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Surface Sensing of Atomic Behavior of Polymer Nanofilms via Molecular Dynamics Simulation

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Abstract : Surface-sensing devices such as atomic force microscope have been widely used to characterize the surface structure and properties of nanoscale polymer films. However, using molecular dynamics simulations, we show that there is intrinsic and unavoidable inelastic deformation at polymer surfaces induced by the sensing tip. For linear chain polymers like perfluoropolyether, such tip-induced deformation derives from the differences in the atomic interactions which are atomic specie-based Van der Waals interactions, and resulting in atomic shuffling and causing inelastic alternation in both molecular structures and mechanical properties at the regions of the polymer surface. For those aromatic chain polymers like epoxy, the intrinsic deformation is depicted as the intra-chain rotation of aromatic rings and kinking of linear atomic connections. The present work highlights the need to reinterpret the data obtained from surface-sensing tests by considering this intrinsic inelastic deformation occurring at polymer surfaces.

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