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TÉMA

AFM on a Hydrogenated Si 7x7 Surface: exploring different interaction regimes

Mgr. Martin Ondráček, Ph.D.

Institute of Physics ASCR, Prague, Czech Republic

The non-contact atomic force microscope (nc-AFM) allows us to probe forces acting between the apex of the AFM probe and the surface of the sample on the atomic scale. Especially when the imaging mode is combined with an on-site force spectroscopy, valuable information on the character of inter-atomic forces can be obtained. However, the detected forces and the mechanism by which they arise may differ markedly depending on the structure and reactivity of the AFM-tip termination. Here we have explored the interaction between an AFM probe and the Si (111)-7x7 surface exposed to a low-coverage of atomic hydrogen at RT, both experimentally and theoretically. We have identified two profoundly different types of tip termination, distinguished by the image contrast as well as the interaction forces measured over the hydrogen-passivated and non-passivated Si adatoms. The statistics of the tip-dependence of the measured forces, which are obtained using various tip states with different cantilevers, reveals the typical values of the force and their distribution in the two characteristic interaction modes. Our experimental results were corroborated by density functional theory (DFT) calculations performed for different atomic models of tips in order to interpret the observed force curves.

In this contribution, we will point out the role of the chemical reactivity and the van der Waals forces in terms of chemical composition of the tip-apex termination. Finally, we will also discuss the mechanisms of interaction forces by combining the projected density of states (PDOS) calculations with the maps of electron density redistribution at the tip-sample interface.

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

Zsolt Majzik, MSc.

Institute of Physics ASCR, Prague, Czech Republic

In STM, the tunneling current I usually obeys the exponential dependence on tip-sample distance z, I~exp(-Azvω), where the decay length is controlled by the so called apparent barrier height ω. 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) with atomic scale resolution 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 on the Si(111)–7×7 surface.

odborný garant: *Ing. Pavel Jelínek, Ph.D.*