

Abstract Submitted  
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**Effect of interaction on the exfoliation and dispersion of a stack of platelets in a dynamic polymer matrix and solvent particles by a coarse-grained Monte Carlo simulation**<sup>1</sup> BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — We consider a stack (layer) of four sheets in host matrix of mobile polymer chains and solvent particles and study their exfoliation and dispersion on a discrete lattice. Sheets and chains are created by tethering particles (nodes) by the bond-fluctuation mechanism. Each component interacts and executes their stochastic motion via Metropolis algorithm. Entropic constraints (excluded volume and entanglement [1]) play a critical role in a relatively dense matrix. Therefore, the density of these constituents and their molecular weight are carefully selected to make this study feasible. Exfoliation of the sheets is examined by varying the interactions among different components, i.e., solvent particles, polymer chains, and platelets. The relaxation time for dispersion in the self-organizing dynamic mixture increases on increasing the molecular weight. Exfoliation ceases in a matrix with chains beyond a certain length. [1] R.B. Pandey and B.L. Farmer, J. Polym. Sci. Part B 46, 2696 (2008).

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