

Abstract Submitted
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Thermodynamics of Polymer-Clay Nanocomposites Revisited: Compressible Self-Consistent Field Theory Modeling of Melt-Intercalated Organoclays VALERIY GINZBURG, PRASANNA JOG, JEFFREY WEINHOLD, RAKESH SRIVASTAVA, Dow Chemical Company — We formulate a “compressible” version of lattice self-consistent field theory (SCFT) to describe thermodynamic behavior of organically modified clays in polymer melt. The melt consists of the homopolymer matrix and a fraction of end-functionalized “active” chains, each chain having a single “sticker” end-group with strong affinity to the clay surface. We calculate the phase map for this system as function of the melt composition and the strength of the “sticker” adhesion to the clay. It is shown that within the compressible SCFT model, intercalated morphologies are favored in a significantly broader parameter range than was expected based on the incompressible SCFT analysis. We provide a qualitative analysis of this result and discuss implications for the physics of nanocomposites in general.

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