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Polymer translocation through a nanopore: Impact of fluctuations on dynamical scaling

Vakhtang G. Rostiashvili[1]*, **Johan L. Dubbeldam**[2], **Andrey Milchev**[1], **Thomas A. Vilgis**[1]

[1]Max-Planck Institute for Polymer Research, Mainz, Germany
[2]Delft University of Technology, Delft Institute of Applied Mathematics (DIAM), Delft, The Netherlands
*rostiash@mpip-mainz.mpg.de

We suggest a theoretical description of the force-induced translocation dynamics of a polymer chain through a nanopore. Consideration is based on the tensile blob picture of a driven chain and the notion of a propagating front of tensile force along the chain backbone, suggested by Sakaue (Phys. Rev. E 81, 041808 (2010)). The driving force is associated with a chemical potential gradient that acts on each chain segment inside the pore. Depending on its strength, different regimes of polymer motion (named after the typical chain conformation, "trumpet", "stem-trumpet", "stem") occur. Assuming that the local driving and drag forces are equal (i.e., in a quasi-static approximation), we derive an equation of motion for the tensile front position. We show that the scaling law for the average translocation time versus chain length changes as the driving force f grows. As a result the corresponding scaling exponent increases with f. This and other predictions are tested by Molecular Dynamics (MD) simulation. Data from our computer experiment indicate indeed that the translocation scaling exponent increases with the pulling force f albeit the observed exponent stays systematically smaller than the theoretically predicted value [1]. In order to study the role of fluctuations (which are ignored in the quasi-static approximation), we assumed that the translocation coordinate $s(t)$ is a random process governed by the so-called velocity Langevin (V-Langevin) equation [2]. With this in mind we have derived the corresponding Fokker-Planck equation (FPE) for the translocation coordinate probability distribution function $W(s,t)$ which has a nonlinear drift term and time-dependent (running) diffusion coefficient $D(t)$. Our direct MD-simulation performed in 3D shows that the driven translocation follows a super-diffusion with a running diffusion coefficient $D(t)$. This finding being used in the numerical solution of FPE demonstrates an important conclusion: under relatively small driving forces fluctuations can facilitate the translocation dynamics [3]. Moreover, the effective translocation exponent becomes smaller. In the undriven case the translocation is slightly sub-diffusive and can be treated within the framework of fractional Brownian motion (fBm) [4]. In particular, this means that $W(s,t)$ is Gaussian but with a time-dependent variance which grows sub-diffusively. These results are supported by extensive MD-simulation.

References

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