyword Scheme for the Description of Materials

– Keywords for the Description of Microstructures –

ICME 2016

**G.J.Schmitz*, B.Böttger, M.Apel, J.Eiken, G.Laschet, R.Altenfeld,
R.Berger, G.Boussinot, A.Viardin**

[*] MICRESS® group at Access e.V., Intzestr. 5, D-52072 Aachen, Germany
*g.j.schmitz@micress.de

ABSTRACT

The property of any material is essentially determined by its microstructure. Numerical microstructure models thus get increasingly into the focus of modern engineering as helpful tools for tailoring and optimization of custom-designed microstructures by suitable processing and alloy design. Nowadays, a huge variety of software tools is available to predict various microstructural aspects for different materials. In the general frame of an Integrated Computational Materials Engineering (ICME) approach, these microstructure models provide the link between models operating at the atomistic or electronic scales, on the one hand, and models operating on the macroscopic scale of the component and its processing, on the other hand. In view of an improved interoperability of all these different tools it is highly desirable to establish a standardized nomenclature for the exchange of microstructure data. The scope of this presentation is to present and to discuss a comprehensive system of metadata keywords for the description of a 3D microstructure. The presented keywords are limited to a mere geometric description of a static microstructure and have to be complemented by further keywords e.g. for properties, for numerical representations, for kinetic data and others in the future. Further attributes to each keyword e.g. on data origin, on data uncertainty, on data validity range and others currently are defined in on-going work. The proposed keywords are meant to be independent of any specific numerical representation. The keywords defined in this presentation may serve as a first basis for standardization and will simplify the data exchange between different numerical models, as well as promote the integration of experimental data into numerical models of microstructures. A description of an HDF5 template data file for a simple, three phase Al-Cu microstructure being based on the defined keywords finalises this presentation.

REFERENCES

[1] G.J.Schmitz, B.Böttger, M.Apel, J.Eiken, G.Laschet, R.Altenfeld, R.Berger, G.Boussinot, A.Viardin: *Towards a Metadata Keyword Scheme for the Description of Materials – Keywords for the Description of Microstructures* – under preparation

[2] G.J.Schmitz: "Microstructure Modeling in Integrated Computational Materials Engineering (ICME) Settings: Can HDF5 Provide the Basis for an Emerging Standard for Describing Microstructures?" JOM, Vol. 68, No. 1, (2016) 77, DOI: 10.1007/s11837-015-1748-2