

SIMULATION OF SCRATCHING BEHAVIOR IN POLYMERS THROUGH MOLECULAR DYNAMICS

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ABSTRACT

In spite of some accumulation of experimental evidence [1 - 3], scratch resistance is still not sufficiently understood. Thus, part replacement and repair in structures with moving parts because of scratchability and wear lead to very high maintenance costs. We have studied scratch resistance of amorphous polymeric materials through molecular dynamics [3] computer simulations. As a first approach, a coarse grain model was created for high density polyethylene (HDPE) at the mesoscale. The obtained results include analysis of penetration depth, residual depth and recovery percentage related to indenter force and size. Our results show there is a clear effect from these parameters on the tribological properties. We also discuss geometric features in the scratched surface topology and the reasons for their appearance.

Keywords: polymers, nano-scratching, molecular dynamics simulations

References:

1. W. Brostow, J.-L. Deborde, M. Jaklewicz & P. Olszynski, Tribology with emphasis on polymers: Friction, scratch resistance and wear, *J. Mater. Ed.* 2003, 25, 119-132.
2. N.K. Myshkin, M.I. Petrokovets and A.V. Kovalev, Tribology of polymers: friction, wear and mass transfer, *Tribology Internat.* 2005, 38, 910-921.
3. W. Brostow, V. Kovacevic, D. Vrsaljko & J. Whitworth, Tribology of polymers and polymer based composites, *J. Mater. Ed.* 2010, 32, 273-290.
4. W. Brostow & R. Simões, Tribological and mechanical behavior of polymers simulated by molecular dynamics, *J. Mater. Ed.* 2005, 27, 19.