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Effects of Grafted Chain Density on Nanoparticle and Melt Structure JOSHUA KALB, SANAT KUMAR, Columbia University, ROBERT S. HOY, University of California, Santa Barbara, GARY S. GREST, Sandia National Laboratories — Applications of nanoparticles have increased dramatically over the last few years with uses ranging from scratch proof glass to lubricants to fighting cancer. Grafting polymer chains to these systems further increases the range of their properties, but still much remains to understand about the behavior of 'brush grafted nanoparticle' systems, particularly in their interaction and entanglement with a polymer melt. Previous works where polymer brushes were attached to a flat surface have demonstrated that entanglements between the attached chains and the polymer melt depend strongly on coverage and length of the attached chains. Allowing for a curved grafted nanoparticle surface allows for a wider range of interactions with the melt. Here we present molecular dynamics simulations of the structure of grafted nanoparticles and their entanglements with a highly entangled melt. Individual entanglements are identified using a modified version of primitive path analysis.

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