B2: MEPP based modelling and simulation of phase transformation and phase formation in the LAS system by considering mixed kinetic phenomena during solidification

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Overview

For developing tailored Li-Al-Si-O (LAS) slag designs by triggering initial slag compositions in the liquid state and time-dependent cooling paths, to gain high Li-containing crystal phases during solidification, fundamental knowledge of the impact of mixed kinetic phenomena on the time-dependent phase transformation and phase formation is necessary (Schirmer, et al. 2020), (Wittkowski, et al. 2021). A deep understanding of the structure, property and process relationship is required for successful engineering of artificial minerals (EnAM) (Li, et al. 2022). Today, no thermodynamic model exists, which is capable of capturing mixed kinetic phenomena occurring in this system in a holistic way, such that liquid-solid, as well as solid-state reactions and the time-dependent phase formation, can be qualitatively and quantitatively predicted for this system. The basic idea of this project is to develop a non-equilibrium thermodynamic model based on the maximum entropy production principle (MEPP) to simulate the time-dependent and non-isothermal phase transformation and phase formation in the LAS system during solidification. The complex multiphase character of the LAS system is challenging and taken into account by the model. Additionally, four different kinetic phenomena, i.e., reactive diffusion, interface migration, vacancy generation and annihilation and time-dependent processing conditions in terms of cooling rates and retention times and levels, are considered (Figure 1).

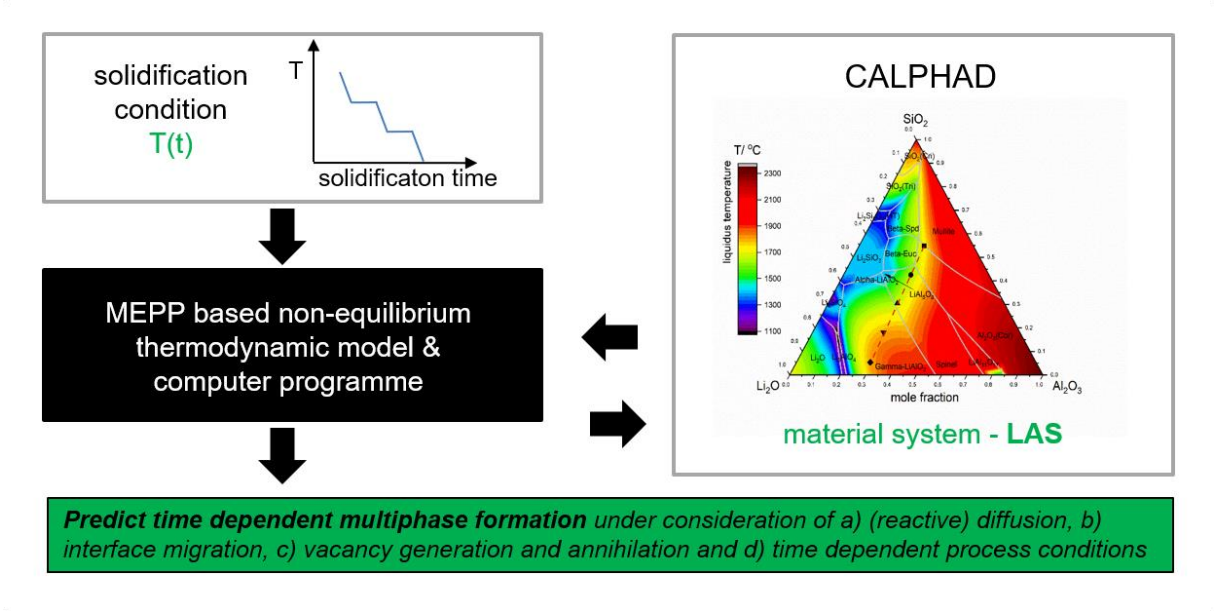

Figure 1: Schematic representation of the non-equilibrium thermodynamics model procedure accompanied with the considered mixed kinetic phenomena during solidification

The kinetic evolution equations as well as the phase selection criterion for growth processes of the respective phases are developed systematically within MEPP framework. The kinetic coefficients of the developed non-equilibrium thermodynamic model are determined by inverse parameter determination based on solidification experiments. Experimental measurements are carried out to obtain thermodynamic data combined with chemical composition and phase structure information, which are used for parameter identification on the one hand and model validation on the other hand. With the experimentally validated model, calculations are performed to develop an optimal initial slag composition in the liquid state and a tailored time-dependent solidification path for LAS to obtain high Li-containing crystal phases.

References

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