

Chemical structure of molecules in topographic images

Y. Yasui[#] and Y. Sugimoto

¹*Department of Advanced Materials Science, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8561, Japan*

[#] Presenting author's e-mail: yasui@k.u-tokyo.ac.jp

The chemical structures of organic molecules have been investigated with atomic force microscopy (AFM) using CO-terminated tips [1]. Those measurements were generally taken with constant-height scans using the qPlus sensor. Its large spring constant allows for an oscillation amplitude as small as 100 pm, enabling good sensitivity to the short-range repulsive force.

Here, we demonstrate that the chemical structure of molecules is resolved in AFM topographic images [Fig. 1(a)]. This was achieved using an optical interferometry technique with Si cantilevers [2, 3]. Compared to quartz oscillators, Si cantilevers are more sensitive to force due to their soft spring constant and fast resonance frequency, which multiply the conversion factor from force to frequency shift. We used 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) molecules deposited onto Au(111) substrates as an example of a molecule. Measurements were performed at 5 K. AFM topographic images were obtained with a traditional frequency-modulation AFM operated in the constant-frequency-shift mode. The relatively large oscillation amplitude of 1.46 nm allowed us to detect both the short-range repulsive force and the long-range van der Waals force [Fig. 1(b)]. This facilitates the chemical-structure imaging in topographic images. The current approach prompts a subsequent examination of the chemical structure of non-planar molecules.

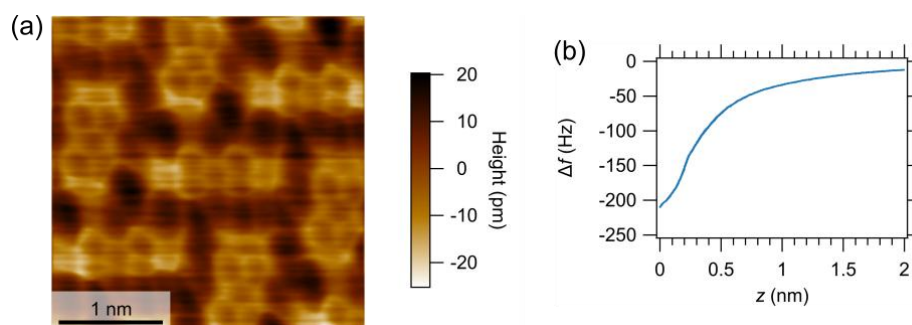


Figure 1. (a) AFM topographic image of a PTCDA monolayer on Au(111). The set-point frequency shift is -90.2 Hz, the sample bias is 600 mV, the oscillation amplitude is 1.46 nm, the scan speed is 5.1 nm/s, the resonance frequency is 987 kHz, and the spring constant is 1200 N/m. (b) Frequency shift as a function of tip-sample distance measured on Au(111) substrate with the CO-terminated tip.

Reference

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