The role of the bias voltage and the atomic thermal movements on the STM/FM-AFM images: how is a Si tetramer observed on the Si(111)-7×7 surface?

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It is well known that both bias voltage and dynamical effects should be taken into consideration on the interpretation of STM images [1,2]. In this work we present a combined experimental and theoretical study on the influence of the bias voltage and the atomic thermal movements on both the STM and the FM-AFM images of a Si tetramer on the Si(111)-7x7 surface [3].

Using the FM-AFM atomic manipulation ability [4] we have built up the Si tetramer. Topographic STM, CITS and constant high simultaneous FMAFM/STM images at RT show the Si4 atoms forming a symmetric structure (Fig. 1). Numerical simulations based on DFT show that the system is bistable, there are two solutions characterized by a rhombohedral tetramer with one of the atoms protruding over the other three (Fig. 1c). The corresponding STM simulated image displays this asymmetric structure. Molecular dynamic as well as energy barrier calculations disclose that, at RT, the tetramer is moving between the two solutions. LT-STM experiments shows the two stable solutions at low voltages (< 0.3 eV) but recover the symmetric tetramer at bias larger than 0.7 eV. Therefore, RT-STM or high-voltage STM images are in fact an average of the two atomic configurations of the bistable system resulting in images displaying a symmetric structure. Explanation of the FM-AFM measurements is more complicate, simulations shows how not only the thermal or voltage-induced fluctuations but also the tip-surface interaction are playing an important role: at long tip-surface distances SR forces are negligible -no Δf contrast, standard STM image-, but at closer distances the outermost apex atom attracts its closer surface atom fixing the fluctuating tetramer in a particular solution (with that closer atom being the higher of the tetramer), consequently both FM-AFM and STM images show the symmetric “on atom” solution.

References

[1] J. Avila et al, Phys. Rev. Lett. 82, 442-445 (1999)

[2] B.C. Stipe, et al, Phys. Rev. Lett. 78, 4410 (1997)

[3] H. Tanaka et al., Jpn. J. Appl. Phys. 33, 366 (1994)

[4] Y. Sugimoto et al, Phys. Rev. Lett. 98, 106104 (2007)

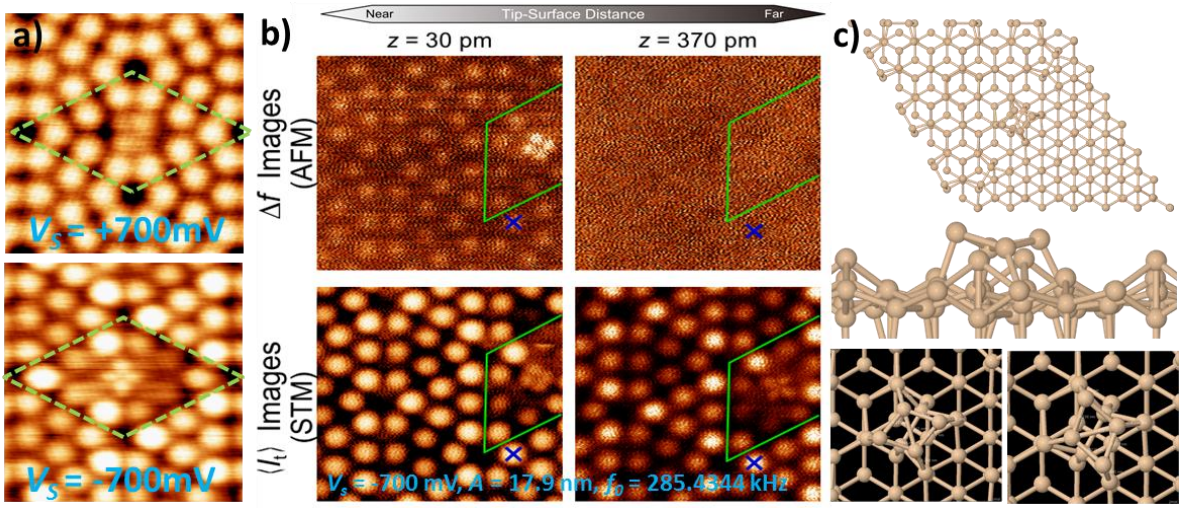

Figure 1: a) RT-STM show a symmetric “on atom” structure for empty states and a cross-like image for the filled ones. b) Constant high simultaneous FM-AFM/STM for negative bias: STM images evolve for the cross-like structure to the “on atom” image upon tip-surface approximation. c) The asymmetric atomic structure calculated with the DFT method.