

Elemental contrast in noncontact atomic force microscopy on a boron-nitride monolayer

F. Schulz^{1,2} J. Ritala² A. P. Seitsonen³ A. S. Foster² P. Liljeroth²

¹IBM Research, Zurich Research Laboratory, 8803 Rüschlikon, Switzerland

²Department of Applied Physics, Aalto University School of Science, 00076 Aalto, Finland

³Département de Chimie, École Normale Supérieure, 75005 Paris, France

Elemental contrast with atomic resolution is a key aspect of cutting-edge microscopy, enabling materials research at the nanoscale. Transmission electron microscopy (TEM) offers chemical sensitivity through different modes, most strikingly as Z-contrast and via atomically resolved electron energy loss spectroscopy (EELS) in scanning TEM [1]. However, due to the high-energy electron beam, TEM is not suitable for more sensitive structures such as small organic molecules. A less destructive alternative might be noncontact atomic force microscopy (nc-AFM). Though not yet capable of chemical fingerprinting as powerful as EELS, elemental contrast is one of the most-studied topics in nc-AFM. In a seminal contribution, Sugimoto et al. identified different atomic species in a surface alloy by comparing the maximum attractive forces on different lattice sites in $\Delta f(z)$ spectroscopy [2]. Measurements of the local contact potential difference (LCPD) in Kelvin probe force microscopy, either via an AC modulation of the tip-sample voltage or through $\Delta f(V)$ spectroscopy, is another avenue that achieved chemical resolution, in particular on ionic systems [3–5]. Here, we employ nc-AFM with CO-functionalized tips [6] to investigate the atomic-scale contrast on a monolayer of hexagonal boron nitride (hBN) on Ir(111) [7]. hBN constitutes an interesting model system, as it is a mostly covalently bonded insulator with a nearest-neighbour distance of only ~ 145 pm. Yet constant-height maps of both frequency shift and local contact potential difference reveal strong contrast between the boron and nitrogen sub-lattices. nc-AFM simulations based on the density functional theory-optimized hBN/Ir(111) geometry allow us to match the two distinct atomic sites with the different elements and shine light on the origin of the atomic-scale contrast. Our combination of constant-height images and atomically resolved LCPD maps offers a robust method to identify different chemical species in nc-AFM.

[1] K. W. Urban, *Science* **321**, 506 (2008).

[2] Y. Sugimoto et al., *Nature* **446**, 64 (2007).

[3] F. Bocquet et al., *Phys. Rev. B* **78**, 035410 (2008).

[4] G. H. Enevoldsen et al., *Phys. Rev. Lett.* **100**, 236104 (2008).

[5] L. Gross et al., *Phys. Rev. B* **90**, 155455 (2014).

[6] L. Gross et al., *Science* **325**, 5944 (2009).

[7] F. Schulz et al., *Phys. Rev. B* **89**, 235429 (2014).