Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Polymer-Grafted Nanoparticles in Polymer Melts: Modeling using Combined SCFT-DFT Approach VALERIY GINZBURG, Dow Chemical Co — Nanoparticles (silica, carbon black, etc.) are often used as fillers to improve physical (thermal conductivity, coefficient of thermal expansion) and mechanical (modulus, strength) properties of polymer materials. In many cases, however, lack of nanoparticle dispersion in the polymer limits the utility of a resulting nanocomposite material. To improve dispersion, one often grafts organic chains ("ligands") onto the surface of the particles; if the ligands are chemically miscible with the matrix polymer, it helps the particles to disperse more uniformly. In recent years, many new morphologies ("wires", "sheets", "networks", etc.) were observed in such nanocomposites. Here, we adapt our earlier formalism combining Self-Consistent Field Theory (SCFT) for polymers with Density Functional Theory (DFT) for the particles; the modified formalism explicitly incorporates the grafted chains into SCFT. We then perform several simulations to study the dependence of morphology on the length and density of grafted chains, as well as the nanoparticle loading. The results are in qualitative agreement with predictions of earlier theories in the limit of lower particle loadings, and predict new morphologies ("bundles of wires") for the case of larger particle loadings. The method can be easily extended to more complex cases (for example, where the matrix and/or ligand itself is a blend or block copolymer).

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Date submitted: 31 Oct 2013 Electronic form version 1.4