Exfoliation of layered platelets and intercalation of polymer chains: effects of molecular weight and quality of polymer solvent

Ras B. Pandey, University of Southern Mississippi, Hattiesburg, MS
Barry L. Farmer, Air Force Research Laboratory, WPAFB, Dayton, OH

Abstract

A Monte Carlo simulation is used to investigate the dispersion of layered platelets in a polymer matrix on a discrete cubic lattice with a coarse-grained model. A polymer chain is a set of L_c nodes tethered together by fluctuating bonds while a platelet (sheet) is described by a set of L_s^2 nodes tethered together by flexible bonds on a square grid. A stack of layered sheets is placed in the center followed by a random distribution of polymer chains on a fraction of lattice sites. Chains and platelets interact and execute their stochastic motion via Metropolis algorithm. Dispersion of sheets and intercalation of chains are studied as a function of molecular weight of polymer chains for attractive and repulsive interaction between polymer and platelets. We find[1] that, with the low molecular weight polymer solvent, the sheets exfoliate in presence of polymer with repulsive interaction while maintain layered structure with attractive interaction via solvent induced interaction. The system becomes much more complex on increasing the molecular weight of polymer as the interplay between the interaction thermodynamics and structural entropy sets in.

1. R.B. Pandey and B.L. Farmer, J. Polym. Sci. B, Polymer Physics (accepted for publication).