

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

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**Key words:** *Multiscale modeling, Molecular dynamics, Surface elasticity, Polymer.*

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

- [1] D. Davidov, A. Javili and P. Steinmann P. On molecular statics and surface-enhanced continuum modeling of nano-structures, *Computational Materials Science*, Vol. **69**, 510–519, 2013.
- [2] J. Yvonnet, A. Mitrushchenkov, G. Chambaud and Q.-C. He. Finite element model of ionic nanowires with size-dependent mechanical properties determined by ab initio calculations. *Computer Methods in applied Mechanics and Engineering*, Vol. **200**, 614–625, 2011.