Multiscale Modelling and Molecular Dynamics Characterization of Size Effects in Thin Polymer Films

F. Detrez*, J. Yvonnet* and Q.-C. He*

*MSME UMR 8208 CNRS, Université Paris-Est Marne-la-Vallée
5 Bd Descartes 77454 Marne-la-Vallée CEDEX 2, France
Email: fabrice.detrez@u-pem.fr

ABSTRACT

A multiscale model of thin polymeric films with size effects is constructed and characterized by molecular dynamics simulations. For this purpose, a continuum model including nonlocal elasticity is employed, whose elastic coefficients are identified by MD simulations on slab models of linear monodisperse polyethylene. Due to long-range effects in such materials, a procedure inspired from Yvonnet et al [1] is employed with different slab thickness to deduce the elastic coefficients. The continuum equations are solved by a FEM discretization and compared to the full MD model.

REFERENCES