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Nano-scale stripe structures on FeTe observed by low-temperature STM/STS

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Abstract

We have investigated the nano-scale stripe structures on a parent compound of the iron chalcogenide superconductor Fe$_{1-x}$Te ($d$=0.033) by using low-temperature scanning tunneling microscopy (STM). The STM topographies and the $dV/dI$ maps show clear stripe structures with the period of twice as large as the Te-Te atomic displacement ($\sim$0.76 nm $\sim 2a_0$, $a_0$ is lattice constant), in addition to weak modulation with the same period of lattice constant ($\sim$0.38 nm). The bias-voltage dependence of both STM topographies and $dV/dI$ maps show the several kinds of the stripe structures. The $2a_0$ modulations are similar to the biquadratic spin order of the parent compound FeTe, indicating the possibility of the coupling with spin density wave and electronic structures.

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1. Introduction

Recently discovered iron-based superconductors [1] have been giving a great impact in its highest critical temperature $T_c$ of $\sim$ 55 K, which is the highest value among the non-cuprate superconductors. The materials of the simplest crystal structure among Fe-based superconductors are the iron-chalcogenide compounds (the 11-type) [2]. These 11-type superconductors have no charge reservoir layer, hence, the electronic properties including superconductivity are tunable by modifying the lattice structures such as the replacement of chalcogen elements and/or applying the high pressure. The parent compound Fe$_{1-x}$Te of 11-type superconductor has the biquadratic antiferromagnetic order along the 45 degrees away from the Fe-Fe square network as shown in the schematic view of Fig. 1(a) [3,4]. The superconductivity would occur after the destruction of the magnetic order by certain amount of doping. Therefore, it is important to investigate these parent compounds with the microscopic scale because the nano-scale features at the superconducting - nonsuperconducting phase boundary may provide us how the superconductivity relates magnetism of parent compounds. In this paper, we show the STM/STS observation on a parent compound of the iron chalcogenide superconductor, Fe$_{1-x}$Te, including the nano-scale stripe modulations.

2. Experimental

The single crystals of Fe$_{1-x}$Te were synthesized by a self-flux method using the double-sealed quartz tubes with the use of Fe (99.9%) and Te (99.99%) powders [5]. The actual composition of the crystal measured by electron probe micro analyzer (EPMA) is Fe$_{1.03}$Te ($d$=0.033). The temperature dependence of the resistivity shows the noticeable drop at $T$=72 K, which is related to the structural and magnetic phase transitions. The STM apparatus used in this experiment is a modified Omicron LT-UHV-STM system [6,7]. The sample was cleaved in situ at $T$ = 77 K in an...
ultra-high vacuum chamber of $\sim 10^{-8}$ Pa to obtain unaffected crystal surface. The Pt/Ir tip was cleaned by high-voltage field emission process with Au single crystal target before the scanning operation. The all STM/STS measurements were carried out at $T = 4.9$ K under condition of $\sim 10^{-8}$ Pa evacuated by ion pump. Before the STM observation, the measurement of the local barrier height (work-function) by the tunnelling current $(I)$ – tip-sample distance $(z)$ method [6] was done and it showed high enough barrier height, $\phi \sim 5.1$ eV, indicating that the tunnel conditions are good enough to ensure the atomic resolution. A constant-current mode was adopted to obtain the STM images. The $dI/dV$ curves were obtained by numerical differentiation of the measured $I–V$ characteristics with the interval of $\sim 0.12$ nm.

3. Results and discussion

Figure 1(b) shows a typical STM topography of the cleaved Fe$_{1-x}$Te surface with the sample bias voltage of $V = -30$ mV at 4.9 K. The image shows regular atomic arrangement together with the large bright spots. The regular atomic structure is considered to be due to topmost chalcogen atom Te, which had been discussed in previous reports [5,8,9]. The period of the regular atomic arrangement along the $a$-axis direction is about $\approx 0.38$ nm, which is consistent with the Te-Te atomic length that corresponds to the previously reported lattice constant $d_0 \approx 0.38$ nm [4]. (The $b$ axis length is slightly smaller than $a$-axis.) On the other hand, the large bright spots are considered as the position of excess Fe. The average rate of these large bright spots from various STM topographies on this specimen was approximately $\sim 0.31 \; (1/\mathrm{nm}^2)$ i.e., about 4% of the unit-cell, which is good agreement with the EPMA results of excess iron, 3.3% of the unit-cell. Furthermore, the most characteristic feature in this STM topography is that there are the alternate bright streak (chain) patterns running along the vertical direction, which are indicated by dashed lines in Fig. 1(b). This pattern modulates along the $a$-axis direction and forms the stripe structure with the period of $\approx 0.76$ nm, two-times of $a$-axis constant $2d_0$. It is noted that this period corresponds to that of the bi-collinear spin order of diagonal direction to Fe-Fe network, as shown in the schematic model of Fig. 1(a).

In order to examine the properties of these stripe structures, the STM topographies are shown in Fig. 2(a) - (f) with various $V = -200$ mV to $+200$ mV. The $2d_0$ stripe structures are clearly visible at the bias voltage from $-30$ mV to $+200$ mV among the basic atomic corrugation and large bright spots, while they are not clear at $V = -200$ mV and $-100$ mV. To exhibit the details of the morphology of these stripe structures, the cross sectional profiles of the topographies visualized from dashed squares are shown in Fig. 3(a). These curves show the atomic corrugations and the $2d_0$ stripe structures. However, the shapes of these structures vary with the bias voltages. At the bias voltages of $\pm 200$ mV to $\pm 30$ mV, the $2d_0$ stripe structures are formed by the combined two neighbouring atoms, while the only one (left) -

![Fig. 1](https://via.placeholder.com/150)

![Fig. 2](https://via.placeholder.com/150)
side atom is enhanced at \( V = -30 \text{ mV} \) (enhanced atomic side positions are depicted with vertical dashed lines in Fig. 3(a)). At \( V = -100 \text{ mV} \), there are no clear \( 2a_0 \) streak modulation patterns and only the regular atomic corrugation (or \( a_0 \) streak modulation) is visible, then, the \( 2a_0 \) stripe was slightly recovered at \( V = -200 \text{ mV} \). The two-dimensional first Fourier transformation (FFT) power spectrum images are shown in the inset of Fig. 2. This gives additional information of the spatial frequency of the surface structures. In the FFT images, two kinds of the basic peaks, \( q_1 \) peaks (\( a \)-axis Bragg peak) and \( q_2 \) peaks (\( b \)-axis Bragg peak) are commonly recognised in all bias voltages, which are representatively indicated by the circles in Fig. 2(f). At the bias range from \(-30 \text{ mV} \) to \(+200 \text{ mV} \) (Fig. 2(c)-(f)), the \( q_{1/2} \) spots corresponding to the \( 2a_0 \) stripe modulation are clearly seen (indicated by red-dashed circles), while they are not recognised at the bias voltage of \(-200 \text{ mV} \) and \(-100 \text{ mV} \) (Fig. 2(a) and (b)). To demonstrate the variation of \( q_1 \) and \( q_{1/2} \) peaks, the line-cut of the \( q_1 \) direction in FFT images (indicated by black arrow in Fig. 2(f)) are shown in Fig. 3(b), together with the plot of the magnitude of \( q_1 \) and \( q_{1/2} \) peak heights at each voltage in the inset. The \( q_1 \) Bragg peak is persistently observed with all bias voltages. The intensive \( q_{1/2} \) peak found at \( V = -30 \text{ mV} \) becomes quite low at \( V = -200 \text{ mV} \) and \(-100 \text{ mV} \). At the positive bias voltages, the \( q_{1/2} \) peaks were continuously observed up to \( V = +200 \text{ mV} \). These results together with the variation of the topographic shapes show that the feature of the modulation changes around \( V = -30 \text{ mV} \) and \(-100 \text{ mV} \). The details will be discussed later.

Generally, an STM topography shows the convolution of the surface morphology and the integration of the local density of states (LDOS). Therefore, to obtain the real features of the surface electronic structures with various bias voltages, the measurements of \( dI/dV \) spectrum, which is proportional to the LDOS, were carried out. Fig. 4(a) and (b) show the \( dI/dV \) map at \( V = 0 \text{ mV} \) and the line profiles of \( dI/dV \) along the dashed arrow in Fig. 4(a), respectively. In the \( dI/dV \) map, the stripe structure, which corresponds to that of observed in the topographies, were clearly observed. Such \( dI/dV \) maps were obtained in all the bias ranges of \( |V| < 150 \text{ mV} \). In the \( dI/dV \) curves in Fig 4 (b), the spatial corrugations originated from the stripe structures were recognised among the regular \( V \)-shaped back ground especially at the bias range from \(-30 \text{ mV} \) to \(+150 \text{ mV} \). Fig. 4(c) shows the FFT image of the \( dI/dV \) map of Fig. 4(a). The relatively-higher FFT peaks of \( q_{1/2} \), corresponding to the spatial period of \(-0.76 \text{ nm} = 2a_0 \), are clearly seen, which is indicated by red circles in Fig. 4(c). The small peaks of \( q_1 \) are also visible while the \( q_2 \) peaks are quite low. The bias dependence of the peaks of \( q_{1/2} \) and \( q_1 \) are shown in Fig. 4(d), together with the data from that of the topographies in Fig. 3(b). In Fig. 4(d), the \( q_{1/2} \) signal shows significant asymmetric features with respect to the bias polarity, i.e., quite low signal level (nearly background level) at the negative bias of \(-30 \text{ mV} \) \(-100 \text{ mV} \), while it shows high signal level with monotonically increasing intensity with the increase of positive bias. Furthermore, there are small peak and dip around the zero bias. From the \( q_{1/2} \) intensity of Fig. 4(d) and shape of streak pattern in Fig 3(a), the observed bias range \((-150 \text{ mV} < V < +150 \text{ mV} \) can be divided into four different types of the modulation as shown by A - D in Fig.
In the region A ($V<-100\text{mV}$), very weak $2a_0$ stripe structure is shown in a moderate background. In the region B ($-100\text{mV}<V<-30\text{mV}$), only the weak $a_0$ stripe modulation is visible and there are no apparent $2a_0$ structures. It is noted that the $a_0$ modulation was also observed by other groups in the wider energy range [9]. In the region C ($-30\text{mV}<V<-10\text{mV}$), the strong $2a_0$ stripes are observed as the asymmetric double-peaked streak patterns. Finally, in the region D ($V>-10\text{mV}$), there are $2a_0$ stripes with double-peaked shallower hump structures.

The origin of the bias-dependent stripe structures is unclear at present. However, it is possible to consider that these streak patterns are due to the charge density wave (CDW) formation. In fact, the STM observation of the conventional CDW compound such as NbSe$_2$ [10] showed the bias dependent modulation, which is related to the properties of the CDW gap and the band structures. It is difficult to explain the $2a_0$ stripe structures by inter-band nesting because the band structures from the band calculation [11] as well as the angle-resolved photoemission spectroscopy (ARPES) [12] on Fe$_{1+\delta}$Te show mainly ($\pi$, 0) scattering, which is 45 degree away from our observed modulation direction (diagonal direction to the Fe-Fe network, ($\pi/2$, $\pi/2$)). It is generally considered that all Fe (or Te) atoms in FeTe are basically equivalent in terms of charge property. However, the asymmetric double-peaked streak patterns seen in the region C mean that one specific atomic site is enhanced that possesses the different electronic states from other neighboring sites. Therefore, there exist some origins of forming such non-equivalent atomic circumstances. One of the possible candidates for such origins is due to the spin structures of Fe-Fe network. As mentioned above, the period of $2a_0$ corresponds to that of the bi-collinear spin order of diagonal direction to Fe-Fe network, as shown in Fig. 1(a). The neutron scattering study suggested the commensurate ($\pi/2$, $\pi/2$) magnetic order in monoclinic Fe$_{1.08}$Te and the tunable magnetic order by varying the excess Fe in orthorhombic Fe$_{1.4}$Te. Taking into account the rate of the excess Fe of our observed specimen $d=0.033$, the observed results may reflect the commensurate ($\pi/2$, $\pi/2$) magnetic order of monoclinic lattice. It is unknown how the spin order is coupling with the charge order at present. For the conventional-monodomain spin density wave (SDW) state, the momentum of the CDW modulation is twice as short as that of SDW and indistinguishable from the lattice period ($-q_g$). However, recent theoretical studies predicted that the multidomain SDW, which would be induced by defects and/or strain in practical compounds, could produce the distinguishable CDW signatures of variable periods in Fe based superconductors [13]. Our results were not inconsistent with these predictions by concerning such conditions. Further STM/STS measurements of the various excess-Fe compounds may lead us to understand these phenomena.

4. Summary

The STM observation on the parent compound of the iron chalcogenide superconductors Fe$_{1+\delta}$Te has been carried out. The STM topographies and the $dV/dI$ maps show clear stripe structures with the period of $2a_0=0.76$ nm. The bias-voltage dependence of both STM topographies and $dV/dI$ maps shows several kinds of the stripe modulations. These structures are similar to the biconicalline spin order of the parent compound FeTe, indicating a possible coupling between the magnetism and electronic states.

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