Crystallization of Oxide Melts: A Phase Field Model Coupled With ChemApp

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Abstract

Partial or full solidification of metallurgical slags occurs in many industrial pyro-metallurgical processes. To enhance the fundamental knowledge of this phenomenon, this research focuses on the simulation and in-situ observation of crystallizing minerals in oxide melts. The isothermal crystallization of Wollastonite ($CaO.SiO_2$) in a ternary CaO-Al_2O_3-SiO_2 melt is investigated. We used a confocal laser microscope (CLSM) to observe the dendritic crystallization and measured the dendrite tip radius and its velocity as a function of undercooling. The phase field method is chosen to model and simulate the crystallization, because it has proven its power for phase transformations in metals. The phase field model uses a vast number of physical input data, such as Gibbs energies of the phases, diffusion coefficients of the components and the interfacial energy of the solid-liquid interface. The thermodynamic data is retrieved from the *FactSage* database for oxide systems using *ChemApp*. By comparing experimental values for the dendrite tip velocity with values obtained with simulations, the influence of surface energy and diffusion coefficients on the crystallization behavior can be assessed.