MULTISCALE MODELING AND MOLECULAR DYNAMICS CHARACTERIZATION OF SURFACE EFFECTS IN POLYMER THIN FILMS

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A multiscale model of polymeric thin films with surface effects is constructed and characterized by molecular dynamics simulations. For this purpose, a continuum model including surface elasticity energy (see e.g. [1]) is employed, whose surface coefficients are identified by MD simulations on slab models of linear monodisperse polyethylene thin films. Due to long-range effects in such materials, a procedure proposed in [2] is employed with different slab thickness to deduce the surface energy and the related elastic terms. The continuum equations are solved by a FEM discretization and compared to the full MD model.

REFERENCES
