diffusion-fundamentals.org

The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Determining surface diffusion properties from signal fluctuations

Susanne Hahne*, Philipp Maass

Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany
*shahne@uni-osnabrueck.de

To describe growth kinetics of adsorbates on surfaces, knowledge of diffusion coefficients of atoms and molecules on the surface is of vital importance, especially for controlling the self-assembly of organic molecules. These usually have high mobilities and sizes large compared to the lattice constant of the substrate. In this situation, not all techniques are equally well suited for determining the diffusion coefficient. A convenient and powerful method is the recording of temporal signal fluctuations of a locally fixed probe as, for example, the current of a scanning tunneling microscope or the frequency/height modulation of an atomic force microscope. Origin of the respective fluctuations are single molecules passing the probe. This method is limited neither to sufficiently small mobilities nor to large defect-free areas.

Signal fluctuations from a fixed probe show well-defined peaks with stochastically varying widths and interpeak intervals. After transforming the signal into a rectangular one via a suitable noise-eliminating threshold value, a distribution of peak widths (Ψ_w) and interpeak distances (Ψ_d) can be obtained. In addition, the autocorrelation function (C) of the signal can be studied. We present a theory for these distributions[1], and, in extension to earlier treatments [2], for the autocorrelation function, that allows one to extract various diffusion parameters. Monte Carlo simulations of the problem are carried out for comparison with the theoretical predictions. Figure 1 shows representative examples for Ψ_w and Ψ_d, which exhibit distinct scaling behaviours in different time regimes in agreement with the theory.

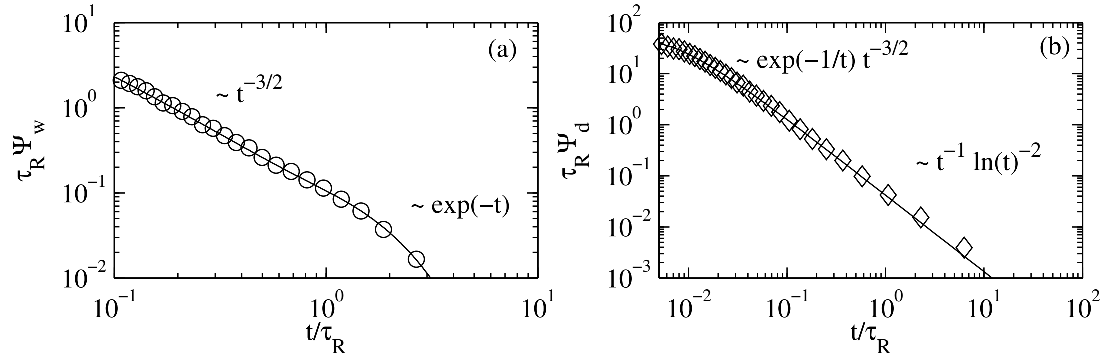

Figure 1: Analytical results (solid lines) in comparison with Monte Carlo data for (a) Ψ_w and (b) Ψ_d for a representative example. The distributions and time t are scaled with the characteristic time $\tau_R = R^2/D$, where R is the molecule radius and D the diffusion coefficient.

With respect to the applicability of the approach one has to note that Ψ_d is influenced by exchange processes of distinct particles at long times, which can only be captured approximately by the theory. The autocorrelation function is also affected by these exchange processes. Ψ_w on the other hand is governed solely by the diffusion of a single particle, but a good time resolution is necessary to resolve the peaks with high accuracy. Furthermore, Ψ_w and C can be influenced by the probe, while this influence can be neglected for Ψ_d. It is therefore advisable to use a combination of all three methods to utilize their strengths and minimize their weaknesses. This combined analysis has successfully been applied recently to the diffusion of CuPc molecules on Ag(100) [1].

References

[1] S. Hahne, J. Ikonomov, M. Sokolowski, P. Maass: *Determining molecule diffusion coefficients on surfaces from a locally fixed probe: Analysis of signal fluctuations*. Phys. Rev. B **87**, 085409 (2013)

[2] M. Sumetskii, A. Kornyshev: *Noise in STM due to atoms moving in the tunneling space*. Phys. Rev. B **48**, 17493 (1993)