The Effects of Signal Processing on Higher Harmonics for Subatomic Resolution in NC-AFM

C. Alan Wright and Santiago Solares
Department of Mechanical Engineering, University of Maryland, College Park, USA
Email: ssolares@umd.edu

Detailed information about the tip-sample interaction in dynamic AFM is encoded in the higher harmonics of the cantilever response [1]. As such, higher harmonics have been employed for both tip-sample force reconstruction and increased image contrast. While force reconstruction is a relatively straightforward mathematical consequence of the sinusoidally-driven cantilever in a nonlinear force field, the limit of attainable resolution via higher-harmonics AFM remains an open question. At the forefront of this debate are the experimental images reported by Hembacher *et al*. in 2004 [2]. The authors performed simultaneous STM/AFM on a graphite surface using a tungsten tip, and maps of the higher harmonics revealed features of subatomic size (Figure 1A). These features were attributed to the electronic structure of the foremost tungsten tip atom – an interpretation that raised two important questions: Can NC-AFM spatially resolve subatomic features on a surface? And, can those features be seen as maps of the charge density? We recently developed a simulation method to show that the subatomic features are *fundamentally* feasible under *ideal* conditions [3]; however, a definitive connection to the charge density of the apex tungsten atom has not been made. In this work we continue our bottom-up theoretical approach. Specifically, we explore the most significant point of contention regarding the interpretation of Hembacher's images: the signal processing used to collect the harmonics, which consisted of both filtering and averaging the harmonics (in the form of an rms). Our simulations suggest that, while there are no imaging artifacts inherent to the filtering process, harmonics averaging is not an appropriate method for obtaining increased contrast due to variations in the harmonics ratios across the surface [4]. However, a promising approach may be the individual mapping of the first or second harmonics, which are expected to dominate the contrast under the conditions studied by *Hembacher et al*.

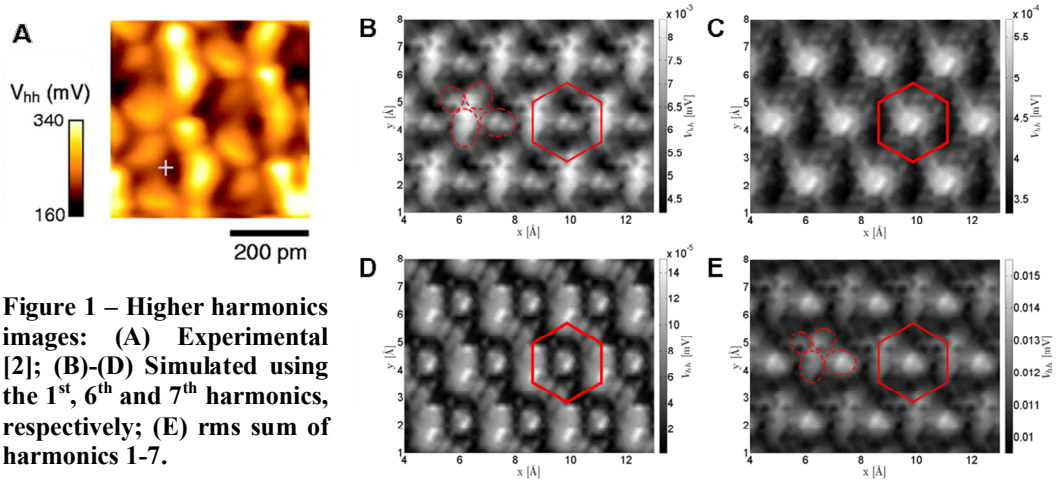

Figure 1 – Higher harmonics images: (A) Experimental [2]; (B)-(D) Simulated using the 1st, 6th and 7th harmonics, respectively; (E) rms sum of harmonics 1-7.

[1] Sahin, *et al*., Springer Handbook of Nanotechnology, 3rd ed, (2010).
[2] Hembacher, S., Giessibl, F. J., and Mannhart, J., Science, 305, (5682), (2004).
[3] Wright, C. A., and Solares, S. D. Nano Letters, 11, (11), (2011).
[4] Wright, C. A., and Solares, S. D. Appl. Phys. Lett., in press.