

Abstract Submitted
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Effects of molecular weight and entanglement on the dispersion of a layer of platelets in a polymer chain matrix¹ BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — A stack of thin sheets (a model for clay platelets) is initially placed in a matrix of polymer chains. How the dynamic polymer chain matrix (purely entropic constraints) affects the dispersion of sheets is the subject of this computer simulation study. A stack of four sheets constitutes the layer with a small initial inter-layer distance on a discrete lattice. A fraction of the lattice sites are randomly occupied by the polymer chains. Both sheets and chains are modeled by the bond-fluctuation mechanism. Coarse-grained chains and platelets interact and execute their stochastic motion via Metropolis algorithm. Dispersion of the sheets is examined by varying the molecular weight of the polymer chains which form the dynamic network, including entanglements. The relaxation time for dispersion increases on increasing the molecular weight. Exfoliation almost ceases in a matrix with chains beyond a certain length.

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