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Computational modeling of mineral unmixing and growth

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A new finite element based simulation technique for mineral growth governed by the classical Cahn-Hilliard equation is presented. The particular format of the underlying Flory-Huggins free energy for non-ideal mixtures is characterized through a double-well potential. It allows for uphill diffusion driven by gradients in the chemical potential and thus provides the appropriate framework to simulate phase separation typically encountered in mineral unmixing and growth. For the finite element discretization, the governing fourth order diffusion equation is reformulated in terms of a system of two coupled second order equations. For the temporal discretization, a heuristic adaptive time stepping scheme is applied in order to simulate not only the early stages of phase separation but also the long term behavior of ageing and grain fusion. The basic features of the Cahn-Hilliard equation are elaborated by means of selected geologically relevant examples. In particular, isotropic and anisotropic mineral growth and symplectite formation are studied and the long term response in the sense of Ostwald ripening is elaborated.