

Frequency shift approximation in simulations of HR-AFM images with a CO-functionalized tip

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Image simulations of High-Resolution Atomic Force Microscopy with a CO-functionalized tip have greatly improved as we better understand the theory of such images [1,2,3]. Models such as the FDBM allow us to calculate the tip-sample interaction force (F_{ts}) in a sizable 3D space. Nevertheless, AFM experiments can only directly measure changes in the tip's oscillation frequency (frequency shift, Δf). So, to properly compare simulated AFM data to real-world experiments, we must further change the theoretical F_{ts} to a theoretical Δf [4]. The straightforward way to achieve this is to integrate the F_{ts} numerically, along the complete length of the tip oscillation, as described in [5]. However, this method requires the F_{ts} to be calculated at many different points along the z -axis, making the calculations grow considerably. An option that avoids this inconvenience is approximating the Δf with the force gradient ($\nabla_z F_{ts}$) calculated at a single point in the z -axis, which works well for the small oscillations in tuning force AFM. Still, different HR-AFM experiments have oscillations between 0.2 and 1 Å, where the force gradient approximation may not hold. For the last case, we further propose a F_{ts} -based Δf approximation, considering the force at the point of the closest approach of the tip. Meanwhile, the $\nabla_z F_{ts}$ approximation, only considers the mean average position of the tip through a complete oscillation cycle. With FDBM [1], we then simulated the HR-AFM data of different experimentally-relevant molecules (such as trimesic acid [6], pentacene, and pyridine) and calculated the Δf with the three methods previously described. We observed that the integral function and the F_{ts} approximation have similar results, but the $\nabla_z F_{ts}$ approximation does not, as shown in Fig. 1. The difference comes from the CO tip relaxation, as the shape of the force curve changes in a few fractions of an Å due to the CO molecule's deflection. So using the $\nabla_z F_{ts}$ approximation does not fare well because the data of the average plane of the oscillation does not relate to the data at the point of closest approach. In conclusion, the proposed force approximation yields very similar results to the complete integral. Also, it has the advantage that it does not require a wide range of z distances to approximate the Δf .

References

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Figures

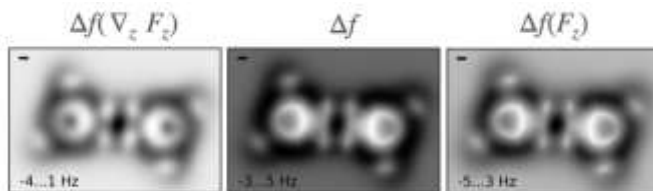


Figure 1: Theoretical frequency shift approximations of a trimesic acid dimer, where carboxyl groups form a double H bond. (left) Approximation based on the force gradient at the mean tip-sample distance, (center) exact calculation as the integral of force versus distance curves, (right) approximation based on the force at the distance of closest approach. Tip-sample distance is 3.17 Å, amplitude is 0.55 Å, scalebar length is 1 Å.