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

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It is well known that dynamical effects should be taken into consideration on the interpretation of STM images [1]. In this work we present a combined experimental and theoretical study on the influence of the atomic thermal movements on both the STM and the FM-AFM images of a Si tetramer on the Si(111)-7x7 surface at RT [2].
Using the FM-AFM atomic manipulation ability [3] we have built up the Si tetramer. Topographic STM, CITS and constant high simultaneous FMAFM/STM images show the Si4 atoms forming a symmetric structure (Fig. 1). However, numerical simulations based on DFT lead to 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 4 nonequivalent solutions (each one corresponding to a different Si tetramer atom being the highest). Therefore, the **STM is in fact sensing an average of the different atomic configurations** resulting in images displaying a symmetric structure. Explanation of the **FM-AFM measurements** is more complicate, simulations shows how **not only the thermal 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.

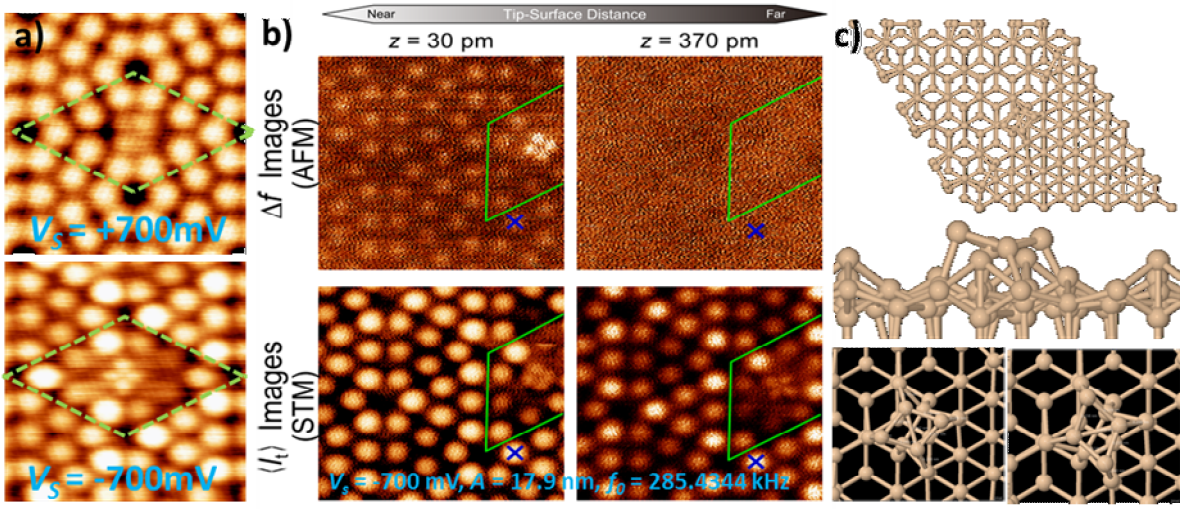

Fig. 1: a) STM show a symmetric "on atom" structure for empty states and a cross-like image for the filled ones. b) Constant high simultaneous FM-AFM/STM for negative bias: STM images evolve for the cross-like structure to the "on atom" image upon tip-surface approximation. c) The asymmetric atomic structure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

References

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