Summary

The dynamic behavior of a liquid front moving across a solid, i.e. wetting, has been studied extensively over the past decades, for academic and industrial reasons. Two main mechanisms for wetting have been proposed in the literature, which are entirely different in their approach.

On one hand, many authors adopted a hydrodynamic approach, where the viscosity and the liquid-vapor interfacial tension are the key parameters. For non-zero contact angles, this approach leads to a mathematical singularity at the contact line. Generally, some mechanism, such as slip, has to be assumed to avoid the singularity. The resulting equations have been verified in many different experiments. On the other hand, some authors have adopted a molecular-kinetic approach, to describe exactly the contact line region at a molecular scale. The main parameters are then the liquid-vapor surface tension and various molecular characteristics of the liquids and solid involved. This approach leads to equations which describe a wide range of experiments equally well. The molecular characteristics which stem from this approach were, however, not accessible independently until now.

To deal with the shortcomings in both existing models, we propose an original approach to describe the dynamics of partial wetting, by combining the different dissipation channels such as friction with the solid and viscosity. It is shown that this approach leads to a succession of different regimes, depending on the characteristics of the system under study and on the time frame over which the experiments are made. This new model gives a possible answer to the long-standing question of why the two basic, but completely different models of partial wetting in the literature, can be used to describe experimental results in particular cases.

To verify the validity of the different models by experiment, we have built a set-up to measure the dynamics of spreading drops. In our set-up, we analyze the changing shapes of drops during spreading. From this analysis, we acquire the contact angle relaxation in time, which is characteristic of the wetting behavior. We compare the experimental data with the different existing models of wetting and with the model proposed in this work. We show that indeed the new model can help us understand better the complete mechanism of wetting, and interpret the exact physical meaning of the different microscopic parameters involved. A particular case of static wetting by liquid drops is also discussed, experimentally as well as theoretically. We study the shape of drops consisting of a mixture of two, partially imiscible, molten metals, under the condition of complete wetting. By analyzing this system in detail, we are able to measure the interfacial tension between the two metals. This analysis shows in particular the accuracy and possibilities of our experimental set-up.

To verify independently the assumptions about the microscopic phenomena of wetting, we use large-scale molecular dynamics simulations. First, it is shown that molecular dynamics simulations, if the systems are large enough, indeed reproduce the spreading of a liquid drop in contact with a solid. All the relevant characteristics, such as the surface tension, the viscosity, the contact angle and the friction near the solid are measured. For the first time, the basic assumptions underlying the molecular-kinetic model are directly verified and the details of the contact line displacement can be scrutinized. Implicitly, the assumptions within the newly proposed model for partial wetting are also verified. Also on the basis of molecular dynamics simulations, the wetting behavior on heterogeneous substrates is analyzed and we propose a new model which describes well the results in terms of molecular friction with the solid substrate. We briefly report on simulations of complete wetting systems.