Available at www.sciencedirect.com
ScienceDirect
journal homepage: www.elsevier.com/locate/carbon

Scanning tunneling microscopy evidences for surface electron scattering by underlying atoms

Junting Wang [a,b], *Weifeng Ge* [a,b], *Yubin Hou* [a], *Qingyou Lu* [a,b,*]

[a] *High Magnetic Field Laboratory, Chinese Academy of Sciences and University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China*
[b] *Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China*

ARTICLE INFO

Article history:
Received 26 May 2014
Accepted 22 November 2014
Available online 28 November 2014

ABSTRACT

We have used a homebuilt scanning tunneling microscope (STM) to observe an atomically resolved underlying edge dislocation that occurred in the second layer of graphite. It showed evidence of variable interactions between the topmost two layers near the dislocation edge. Through a special thermal process, we will further demonstrate a variety of STM features scanned near grain boundaries. A collective interference model was proposed to explain these features. It views an STM image as the interference result of the electron waves in the first layer scattered by the potentials that come from the atoms in the first two layers with the second layer contribution being modified by some interlayer interaction factors. This model could correctly simulate all the observed features and revealed that the degree of the interlayer interaction could be quantitatively reflected by the bright-to-dark size ratio of the bright-dark pair at a lattice site. It thus provides a method of quantitatively studying interlayer interactions at the atomic level.

1. Introduction

The surface electronic state is important because of its comparability with theory, its impact on the performance of surface devices, its intimate relationship with bulk properties and especially its direct accessibility by the scanning tunneling microscope (STM). Accordingly, it has been extensively studied by the STM. However, it is still poorly understood how the underlying atoms interplay the surface electronic structure. Even for the materials such as graphite with weak interlayer interactions, the influence of the underlying atoms on the STM image is not well interpreted. It has long been believed that the triangle lattice structure of the graphite STM image is related to the impact of the α-site atoms in the underlying layer [1]. However, a quantitative study of how the graphite image varies as a function of the interlayer interaction strength is missing. As a result, there has been a long time argument on why both honeycomb and triangle lattices can coexist in a graphite image [2]. Up to recent times, the controversial explanations of this issue mainly include: tip artifacts [3], top layer sliding [4–6], and tip-sample interaction [7–8].

It is not easy to settle the controversies unambiguously; doing so requires scanning a special graphite surface structure in which the interlayer interaction strength varies continuously at atomic scale. In this paper, we present the STM image of an edge dislocation in the second layer (EDSL) of graphite where the imaged periodicity is not distorted across the

* *Corresponding author at:* High Magnetic Field Laboratory, Chinese Academy of Sciences and University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China.
E-mail address: qxl@ustc.edu.cn (Q. Lu).
http://dx.doi.org/10.1016/j.carbon.2014.11.046
0008-6223/

entire dislocation zone. This is the first report on imaging an atomically resolved EDSL in real space, which is itself important in both crystallography and scanning tunneling microscopy. It provides a circumstance where the spacing between the first two layers varies continuously across the edge dislocation (see Fig. 1(a)). Indeed, both the upper and lower reaches show the normal triangle lattice except the middle of the transition zone, which show the honeycomb structure. This is direct evidence that the honeycomb structure is due to the reduced interlayer interaction.

In addition, we will present quantitative studies on how the underlying atoms with various interlayer interactions impact the surface electronic state. We will first show how we thermally process the highly oriented pyrolytic graphite (HOPG) to create high-density of surface defects and report rich and distinctive local electronic structures in the STM images scanned near these defects using a homebuilt high-quality STM. To explain these features, we will introduce a collective interference model. It considers all atoms in the topmost two layers (not just the surface atoms [9–10]) as the scattering potentials with appropriate impact factors for the underlying atoms. The model can correctly simulate all the measured images and further predicts the “O-ring” superstructure which is also experimentally observed near a grain boundary (GB). It thus provides a method of studying interlayer interactions with an STM.

2. Experimental

To prepare the HOPG sample, it was first cleaved in air by tape and then heated at 400 K in the load-lock chamber (6×10^{-6} torr) for 72 h. It was then cooled down to room temperature naturally. The processed HOPG sample was loaded onto the STM in the main chamber (3×10^{-9} torr). Even though 400 K is far below the melting point of graphite, it is equivalent to about 34.5 meV lattice energy which is above graphite’s interlayer binding energy both in experiment (31 ± 2 meV) [11] and theoretical calculation (24 meV) [12]. Therefore, this heat treatment could change or impact the interlayer interactions, especially near energetic defects like GBs. As a result, rich features can be seen in the STM images near the GBs due to variable interlayer interactions in this paper.

The sample was scanned under constant height mode at room temperature, whose superior imaging quality comes from a unique scan head in which the tiny scanner is completely separated mechanically from the driving piezo motor after the coarse approach by means of slightly retreating the sliding piece of the inertial piezo motor [13]. The tip

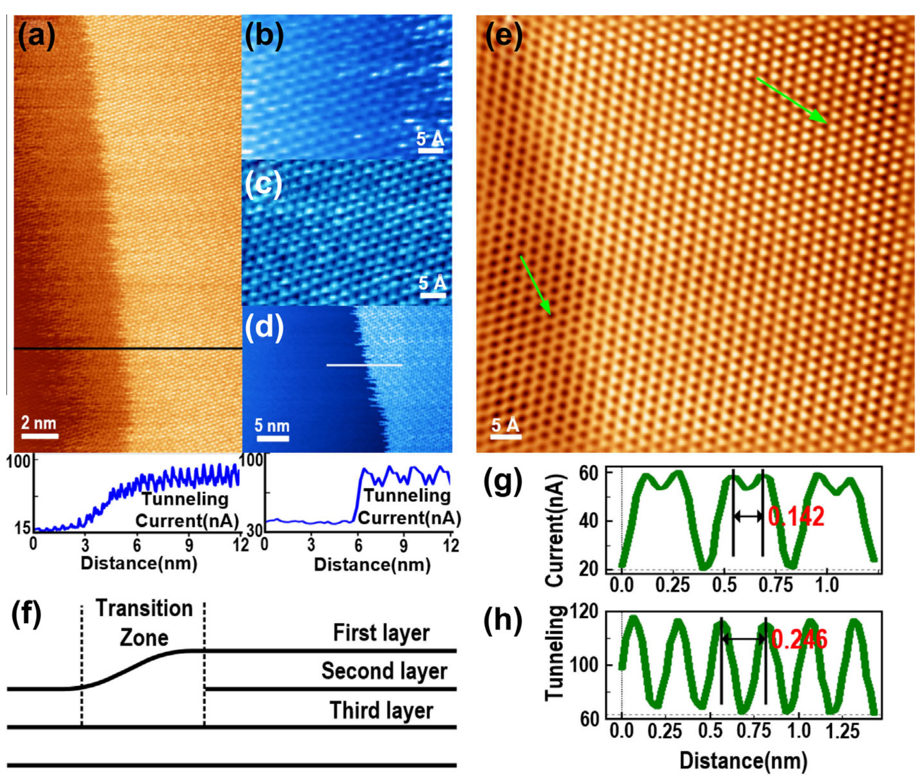

Fig. 1 – (a) Large area STM image across an edge dislocation in the second layer (EDSL), in which the transition zone is marked by the two dashed lines in (f). The profile shows the tunneling current across the transition zone. (b) A zoom-in of the lower reaches of (a) showing a triangle lattice structure (normal graphite image) which is the same as that in the upper reaches (c). (d) A surface step where there is no transition zone. The profile shows the tunneling current with a sudden jump across the step. (e) A zoom-in scan of the EDSL. (f) The side view of the EDSL. (g) Profile along the left arrow in (e) (in the transition zone) showing honeycomb characteristic. (h) Profile along the right arrow in (e) (in the upper reaches) showing the normal graphite characteristic. The tunneling current ranges for (a)–(e) were: 0–120 nA, 16–40 nA, 59–100 nA, 33–97 nA, 10–130 nA. (A color version of this figure can be viewed online.)