STM contrast stability of HOPG: Role of the tip-orientation

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Highly oriented pyrolytic graphite (HOPG) is an important substrate in technological applications, and is routinely used in scanning tunneling microscopy (STM) calibration. Therefore, the accurate interpretation of the experimentally observed STM image contrasts is very important [1]. Using a three-dimensional Wentzel-Kramers-Brillouin tunneling model [2,3] combined with fi

rst principles electronic structure calculations, we demonstrate that the tip orientation has a considerable effect on the simulated STM images. Our simulations indicate that local tip-rotations maintaining a major contribution of the $d_{3z^2-r^2}$ tip-apex state to the tunneling current affect only the secondary features of the HOPG STM contrast. On the other hand, tip rotations leading to enhanced current contributions from $m \neq 0$ tip-apex electronic states can cause a triangular-hexagonal change in the primary contrast. By comparing STM topographic data between experiment [1] and large scal e simulations, we can determine particular tip orientations that are most likely present in the STM experiment.

[1] G Teobaldi et al., *Phys. Rev. B* **85**, 085433 (2012).
[2] K Palotas et al., *Phys. Rev. B* **86**, 235415 (2012).
[3] G Mandi et al., *J. Phys. Condens. Matter* **25**, 445009 (2013).