Relation between the apparent height barrier, the chemical force and the local contact potential difference in atomic scale

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In STM, the tunneling current I usually obeys the exponential dependence on tip-sample distance z, $I \sim exp(-Az\sqrt{\omega})$, where the decay length is controlled by the so called apparent barrier height ω [1]. In a far distance limit, the apparent barrier height ω tends to the surface work function W. On the other hand, Kelvin Force Probe Microscopy (KPFM) [2] with atomic scale resolution [3] senses a variation of the electrostatic force F_{el} with applied bias voltage V_s and the tip-sample distance z. The electrostatic force is $F_{el} = - dC/dz (V_s - V_{lcpd})^2$, where V_{lcpd} denotes the local contact potential difference. The contact potential difference is nothing else than the difference between work functions of the surface and the probe. It is evident that both quantities, the contact potential difference V_{cpd} and the apparent height of the barrier ω , have direct relation to the sample work function W.



Recent progress in Scanning Probe Microscopy opens the possibility of simultaneous acquisition of the tunneling current, atomic forces and local potential difference with atomic resolution. The aim of this contribution is to discuss a correlation between the apparent barrier height and the local contact potential difference on the atomic scale. In particular, we performed simultaneous site-specific AFM/STM measurements using a qPlus sensor on the prototypical Si(111)–7×7 surface with low coverage of atomic hydrogen. We will show how the chemical force, the apparent barrier height and local contact potential difference change according to the tip-sample distance and atomic site (H, Si-adatom, corner hole). Consequently, we will check the relation between these quantities. We will also analyze the capacitance C and its dependence on the quantities. In addition, we carried out DFT simulations to understand how the formation of the chemical bond affects electronic structure and charge distribution [6] on the Si(111)–7×7 surface.

References

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