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Effects of Anisotropic Coherency Strain on Intercalation in Phase-Separating Crystals[1] LIAM STANTON, Lawrence Livermore National Laboratory, MARTIN BAZANT, MIT — We consider the self-organization of intercalating particles within crystals induced by spinodal decomposition and the anisotropy of coherency strains, motivated by recent Li-ion battery materials. A phase-field model is developed which incorporates the energetic contributions from the entropy, enthalpy and elastic properties of the host material. Bulk dynamics of the system is then analyzed using linear stability theory to obtain spinodal regions in the parameter space, and numerical simulations are used to predict long-term evolution and relaxational steady-states. These results may explain the alignment of the phase boundary with phosphate planes in LiFePO4, as assumed in recent models and observed in experiments.

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