Probing Crystallography-induced Anisotropy and Periodic Property of Atomic Friction in MoS2 via Fast Fourier Transform Processing

Meng Li1,2, Lianqing Liu1,*, Niandong Jiao1, Peng Yu1, Ning Xi1,Yuechao Wang1
1State Key Laboratory of Robotics, Shenyang Institute of Automation, Chinese Academy of Sciences, Shenyang 110016, China
2University of Chinese Academy of Sciences, Beijing 100049, China
lqliu@sia.cn

Abstract—An theoretical and experimental study on friction anisotropy and 120 degree periodicity variation in atomic friction of MoS2 is presented in this paper. To clearly clarify these properties, fast Fourier transform(FFT) is utilized by Matlab software to perform the frequency variation of the actual friction signal wave acquired from the lateral friction experiment. Characteristic of the computed frequency ratios periodically varying with lattice orientation is clearly observed and well explained in terms of the periodical variation in atomic friction. The consistency between the theoretical analysis and experimental result ultimately verify the validity of the assumption. The discovery of this paper promises future application in real-time crystallographic orientation detecting.

Keywords—MoS2, crystallography-induced anisotropy, periodic property

I. INTRODUCTION

Recent advances in two-dimensional (2D) nanomaterial has triggered significant attention to its possible application in next-generation nanodevices. Graphene, a high-potential 2D material, exhibits outstanding electric and optical properties compared to its bulk counterpart [1–4]. Unfortunately, its future development in semiconducting devices has been greatly hindered due to the lack of bandgap [5, 6]. Many strategies, therefore, have been employed to overcome this obstacle: open up the bandgap [7, 8] or find an ideal substitute with intrinsic bandgap.

Molybdenum disulfide (MoS2), one kind of transition metal dichalcogenides, is currently being explored as a promising material due to its large intrinsic bandgap [9–11]. Theoretical studies have showed the physical properties of MoS2 closely rely on its chirality [12, 13]: Zigzag edges of monolayer MoS2 and other transition-metal (TM) dichalcogenides are experimentally shown to exhibit strong photoluminescence [14]; Zigzag nanoribbon has spin-dependent conductance [15], whereas the armchair nanoribbon was nonmagnetic and semiconducting [16]; Armchair nanotube has a higher Young’s modulus and Poisson ratio than its zigzag counterpart [17]. In view of the distinctive properties in different lattice orientation, it is critically important to develop an effective technical measure to detect the lattice orientation. To date, polarization dependent Raman spectroscopy [18] and optical second-harmonic generation (SHG) [19] have been utilized to study the crystallographic orientation of MoS2. Nevertheless, these methods either require complicated experimental process or simply reflect the symmetry of the lattice. Moreover, research on friction anisotropy and periodic property of MoS2, which are essential for the research on the lattice orientation have not been found in relevant literature.

The presented study in our paper endeavors to fill the blank in this field. We initially carry out the simulation of friction in various lattice orientation based on the established friction model. Experiment on the lateral friction force is subsequently performed by the technique of lateral force microscopy (LFM). To better demonstrate friction anisotropy and periodic property, fast Fourier transform is adopted to facilitate the analysis and eliminate the external disturbances. The satisfactory agreement between the simulation results and actual friction waves verify the validity of the modeling and ultimately confirmed the periodic property. The comprehensive investigation on the friction anisotropy is expected to pave the way for the realization of a more convenient real-time crystallographic orientation detecting system.

II. THEORY AND SIMULATION

A. Theoretical analysis

MoS2 crystal can be envisioned as a sandwich-like slab, in which Mo and S atoms are hexagonally packed into a trigonal prism [20]. In lateral friction experiment, stick-slip movement will occur between the tip and MoS2 surface according to relevant literature. Then the tip will shuttle between the upper layer, S layer and lower layer, Mo layer. After undertaking a careful analysis of the distinctive structure, depicted in Fig.1, we discover that the atomic configuration varies with the rotating angle of the tip and surroundings of the tip resume to the original state whenever it rotates 120 degree. Thus we firstly envisage that the periodic variation of geometrical position is 120 degree when the tip moves on the surface of MoS2.
To derive the relationship between lattice orientation and friction force, a two-dimension Tomlinson model [21] is necessary:

\[ m_x \ddot{x}_t = k_x (x_M - x_t) - \frac{\partial V(x_t, y_t)}{\partial x_t} - \gamma_x \dot{x}_t \]
\[ m_y \ddot{y}_t = k_y (y_M - y_t) - \frac{\partial V(x_t, y_t)}{\partial y_t} - \gamma_y \dot{y}_t \]  

(1)

Where \( x_t, y_t \) are the actual position of tip at particular time, \( x_M, y_M \) are the equilibrium position of the tip without potential, \( m_x, m_y \) are the effective mass, \( k_x, k_y \) are the elasticity of the tip, and \( \gamma_x, \gamma_y \) are the damping constant of the system.

Furthermore, the interaction potential of MoS2 for all the lattice orientation is needed. According to the analysis regarding the trajectory of the tip on zigzag and armchair orientation we introduced before [22], we assume the interaction potential for zigzag orientation is applicable for other general lattice orientation, such as 10°, 20°, 30°, 40°, 70°, etc.

Zigzag:

\[ V(x_t, y_t) = V_0 \cos \left( \frac{2\pi}{R} x_t \right) \cos \left( \frac{2\pi}{R} y_t \right) \]  

(2)

Where \( x_t, y_t \) are the actual position of tip and also contain the angle of the tip, that is the specific lattice orientation. Notably, when the lattice orientation is 90°, or a specific armchair type, the equation has to be modified considering the particularity of cosine function (cos 90° = 0). Then the interaction potential of MoS2 in all the lattice orientation can be extended as follows:

Lattice orientation except 90°:

\[ V(x_t, y_t) = V_0 \cos \left( \frac{2\pi}{R} x_t \right) \cos \left( \frac{2\pi}{R} y_t \right) \]  

(3)

Lattice orientation is 90°:

\[ V(x_t, y_t) = V_0 \frac{2\pi}{R} x_t \cos \left( \frac{2\pi}{R} y_t \right) \]  

(4)

B. Simulation

According to the theoretical analysis in the previous section, the simulation of lateral force friction in various lattice orientation can be performed with the utilization of Matlab software. To ensure the comprehensiveness of the research, the simulation is carried out every 10 degree in the case of 0 to 110 degree and 120 to 230 degree respectively. Fig.2(a) and Fig.2(b) denote the shapes of the friction wave in the two periods, varying in terms of the lattice orientation. Through the comparison between these simulation results, the roughly identified wave shapes can be observed. Especially in some particular angles, 0°, 30°, 60°, 90° and 120°, 150°, 180°, 210°, the strong resemblance in the wave shapes can be directly observed. Even in other general angles, the slight disparity between the friction waves of the two periods are negligible. Therefore, previous assumption about 120 degree periodical variation can be theoretically confirmed from the comparison of the waves in two periods.

(a) Simulation results of the atomic friction in the first period.
(b) Simulation results of the atomic friction in the second period.

III. MATERIAL AND METHOD

A. Preparation and characterization of MoS2

Molybdenum disulfide (MoS2) bulk sample was purchased from Nanjing XF Nano Materials Technology Company (Nanjing, China. http://www.xfnano.com/). A large numbers of Multilayer MoS2 flakes was obtained by micromechanical cleavage technique and then deposited onto a prepared silicon wafer, which can be identified by HIROX microscope, circled in red in Fig.3(a). Additionally, high resolution tapping mode AFM 3100 instrument was used to confirm the height, size and flatness of the sample we observed through optical microscopy. As shown in Fig.3(b), the samples are around 5*1μm, 9nm in height, respectively.
Friction force measurements were performed on a Digital instrument Multimode Nanoscope AFM in air under ambient conditions (30%-57% relative humidity, 20°C-50°C). Then atomic friction were measured within 10nm scale and the corresponding raw atomic resolution images were obtained and presented in Fig3.(c) . Through the FFT filtering , the lattice structure is shown in Fig 3.(d). With the aid of the lattice structure of MoS2 , we can readily discern the regular distribution of the atomic surface and thereby obtain the friction signal of various lattice orientation.

In order to obtain the direct evidence for the friction anisotropy and periodic property, atomic image of MoS2 is processed by pulling a line along each lattice orientation. For the sake of accuracy, each angle is processed at three different locations of the friction atomic image. As shown in Fig.4, the actual scanning directions in three distinct locations are marked in blue, yellow and green respectively. The white line indicates 0° lattice orientation, then the angle, φ, is the angle between the actual scanning direction and 0° lattice orientation, which remains as a constant in the same friction atomic image.; θ, angle between the red line and white line, is the specific lattice orientation after processed by pulling a line. Then the actual lattice angle is the sum of θ and φ. For comparison purpose, angle θ in each cases.

**B. Fast Fourier Spectrum Transform Analysis**

Unlike the simple analyzing technique adopted for simulation result, straightforward comparison between the actual signal waves in two periods however, is infeasible as the actual friction signals are more prone to be disturbed by the external factors, noise, condition of apparatus and experimental parameters, etc. Hence, appropriate technique should be selected to address this problem.

Fast Fourier transform (FFT), has been proved to be computationally efficient in producing reasonable results for a large class of signal processing [22]. For better displaying the distinction in the actual friction signal waves and eliminate irrelevant external factors that may inevitably affect the normal operation of the experiment, we employ this approach to process all the waves in various lattice orientation obtained from the friction atomic image.

**IV. RESULT AND DISCUSSION**

Following the approach described in previous chapter, twenty-four cases of origin friction signal waves separated by 10 degrees can be obtained, illustrated in Fig.5(a) and(b).
FFT approach, therefore, is employed to process the actual signals of various lattice orientation. Once processed, power spectrum of each lattice orientation can be obtained, as shown in Fig.6(a) and (b), the number of major peaks of the power spectrum diagrams are sorted into table. From the table, it is clear to observe that the number of major peaks of the friction signal wave vary with its lattice orientation. For some special angles, such as 0°, 60°, 120° and 180°, only have one major peak.

| Angle (degree) | Number of the major peaks (Hz) | Angle (degree) | Frequency or Frequency ratio of the major peaks (Hz) | Angle (degree) | Frequency or Frequency ratio of the major peaks (Hz) | Angle (degree) | Frequency or Frequency ratio of the major peaks (Hz) |
|---------------|-------------------------------|---------------|-----------------------------------------------|---------------|-----------------------------------------------|---------------|-----------------------------------------------|
| 0             | 1                             | 60            | 1                                            | 120           | 1                                            | 180           | 1                                            |
| 10            | 3                             | 70            | 3                                            | 130           | 3                                            | 190           | 3                                            |
| 20            | 3                             | 80            | 3                                            | 140           | 3                                            | 200           | 3                                            |
| 30            | 2                             | 90            | 2                                            | 150           | 2                                            | 210           | 2                                            |
| 40            | 3                             | 100           | 3                                            | 160           | 3                                            | 220           | 2                                            |
| 50            | 3                             | 110           | 3                                            | 170           | 3                                            | 230           | 3                                            |

In order to facilitate the analysis, we define frequency ratios as the ratio of the distance for three or two major peaks in each lattice orientation. Two histograms are generated to demonstrate the frequency ratios in various lattice orientation, as shown in Fig. 5(a) and Fig. 5(b). Next, average frequency ratio of each lattice orientation in two periods are summarized in a scatterplot for comparison purposes, as depicted in Fig. 8.

Overall, it is clearly to observe the frequency ratios varying with angle and the nearly identical shapes in two periods significantly verified the periodicity. In this regard, the phenomenon is quite understandable according to the previous analysis on the friction anisotropy and periodic property of atomic friction. Considering the complexity of the experimental conditions in multiple operations, the experimental data always carry with some uncertainties and will unavoidably lead to the bias in various level. Hence, the inconsistence in rare cases is inevitable and irrelevant.

Meanwhile, we notice that the numbers of the major peaks varies with lattice orientation. For instance, 0° and 60° "only have one peak, 30° and 90° have two peaks, while the other angles have three peaks. This peculiarity is also observed in the second period. Rational explanation for this peculiarity is observed in two periods awaits further studied.
experiments provide a solid evidence on the friction relevant experimental data. Both simulations and Fourier Spectrum transform is adopted to process the atomic friction is performed by utilizing Matlab software. Simulation aiming at the variation of the anisotropy and 120 degree periodicity variation in atomic friction of MoS2. Simulation targeting the variation of the anisotropy and periodicity variation of atomic friction in MoS2. Greater insight on the peculiarity of the frequency variation awaits further research.

V. CONCLUSION

In conclusion, we have demonstrated a combined experimental and theoretical study on the friction anisotropy and 120 degree periodicity variation in atomic friction of MoS2. Simulation aiming at the variation of the atomic friction is performed by utilizing Matlab software. Moreover, AFM based experiment is carried out and Fast Fourier Spectrum transform is adopted to process the relevant experimental data. Both simulations and experiments provide a solid evidence on the friction anisotropy and periodicity variation of atomic friction in MoS2. Greater insight on the peculiarity of the frequency variation awaits further research.

REFERENCES

[1] X. Peng, L. Peng, C. Wu, and Y. Xie, “Two dimensional nanomaterials for flexible supercapacitors,” (eng), Chem Soc Rev, vol. 43, no. 10, pp. 3303–3323, 2014.

[2] J. Zhu, K. Sakaushi, G. Clavel, M. Shalom, M. Antonietti, and T.-P. Fellinger, “A general salt-templating method to fabricate vertically aligned graphitic carbon nanosheets and their metal carbide hybrids for superior lithium ion batteries and water splitting,” (eng), J. Am. Chem. Soc, vol. 137, no. 16, pp. 5480–5485, 2015.

[3] C. Soldano, A. Mahmood, and E. Dujardin, “Production, properties and potential of graphene,” Carbon, vol. 48, no. 8, pp. 2127–2150, 2010.

[4] H. Wang and Y. H. Hu, “Graphene as a counter electrode material for dye-sensitized solar cells,” Energy Environ. Sci, vol. 5, no. 8, p. 8182, 2012.

[5] K.-T. Lam and J. Guo, “Bandgap Engineering in Graphene,” in Graphene Optoelectronics, R. b. M. Yusoff, Ed, Weinheim, Germany: Wiley-VCH Verlag GmbH & Co. KGaA, 2014, pp. 149–166.

[6] D. Zhan, J. X. Yan, Z. H. Ni, L. Sun, L. F. Lai, L. Liu, X. Y. Liu, and Z. X. Shen, “Bandgap-opened bilayer graphene approached by asymmetrical intercalation of trilayer graphene,” (eng), Small, vol. 11, no. 9-10, pp. 1177–1182, 2015.

[7] Y.-C. Chen, T. Cao, C. Chen, Z. Pedramrazi, D. Haberer, D. G. de Oteyza, F. R. Fischer, S. G. Louie, and M. F. Crommie, “Molecular bandgap engineering of bottom-up synthesized graphene nanoribbon heterojunctions,” (eng), Nat Nanotechnol, vol. 10, no. 2, pp. 156–160, 2015.

[8] Z. G. Yu and Y.-W. Zhang, “Band gap engineering of graphene with inter-layer embedded BN: From first principles calculations,” Diamond and Related Materials, vol. 54, pp. 103–108, 2015.

[9] D. Lemke, S. Bertolazzi, and A. Kis, “Single-layer MoS2 electronics,” (eng), Acc. Chem. Res, vol. 48, no. 1, pp. 100–110, 2015.