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Generalized Cahn-Hilliard equation for solutions with drastically different diffusion coefficients. Application to exsolution in ternary feldspar

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We address mathematical modeling and computer simulations of phase decomposition in a multicomponent system. As opposed to binary alloys with one common diffusion parameter, our main concern is phase decomposition in real geological systems under influence of strongly different interdiffusion coefficients, as it is frequently encountered in mineral solid solutions with coupled diffusion on different sub-lattices. Our goal is to explain deviations from equilibrium element partitioning which are often observed in nature, e.g., in a cooled ternary feldspar. To this end we first adopt the standard Cahn-Hilliard model to the multicomponent diffusion problem and account for arbitrary diffusion coefficients. This is done by using Onsager's approach such that flux of each component results from the combined action of chemical potentials of all components. In a second step the generalized Cahn-Hilliard equation is solved numerically using finite-elements approach. We introduce and investigate several decomposition scenarios that may produce systematic deviations from the equilibrium element partitioning. Both ideal solutions and ternary feldspar are considered. Typically, the slowest component is initially "frozen" and the decomposition effectively takes place only for two "fast" components. At this stage the deviations from the equilibrium element partitioning are indeed observed. These deviations may became "frozen" under conditions of cooling. The final equilibration of the system occurs on a considerably slower time scale. Therefore the system may indeed remain unaccomplished at the observation point. Our approach reveals the intrinsic reasons for the specific phase separation path and rigorously describes it by direct numerical solution of the generalized Cahn-Hilliard equation.