

Understanding Single-Atom Imaging, Manipulation And Chemical Identification In Atomic Force Microscopy With First-Principles Simulations

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Force spectroscopic measurements [1] have become a fundamental source of information for unveiling the complex phenomena observed in atomic resolution FM-AFM experiments, such as the atomic contrast in the dissipation signal [2], especially when they are combined with large-scale first principles calculations [2, 3]. In this contribution, we further extend this collaboration between theory and experiment in the analysis of force curves measured with room-temperature force spectroscopy [4] in order to assess two key issues in any tip-based microscopy: chemical recognition and access to the real sample structure.

We show that the short-range (SR) interaction force measured over the different atoms composing a heterogeneous semiconductor surface provides information for atomic identification, even when the detected forces have a notable tip-dependence. Single atom chemical recognition is demonstrated in a situation in which a discrimination based solely on topographic measurements would be impossible to achieve.

Our theoretical approach, based on a simple analytic model that combines the relevant chemical interaction between the outermost tip-apex atom and the closest surface atom as well as the elastic response of tip and surface, provides a clear interpretation of the measured short-range interaction forces. According to this model, the intrinsic strength of the short-range force is determined by the chemical interaction between these two atoms while the tip-surface elasticity properties control the overall curve shape. This analysis provides an explanation for the basic experimental findings used for the chemical recognition: both the relative value at the attractive force minima and the distance between them for a set of curves acquired with the same tip over the different atoms at a surface remains nearly constant.

Finally, combining again force spectroscopy and first-principles calculations, we explain the striking variations in the detected topographic height difference between two atomic species at an heterogeneous surface in terms of both the different strength of the short-range chemical interaction and tip-induced atomic relaxations. Our results suggest that the atomic corrugation measured with FM-AFM at low interaction forces, close to the onset of significant short-range chemical interactions, and with tips showing no dissipation signal [2], provides direct access to the real structure of heterogeneous semiconductor surfaces [3].

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