INTERPRETING SCANNING TUNNELING AND ATOMIC FORCE MICROSCOPY IMAGES

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1. INTRODUCTION

In scanning tunneling microscopy (STM) and atomic force microscopy (AFM) studies, one eventually faces the question of how to interpret the observed images especially when they are in atomic or molecular resolution. In the STM studies of metallic samples, the tip-sample electron transfer typically involves the energy levels of the sample lying in the vicinity of the Fermi level $e_f$. To a first approximation, the STM image is described by the spatial variation of the partial electron density $p(r_0, e_f)$ of the sample [1]. In contact-mode AFM measurements, in which the tip-sample repulsive force is probed, all electrons of the sample atoms are involved in the repulsive interactions with the tip. Therefore, the AFM image is described by the spatial variation of the total electron density $p(r_0)$ of the sample.

For a sample of known geometry, it is straightforward to calculate the partial density plot $p(r_0, e_f)$ from its electronic structure. For a large number of organic and inorganic layered materials, the atomic- and molecular-scale features of their STM images are well explained in terms of the $p(r_0, e_f)$ plots [2] calculated with the extended Hückel tight binding (EHTB) electronic band structure method [3]. These $p(r_0, e_f)$ plot calculations reveal that when the height corrugation of the surface is of the order of 0.5 Å, the lower-lying atoms of the surface can dominate the $p(r_0, e_f)$ plot and hence the STM image. When the sub-surface atoms lie more than 1 Å below the surface atoms, the STM patterns are dominated by the surface atoms even if the energy levels around the Fermi level are dominated by the sub-surface atoms.

To be precise, the $p(r_0, e_f)$ and $p(r_0)$ plots respectively simulate the ideal STM and AFM images expected in the absence of the tip-sample interactions. During the scanning, the force exerted by the tip can induce a surface relaxation according to the variation of the surface local hardness [2,4]. The images recorded under this condition are related to the sample surface possessing the tip-force induced corrugation. In principle, therefore, a
comprehensive analysis of STM and AFM images requires the knowledge of the surface deformation induced by the tip force and the associated change in the electron density plots. In this work, the essential aspects of interpreting STM and AFM images are discussed by analyzing the STM images of 1T-TaSe₂ and NbSe₃ as well as the AFM images of 1T-NbTe₂.

2. METAL-ATOM CLUSTERING AND STM IMAGE OF 1T-TaSe₂

Transition-metal dichalcogenide 1T-MX₂ has layers of composition MX₂, which are constructed from MX₆ octahedra by sharing their edges (Figure 1) [5,6]. In each MX₂ layer, a sheet of metal atoms is sandwiched between two sheets of chalcogen atoms, and the metal atoms of an undistorted MX₂ layer form a hexagonal lattice. 1T-TaSe₂ contains d₁ ions and exhibits a √13 × √13 metal-atom clustering (Figure 2) [7]. The clustering in the metal-atom sheets induces a periodic lattice distortion in the sandwiching chalcogen-atom sheets. The crystal structure of 1T-TaSe₂ [7] shows that the Se(1) atoms are farthest away from the

Figure 1. Schematic projection view of an undistorted 1T-MX₂ layer along the c-axis.

Figure 2. Schematic representation of the three different Ta atoms and five different Se atoms of a √13 × √13 cluster in 1T-TaSe₂. The Ta and Se atoms are presented by small filled and large empty circles, respectively. The Se atoms of the bottom Se atom sheet are not shown for clarity. The lines A and B refer to the planes perpendicular to the layer of 1T-TaSe₂.