Role and Descriptions of Chemical Element Distributions in Microstructure Simulation

B. Böttger[*] and J. Eiken[*]

[*] access
Intzestr. 5
52072 Aachen, Germany

ABSTRACT

The simultaneous presence of more than one chemical element in a material has strong impacts on microstructure formation, and thus on the properties. The reason is that alloys, in contrast to pure substances, are subject to the phenomenon of segregation, which reduces the driving force for phase transformation and, in almost all circumstances, drastically restricts the movement of phase interfaces. In many cases, phase transformations then are limited to the element diffusion rate, resulting in microstructures which are finer by several orders of magnitude compared to the case of pure substances.

In the presentation, different aspects of alloying and chemical element distributions related to microstructure descriptions and simulation within an ICME setting are discussed with focus on the multiphase-field software MICRESS®. In the first step, microstructure modelling of alloys often needs related input from external sources: Concentration distributions may be read in from experiments, prior simulation runs or other software tools. Particularly in the case of multicomponent systems, thermodynamic data typically is provided by Computational Thermodynamics tools using Calphad databases. During simulation, the microstructure tool must be able to treat different types of diffusion of chemical elements (chemical diffusion, cross diffusion, interface diffusion, infinite diffusion, far-field diffusion, etc.) as well as redistribution of the elements between phases (including solute trapping, para-equilibrium, LENP). Finally, concentration distributions or derived quantities like average compositions or a segregation index can be stored using standardized formats (e.g. HDF5 or VTK) and be handed over to other tools for simulation of subsequent process steps.

During the talk, microstructure simulation examples for technical multicomponent and multiphase transformation processes like casting, welding, brazing or heat treatments are shown including also complex process chains. The challenges are discussed and the importance of a correct and complete handling of compositions and element distributions in ICME is illustrated.