

Technical University of Denmark



## Polymer friction Molecular Dynamics

Sivebæk, Ion Marius; Samoilov, Vladimir N.; Persson, Bo N. J.

*Publication date:*  
2010

[Link back to DTU Orbit](#)

*Citation (APA):*

Sivebæk, I. M., Samoilov, V. N., & Persson, B. N. J. (2010). Polymer friction Molecular Dynamics. Poster session presented at FANAS workshop, Saarbrücken, .

## DTU Library

Technical Information Center of Denmark

---

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

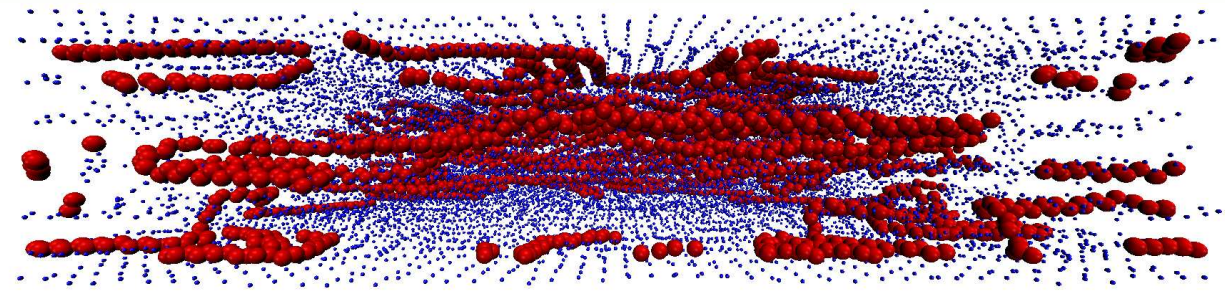
- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# Polymer friction Molecular Dynamics

Ion M. Sivebaek,<sup>\*,†,‡,§</sup> Vladimir N. Samoilov,<sup>†,‡</sup> and Bo N. J. Persson<sup>†</sup>

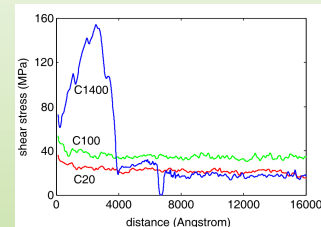
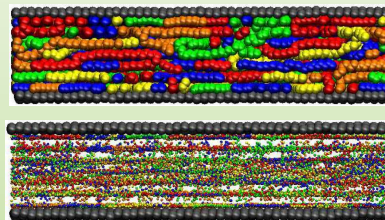
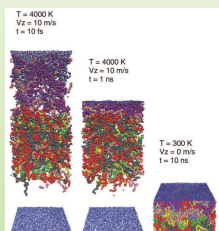
<sup>†</sup>IFF, FZ-Jülich, 52425 Jülich, Germany, <sup>‡</sup>Novo Nordisk A/S, Research and Development, DK-3400 Hillerod, Denmark, <sup>§</sup>Mechanical Engineering Department, Technical University of Denmark, DK-2800 Lyngby, Denmark, and <sup>‡</sup>Physics Faculty, Moscow State University, 117234 Moscow, Russia



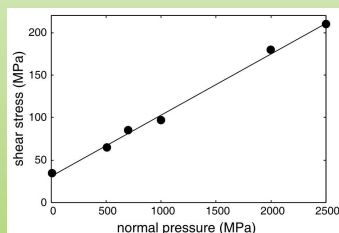
We present molecular dynamics friction calculations for confined hydrocarbon solids with molecular lengths from 20 to 1400 carbon atoms. Two cases are considered: a) polymer sliding against a hard substrate, and b) polymer sliding on polymer. In the first setup the shear stresses are relatively independent of molecular length. For polymer sliding on polymer the friction is significantly larger, and dependent on the molecular chain length. In both cases, the shear stresses are proportional to the squeezing pressure and finite at zero load, indicating an adhesional contribution to the friction force. [ Sivebaek, I.M., Samoilov, V.N., Persson, B.N.J. Eur. Phys. J. E 27, 37-46 (2008). and Persson B.N.J., Sivebaek I.M., Samoilov V.N., Zhao Ke, Volokitin A.I., Zhenyu Zhang. J. Phys.: Condens. Matter 20, 395006 (2008) ]

Concerning the effective viscosity of nanometer thin confined polymer films we find shear thinning effects similar to those seen in Surface Force Apparatus measurements [Yamada S. Tribology Letters, 13 (3), 167 (2002)]. We also find that the temperature alters these shear thinning effects going from solid like state at 0K to a Newtonian liquid at high temperatures [Sivebaek, I.M., Samoilov, V.N., Persson, B.N.J. In preparation].

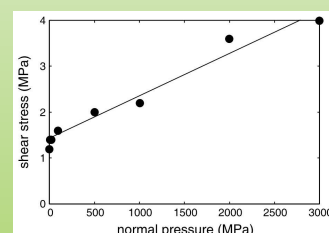
Preparation



Pressure effects



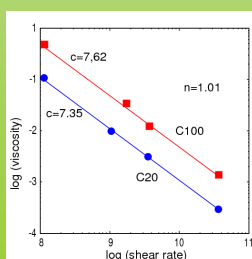
Commensurate



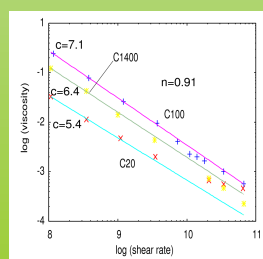
$$\log(\text{viscosity}) = c - n \log(\text{shear\_rate})$$

Effective viscosity

0K



300K



600K

