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Dispersion of Polymer-Grafted Nanorods in Polymer Films
AMALIE L. FRISCHKNECHT, Center for Integrated Nanotechnologies, Sandia National Laboratories, MICHAEL J. A. HORE, RUSSELL J. COMPOSTO, Dept. of Materials Science and Engineering, University of Pennsylvania — Gold nanorods (NRs) exhibit unique optical properties, i.e. their surface plasmon resonances, which can be tuned by the separation between the NRs. One strategy for controlling the assembly of NRs in a polymer film is to coat them with a polymer brush. The resulting dispersion or aggregation of the rods depends on the details of their interactions, which we examine using both theory and experiment. Classical density functional theory (DFT) and self-consistent field theory calculations of the structure of the brush around an isolated NR in a polymer melt predict a gradual transition from a "wet" to a "dry" brush as the NR radius, the grafting density, and/or the ratio of matrix to brush chain lengths is increased. DFT calculations of the interaction free energy between two NRs find an attractive well at intermediate NR separations. The strength of the attraction increases as the brushes become more dry. Including the van der Waals attractions between the NRs gives an estimate of their total interaction free energy, which can be used to predict when the NRs are dispersed or aggregated. A dispersion map shows good agreement between DFT calculations and experimental observations. Our calculations can be used as a guide to the design rules for tuning NR assembly in polymer films.

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