Abstract Submitted for the MAR07 Meeting of The American Physical Society

Entanglements of End Grafted Polymer Brushes in a Polymeric Matrix GARY S. GREST, Sandia National Laboratories, ROBERT S. HOY, Johns Hopkins University — The entanglement of a polymer brush immersed in a melt of mobile polymer chains is studied by molecular dynamics simulations. A primitive path analysis (PPA) is carried out to identify the brush/brush, brush/melt and melt/melt entanglements as a function of distance from the substrate. The PPA characterizes the microscopic state of conformations of the polymer chain and is ideally suited to identify chain/chain entanglements. We use a new thin-chain PPA technique to eliminate spurious non-entangled inter chain contacts arising from excluded volume. As the grafting density of the brush increases we find that the entanglements of the brush with the melt decrease as the system crosses over from the wet to dry brush regime. Results are compared to brush/brush entanglements in an implicit solvent of varying solvent quality. Sandia is a multiprogram laboratory operated by Sandia Corp., a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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Date submitted: 16 Nov 2006

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