SIMULATION OF INDENTATION IN POLYMERS USING MOLECULAR DYNAMICS

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ABSTRACT

The tribological properties of materials are often underappreciated and insufficiently understood, despite their importance to the industry. The indentation process is empirically observed in the laboratory from material hardness tests, e.g. Rockwell, Vickers or Knoop. We have used coarse grain molecular dynamics computer simulations to study indentation resistance of polymers with a chain structure similar to that of high density polyethylene (HDPE). Interaction of statistical segments is defined via Mie potentials to simulate how the interconnected segments respond to an external force imposed by an indenter under different conditions. Results include the time-dependent measurement of penetration depth, recovery depth, and recovery percentage, with respect to indenter force, indenter size, and indentation time parameters. The simulations provide results that are inaccessible experimentally, including continuous evolution of the pertinent tribological parameters during the entire indentation process.

Keywords: polymers, nano-indentation, molecular dynamics simulations