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Thermokinetic modeling and simulation of complex phase transformations in the framework of advanced functional materials

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At present, computational materials engineering is a desired and propagated aim of academia and industry. The usability of computational thermodynamics for physically-based simulations of materials behaviour during technological processing and applications requires a step ahead of classical equilibrium thermodynamic phase descriptions. Theoretic requirements for successful predictions of complex phase evolutions during technological treatments, and related relevant properties, are discussed for two selective, promising functional materials groups. The principles of defect modelling and associated efficiency calculations of complex catalytic materials are discussed for multicomponent nonstoichiometric rare-earth based perovskite oxides. In the functional metals field, simulations of thermo kinetic evolution of metastable precipitates in Ti-Ni based shape memory alloys as function of thermo-mechanical processing is presented. Potentials and limitations of integrated thermo kinetic simulations of phase transformations are highlighted.

Biography

Dr. Erwin Povoden-Karadeniz is an assistant professor at TU Wien, Institute of Materials Science and Technology, Austria at present. His international experience includes various programs, contributions and participation in different countries for diverse fields of study. His research interests as a Scientist reflect in his wide range of publications in various national and international journals.

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