Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A8] Symposium A-8

Chair: Thomas Hochrainer(TU Graz, Austria)
2018年10月31日(水) 16:00 ~ 17:30 Room6

[SY-A8]Coupling multi-component phase field models for oxide systems to thermodynamic databases - breaking the curse of dimensionality

○Inge Bellemans[1], Nico Vervliet[2], Lieven De Lathauwer[2,3], Nele Moelans[4], Kim Verbeken[1] (1.Department of Materials, Textiles and Chemical Engineering, Ghent University , Belgium, 2.Department of Electrical Engineering, KU Leuven, Belgium, 3.Group Science, Engineering and Technology, KU Leuven - Kulak, Belgium, 4.Department of Materials Engineering, KU Leuven, Belgium)

An important focus in creating more realistic phase field models is the incorporation of the thermodynamic driving forces in multicomponent multiphase-field models by coupling to thermodynamic databases. This coupling, which aims at retrieving Gibbs energies and chemical potentials, becomes increasingly intricate as the number of components/chemical elements in the system increases. This is caused by the fact that the number of elements in a tensor increases exponentially with the number of dimensions, and so do the computational and memory requirements. The exponential dependency (and the problems that are caused by it) is called the curse of dimensionality.

Alternatives need to be investigated for the storage and handling of the thermodynamic data required for the phase field simulations. A possible solution for this might be the use of a canonical polyadic decomposition on the tensors containing the thermodynamic data. In this way, the huge tensors are approximated well by compact multilinear models or decompositions. Tensor decompositions are more versatile tools than the linear models resulting from traditional matrix approaches.

This solution promises to be suitable for this challenge and has been applied to a quaternary and quinary metal-oxide system in a multicomponent multiphase-field model which incorporates facetted and dendritic growth and can also treat the boundaries as an open boundary where the melt is locally in equilibrium with the atmosphere at a certain partial oxygen pressure. The results and improvements in computational requirements are compared for various methods to couple to a thermodynamic database.