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Scanning Tunnelling Microscopy/Spectroscopy and Low-Energy Electron Diffraction Investigations of GaTe Layered Crystal Cleavage Surface

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Scanning tunnelling microscopy and spectroscopy (STM/STS) and low-energy electron diffraction (LEED) techniques are used in combination to study the surface structure of GaTe cleavages. Two different structures, hexagonal one on macroscale and monoclinic one randomly distributed on nanoscale, are identified on the crystal cleavage surface. The hexagonal unit cell parameters, $a = b \cong 4.08$ Å, $c \cong 16$ Å, determined by STM are in a good agreement with the bulk ones and, besides, with planar parameters a, b obtained using LEED. The monoclinic unit cell parameters, $a \cong 24$ Å, $b \cong 4$ Å, $c \cong 10$ Å, are consistent with ones of the known monoclinic modifications. LEED and STS data indicate that the GaTe surface is not flat, but is characterized by a well-developed staircase structure formed by cleavage. As concluded, the possibility of partial on-nanoscale reconstruction of base hexagonal structure to the monoclinic one is directly related to the number of surface defects such as loosely arranged steps of one single Te–Ga–Ga–Te packet height.

За допомогою комплексу метод сканівної тунельної мікроскопії та спектроскопії (СТМ/СТС) і дифракції повільних електронів (ДПЕ) досліджено структуру поверхонь сколювання кристалів GaTe. Встановлено існування двох різних структур на поверхні сколювання кристалу: гексагональної в макромасштабі і моноклінної, яка є випадковим чином розподіленою на поверхні в наномасштабі. Параметри гексагональної ґратниці $a = b \cong$ $\cong 4{,}08$ Å, $c \cong 16$ Å, яких одержано за допомогою СТМ, добре узгоджуються з даними для об'єму кристалу, а також із параметрами a, b для поверхні кристалу, одержаними з використанням ДПЕ. Параметри моноклінної ґратниці $a \cong 24$ Å, $b \cong 4$ Å, $c \cong 10$ Å є такими ж, як і для однієї з відомих моноклінних структурних модифікацій. Відповідно до результатів, одержа-

них за допомогою ДПЕ і СТС, встановлено, що поверхня GaTe не є пласкою і характеризується наявністю добре розвиненої східчастої структури, яка утворюється внаслідок сколювання кристалу. Зроблено висновок про те, що можливість локальної в наномасштабі реконструкції базової гексагональної структури в моноклінну пов'язана з кількістю поверхневих дефектів, таких, як довільно розміщені сходинки з висотою, що дорівнює товщині одного пакета Te–Ga–Ga–Te.

С помощью комплекса методов сканирующей туннельной микроскопии и спектроскопии (СТМ/СТС), а также дифракции медленных электронов (ДМЭ) исследована структура поверхностей скалывания кристаллов GaTe. Установлено существование двух различных структур на поверхности скалывания кристалла: гексагональной в макромасштабе и моноклинной, которая случайным образом распределена по поверхности в наномасштабе. Параметры гексагональной решётки $a = b \cong 4{,}08$ Å, $c \cong 16$ Å, полученные с помощью СТМ, хорошо согласуются с данными для объёма кристалла, а также с параметрами a, b для поверхности кристалла, полученными с использованием ДМЭ. Параметры моноклинной решётки $a \cong 24$ Å, $b \cong 4$ Å, $c \cong 10$ Å — такие же, как и в одной из известных моноклинных структурных модификаций. Согласно результатам, полученным с помощью ДМЭ и СТС, установлено, что поверхность GaTe не является плоской и характеризуется наличием хорошо развитой ступенчатой структуры, которая образуется в результате скалывания кристалла. Сделано заключение о том, что возможность локальной в наномасштабе реконструкции базовой гексагональной структуры в моноклинную связана с количеством поверхностных дефектов, таких, как случайно расположенные ступеньки с высотой, которая равняется толщине одного пакета Te–Ga–Ga–Te.

Key words: gallium telluride, layered crystal, scanning tunnelling microscopy, scanning tunnelling spectroscopy, low-energy electron diffraction.

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1. INTRODUCTION

Gallium telluride semiconductor crystal belongs to the layered III–VI group chalcogenides and has been characterized for a long time [1–3]. It is known that these crystals exhibit anisotropic properties [4]. Moreover, the results of structural studies of bulk GaTe crystal indicate the presence of hexagonal and monoclinic structural modifications. The latter one is characterized by a rather wide variety of values of lattice constant. At least, one hexagonal phase of GaTe with unit cell parameters of $a = b = 4.06$ Å, $c = 16.96$ Å [1, 3] and several monoclinic phases of $a = 23.64$ Å, $b = 4.077$ Å, $c = 10.46$ Å, $\gamma = 134.47°$; $a = 17.45$ Å, $b = 10.47$ Å, $c = 4.09$ Å, $\gamma = 104.5°$; $a = 17.34$ Å, $b = 4.06$ Å, $c = 10.61$ Å, $\gamma = 104.44°$ [3, 5] have previously been reported. The results of GaTe thin-film studies are interesting for their model representations of the

structural hexagonal–monoclinic transformations [2].

It is well known that GaTe differs from other III–VI group chalcogenides of similar chemical compositions, such as GaS, GaSe, InSe, by a stronger planar anisotropy that characterizes a single layer of GaTe [4]. In fact, apparently, it might result in the possibility of total or partial reconstructions of the cleavage surfaces, which are known not to be typical of layered crystals and, as it was reported, lead to a broad number of structural phases with different lattice parameters.

The basic prerequisites for this GaTe surface study are the following. Firstly, the conclusion contained in the article [3] about the possibility of phase transformation in the bulk crystal from hexagonal to monoclinic one upon grinding a single crystal to powder for XRD powder diffraction analysis. Obviously, this might be due to an increase in the surface-to-bulk ratio, and thus, a surface structure study is essential. However, it should be noted that paper [6] reports on a completely reverse partial structural transformation on the cleavage surface of GaTe crystal. Secondly, the known result of [2] that hexagonal-to-monoclinic phase transformation occurs in the polycrystalline thin films at elevated temperatures.

A variety of existing structural unit cell parameters is reported. Nevertheless, there is lack of 'direct' observation of evident surface phase transformations at the nanoscale by scanning probe methods such as scanning tunnelling microscopy/spectroscopy (STM/STS). The phase state of the GaTe surface is obviously important to characterize the crystal, which is the aim of our study employing the STM/STS and LEED methods.

2. EXPERIMENTAL

The STM/STS data were acquired using the Omicron NanoTechnology STM/AFM System, at room temperature under ultrahigh vacuum (UHV) conditions ($4 \cdot 10^{-9}$ Pa). The STM images were taken in the constant-current mode. Considering the importance of quantitative data obtained in the step height analyses the STM scanner vertical movement was calibrated using commercial (NT-MDT) 6H-SiC test sample with half of lattice constant (0.75 nm) in [0001] direction steps and in situ prepared Si (100) substrate with single atomic steps (height of 0.14 nm). The STM/STS data processing was carried out using the WS&M v.4.0 of Nanotec Electronica [7].

The LEED data were analysed using the SPECS SAFIRE Diffraction Image Acquisition and Processing System for LEED and RHEED. LEED analysis was carried out using incident beam energies 10–150 eV, and spot size less than 1 mm. Heating the sample *in situ* was possible up to 500–600°C.

GaTe single crystals were grown by the Bridgman method. The sam-

ples for the STM/STS and LEED studies had dimensions of $3\times4\times6$ mm^3 and a special shape suitable for multiple cleavage directly before introducing into the vacuum chamber. Previous bulk-structure investigations indicated the hexagonal structure of the studied GaTe crystals with unit cell parameters $a = b \cong 4.06$ Å, $c \cong 16.96$ Å.

3. RESULTS AND DISCUSSION

Recent GaTe crystal cleavage STM observations revealed only a relatively poor-resolution set of sixfold chains composed of clusters with an average size of 6–8 nm [6]. This size of the experimentally observed structures is clearly not associated with the LEED data dimensions given in the same paper. However, a combination of STM and LEED methods is productive in terms of cleavage surface characteristics and structural phase transformations inherent in GaTe crystals. Generally, integral LEED results confirm the crystallographic data obtained by STM on the nanoscale. STM measurements are crucial, particularly, to identify and assign the satellite spots and streaks to coexistent different superstructures, which might be superposed incoherently in the diffraction pattern.

3.1. STM/STS Results

Figure 1, *a* shows a typical 2*D* STM image with a very weak periodic pattern that could potentially be associated with the GaTe crystal lattice order. We were able to obtain such lattice resolution usually for large-scale images, 21×21 nm^2, as shown in Fig. 1, *a*, and a better one for a negative bias. A lot of areas on the different cleavage surfaces were investigated with a view to dropout a 'tunnel version'. It is also important to see that self-correlation filtering pattern (see inset in Fig. 1, *a*) exhibits a good periodicity with the period $a \cong 11.85$ Å. Figure 1, *b* presents known GaTe structural models described elsewhere [2]. Comparison of these models suggests that the surface of the monoclinic phase in general is less smooth than the hexagonal one. It would manifest itself by the characteristic furrows, and therefore can be easier 'captured' in STM studies.

In accordance with the model presented in [2] on conversion of h-GaTe to m-GaTe, the sheets are still parallel to the surface except now the lattice parameters have changed and some geometric features of the layers are different. The localized twist of every third Ga–Ga moiety in the h-GaTe structure occurs on going to m-GaTe. Thus, furrows observed in top and bottom boundary regions in Fig. 1, *a* and confirmed in the self-correlation filtering pattern are the result of such lattice reorganization when the (–201) plane becomes as the surface

one instead of (001).

Figures 1, *c*, *e* show 2.8×2.6 nm^2 and 5.3×4.5 nm^2 fragments, taken within the 'smooth' central and 'furrowed' upper near boundary areas in Fig. 1, *a*, respectively, obtained by 2dFFT filtering. Figure 1, *c* displays honeycomb structure, which is typical for h-GaTe crystal structure [2]; cf. Fig. 1, *g*. Since we are dealing with the surface of the crys-

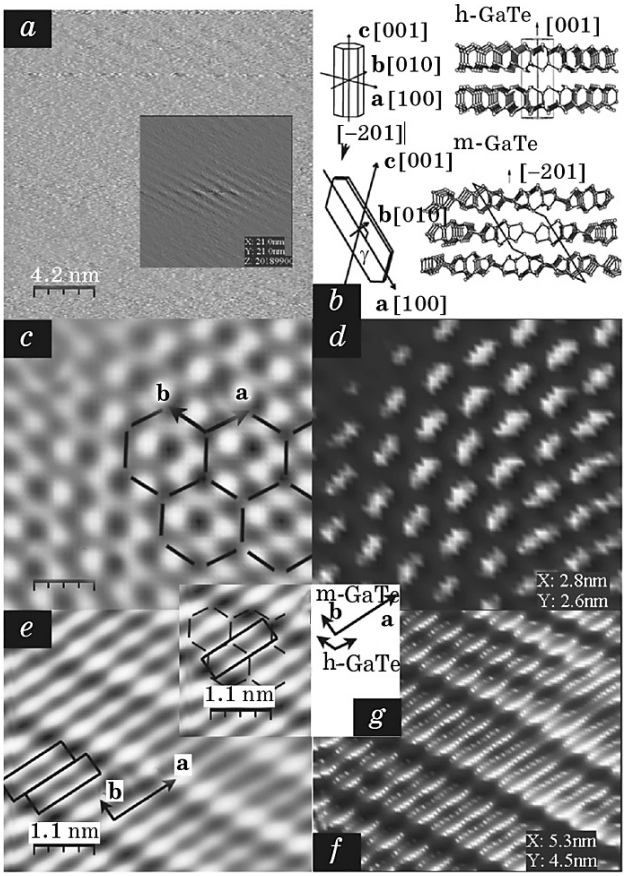


Fig. 1. STM study of GaTe cleavage surface: 21×21 nm^2 2*D* image obtained at –2.3 V bias, 0.122 nA. Inset: self-correlated filtered image (*a*); structural models for GaTe monoclinic m-GaTe and hexagonal h-GaSe or h-GaTe phases [2] (*b*); 2.8×2.6 nm^2 and 5.3×4.5 nm^2 2*D* FFT filtered fragments taken within the 'smooth' central and 'furrowed' upper near boundary areas of (*a*) image (respectively, *c*, *e*), and their corresponding 3*D* visualization (*d*, *f*). The schematic models of the hexagonal and monoclinic GaTe surface unit cells are drawn as guide to the eye. The model hexagons have 4.08 Å length sides. The size of model rectangular is 1.3×0.408 nm^2. Schematic diagram showing the relative directions of unit cells' vectors, **a** and **b**, in the monoclinic and hexagonal GaTe phases (*g*).

tal, which consists of two kinds of atoms, and it is known that the surface is not flat, for better identification of the surface structure, Fig. 1, *d* shows 3*D* image of Fig. 1, *c* represented by the shaded texture, which allows better visualization of hexagonal structure. The presence of hexagonal structure on the surface of GaTe crystal cleavage basically confirms data previously obtained for the bulk of this crystal and as shown below is also confirmed in the LEED study. Analysis of the periodicities observed in Fig. 1, *e*, which actually represents visually 'furrowed' structure in Fig. 1, *a*, suggests the presence of another pattern, that is characteristic in accordance with GaTe structure model representations in [2] for monoclinic GaTe structure. 3*D* visualization of this pattern (see Fig. 1, *g*) clearly illustrates the typical structure of the monoclinic GaTe phase surface, as can be seen in Fig. 1, *b*.

Figures 1 *c*, *e* are supplemented by schematic models of hexagonal and monoclinic unit cells, respectively, that are superimposed on the corresponding structures observed on the surface. The model hexagons have 4.08 Å side lengths. The size of model rectangular is 1.3×0.408 nm^2. However, it should be taken into account that, in fact, the cleavage surface in any of the structural phases is not flat, as can be seen from the Fig. 1, *b*, but, even in this case, there is a good correlation of STM image and relevant unit cells models. Thus, as seen from Figs. 1, *c*, *e* and more strikingly from Figs. 1, *d*, *f*, which are their appropriate 3*D* images, the structure of GaTe surface is not homogeneous even on nanoscale.

The evaluated parameters of 4.08 Å in STM studied hexagonal structure in the surface plane correlate well with lattice constants *a* and *b* of the hexagonal GaTe phase. As for the parameters of the monoclinic structure derived from STM study, the value 0.408 nm is consistent with *b* lattice constant in one of the known monoclinic phases. As for the 1.3 nm periodicity, which apparently does not correlate with any of known bulk structures, it should be noted that the monoclinic unit cell of GaTe, as well as the hexagonal one, consists of two Te–Ga–Ga–Te packets with a different stacking sequence relative to each other (see Fig. 1, *b*). Considering the above, it is possible to estimate the parameter of the monoclinic structure toward the *a* axis, giving a value of 2.6 nm for the GaTe monoclinic lattice parameter. When evaluating a unit cell parameter for the monoclinic structure by STM, it should be also considered a certain angle between [–201] and [100] axes that depends on one or another monoclinic phase. Therefore, we can assume that we were able to identify the monoclinic phase with *a* equal to 23.64 Å.

The schematic diagram showing the relative directions of the surface unit cells **a** and **b** vectors, however, in 'projection' on the certain surface plane, for the monoclinic and hexagonal GaTe phases is presented in Fig. 1, *g*.

The corresponding unit cells models are taken from Figs. 1, *c* and *e* and reduced to a common scale. According to the model representations of h-GaTe towards m-GaTe phase transformation described in [2], two hexagonal cells on the surface are involved in the process of rearrangement into surface monoclinic unit cell. Thus, as mentioned above, the direction and size of the lattice vectors **a** and **b** are changing as it is shown in Fig. 1, *g*.

It should be noted that patterns shown in Figs. 1, *c* and *e* actually obtained for individually selected areas on 'raw' STM image, like Fig. 1, *a*, give reason to believe that we are dealing with two locally distinct 'topographic' structures on the surface of GaTe cleavage, rather than 'electronic' features like local density of states (DOS) oscillation shown by Moiré pattern.

Thus, the detailed STM study of the surface and comparing the obtained distances with known data for bulk structures suggests the coexistence of both hexagonal and monoclinic phase on the surface of the GaTe cleavage, at least on nanoscale.

Another major issue is the possibility of direct observation of not only planar **a** and **b** lattice vectors of GaTe crystal, but also **c** vector which, for the hexagonal structure is normal to the surface plane, and for the monoclinic one does not form normal angles with the plane of the surface (there are several monoclinic structures as mentioned above). For such an STM study, it is important that, besides the difference in the **c** lattice-vector angle relative to the surface plane, the geometric heights of the *h*-GaTe and *m*-GaTe layers are different. Thus, according to the obtained height differences, which can be quite well identified in the vicinity of steps, we succeeded in determining the value of the *c* lattice parameter and, consequently, the structural phase of the surface layer associated with it.

Figures 2, *a*, *d* show 2*D* and 3*D* STM images of rather an elongated step on the GaTe cleavage surface. It should be noted that stepped structure is characteristic of the GaTe crystal cleavage surfaces on macroscale as it will be shown in the LEED study discussed below. Figure 2, *b* shows a typical height profile of the step, which indicates that the average height difference in the vicinity of the step tends to 8 Å. The statistical evaluation of the height differences in the array of image pixels, which could be obtained via standard feature of WS&M application such as that for roughness analysis, is even more reliable. Figure 2, *c* shows a corresponding histogram for height intervals of image pixels in the surface region marked with rectangle in Fig. 2, *a*. It is clear that there is some height distribution of pixels along both sides of the step, which is depicted in Fig. 2, *c* by the 'Bactrian structure', but the actual height difference between the maxima of the distributions is about 8 Å. The above suggests that the monoclinic or hexagonal unit cell of GaTe contains a double Te–Ga–Ga–Te packet. Taking into ac-

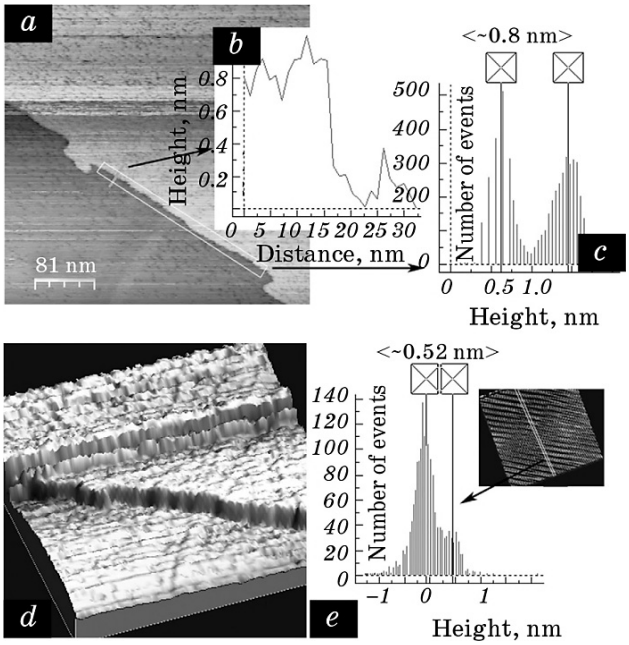


Fig. 2. STM study of the *c* axis unit cell parameter of GaTe crystal: 400×400 nm^2 2*D* (*a*) and 3*D* images (*d*), obtained at 2.3 V bias, 0.303 nA; the subsequent typical height profile indicating the single Te–Ga–Ga–Te packet thickness in hexagonal structure (*b*); height distribution of image pixels obtained from roughness analysis, including both sides in the vicinity of the step as marked with rectangle in Fig. 2, *a* (*c*); height distribution of image pixels obtained from roughness analysis made along the narrow area of Fig. 1, *a* and indicated by inset (only for better visualization the inset shows appropriate 3*D* image of 2*D* FFT filter of Fig. 1, *a*) (*e*).

count the known data on the *c* parameter, we can conclude that have observed a hexagonal structure of the surface layer. Moreover, only individual Te–Ga–Ga–Te packet could form the observed step, because the actual thickness of the GaTe hexagonal packet structure is a multiple of ≅ 8 Å, rather than ≅ 5 Å as would be in the case of a monoclinic one.

The question arises about the nature of the possible partial reconstruction of the hexagonal bulk structure at the GaTe cleavage surface toward the monoclinic one. Thus far, we analysed the height distribution of image pixels along the narrow area that is selected in the central region of Fig. 1, *a*, also by using a roughness analysis tool of WS&M. Such choice of the analysed area is reasonable, since the observed pattern of the central region of Fig. 1, *a* exhibits lack of periodicity, which is inherent in monoclinic structure, while the hexagonal pattern is present. From the obtained height distribution histograms (see Fig. 2, *e*), we were able to identify two characteristic heights sepa-

rated by size of about 5 Å. This value is approximately equal to the typical thickness of a single Te–Ga–Ga–Te packet in the majority of known monoclinic structures, particularly, such as that in Fig. 1.

Consequently, the STM results show that the surface of the crystal cleavage contains local areas of both hexagonal and monoclinic structure, which is indicated by the presence of steps with different heights.

Regarding STS studies of GaTe surfaces, it is known that one of their direct outcomes is the ability to evaluate the energy band gap of semiconductor crystal. However, the obtained value may be characteristic of local points or rectangular regions of the surface, after averaging over some array of points on the nanoscale. It should be noted that local structural inhomogeneity, particularly the steps, could significantly affect the local DOS and, consequently, result in the band gap. Figure 3, *a* shows a typical set of the normalized $(dI/dV)/(I/V) = f(V)$ curves spatially averaged each over an area of 50×50 nm^2. The corresponding STS derived band gap ranges from 1.65 to 1.75 eV.

There are a number of known, but 'integrated' data on GaTe band gap magnitudes obtained by different methods. The values range between 1.65 and 1.7 eV [3, 8, 9] for bulk crystals and between 1.7 and 1.9 eV for GaTe films [2]; and there is evidence of only slight difference in band gap values between monoclinic and hexagonal structures. Our STS data on band gap values (see Fig. 3, *a* and Fig. 3, *b*, curve *2*), obtained for a local nanoscale surface area, correlate well with these data. Thus, the wide apparent band gap, shown as a magnified fragment in Fig. 3, *c*, curve *2*, suggests the absence or a negligible quantity of intrinsic surface states for the fundamental bulk band gap.

Curve *1* in Figure 3, *b* represents the spatially averaged normalized $(dI/dV)/(I/V) = f(V)$ STS spectrum from the averaged electronic structure of the stepped 1×1 μm^2 surface. It is not possible to distinguish spectra of the step edges and the centre of relatively flat areas from each other due to a poor image resolution. However, even the averaged STS spectra from the whole 1×1 μm^2 area give evidence of a significant inhomogeneity of the surface on macroscale. This assertion arises from comparing the zoomed up band gap regions with the normalized dI/dV STS curves averaged over the 1×1 μm^2 and 50×50 nm^2 areas (see Fig. 3, *c*). One could find that the band gap is significantly less for a larger area than the one, which is obtained for a local 50×50 nm^2 surface area and 'narrows' to about 1 eV. Certainly, it must be considered that this effect could arise from the decrease of the transmission coefficient for electron tunnelling with tip/sample separation, leading to a broader range around the zero bias voltage without a detectable tunnel current. However, the actual tip/sample separation for all curves changed only slightly. Thus, so significant differences in the average values of band gap over the studied areas could be explained by availability of significant tails of DOS near the bottom of conduction band and the top of va-

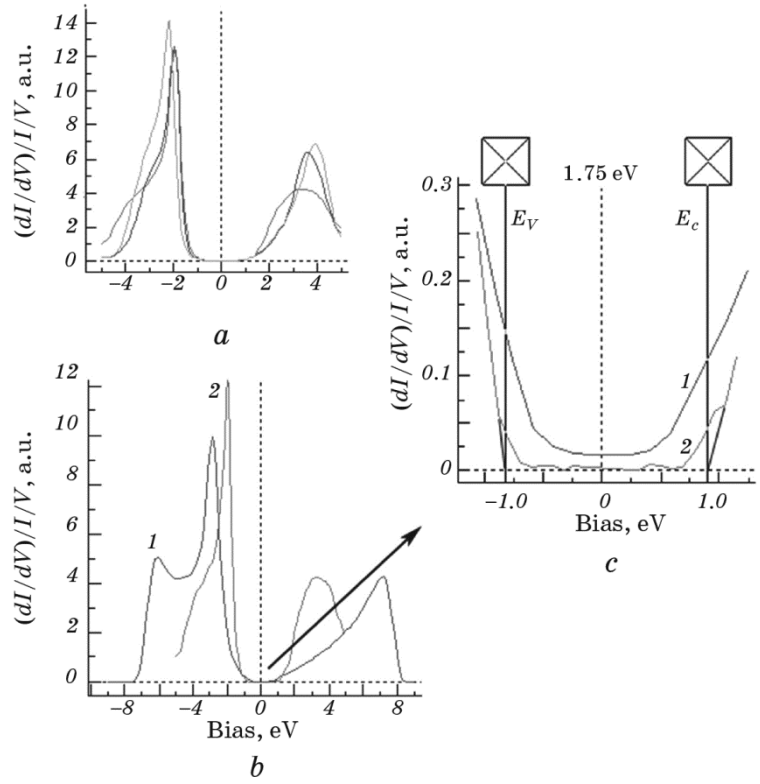


Fig. 3. STS data obtained from the GaTe cleavage given by the normalized $(dI/dV)/(I/V) = f(V)$ curves: STS curves, each one shows the averaged data of 6400 local curves from three different 50×50 nm^2 areas within the relatively large 1×1 μm^2 area, of which an averaged spectrum is given by curve *1* in Fig. 3, *b* (*a*); comparison of averaged STS *1* and *2* curves typical of the large 1×1 μm^2 and small 50×50 nm^2 areas of the surface, respectively (*b*); zoomed up fragment of figure (*b*) showing in detail the region of the GaTe energy gap (*c*).

lence band. Thus, the peculiarities of the local DOS spatial distribution, particularly, in the vicinity of zero bias, are determined by the inhomogeneous distribution of structural defects on the stepped surface of cleavage. The fact that a highly stepped surface provides the major impact on the acquired STS data is also confirmed by our LEED studies of GaTe crystal cleavage.

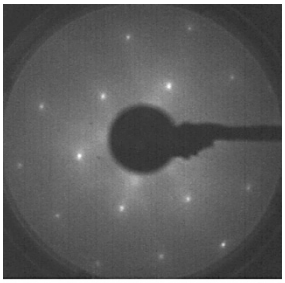
3.2. LEED Results

In order to check the structure of GaTe cleavage surface on the macroscale and get more information about the structures observed by STM on nanoscale, the LEED experiment was performed. Some of the

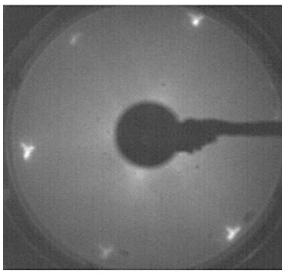
structural periodicities measured by STM are confirmed by diffraction patterns. First of all, the spots of the hexagonal pattern are intense and clearly visible anytime.

Figure 4, *a* shows a typical hexagonal pattern obtained from cleavages, which presents several orders of spots. Diffraction spots indicate a formation of long-range order as concluded from their sharpness. Dimensions of the hexagonal structure lattice vectors, as derived from the reciprocal ones observed in the LEED pattern, are equal to about 4 Å. Thus, they are in accordance with the reported STM local data observed on the nanoscale.

However, we were not able to observe the spots characteristic of the



a



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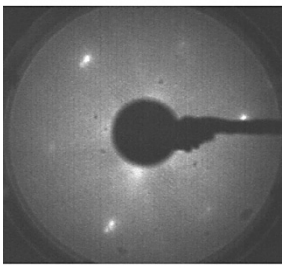

c

Fig. 4. Typical LEED patterns from different areas of the GaTe cleavage surface taken at the primary electron beam energy of: 121.5 eV (*a*), 28 eV (*b*), 52.5 eV (*c*).

monoclinic structure, which, in accordance with our STM data, could be present on the surface of cleavage. Obviously, this one could be related to the random distribution of local areas, where the monoclinic structure could be seen. The additional reason for the lack of monoclinic structure spots under observation might be a relatively weak intensity of this structure spots caused by the fact that, at least, one of the monoclinic structure lattice parameters is sufficiently larger than that of hexagonal one to contribute to a smaller proportion in the surface and, consequently, its spots are much less intense than those of the hexagonal structure and below the camera sensitivity.

However, the detailed STM/STS data on surface structure defects, including the steps on the GaTe surface, are confirmed by LEED data. Generally, the LEED technique provides statistical information about the distribution of defects, because structural defects strongly influence the spot profiles. The randomly distributed height of the steps or terraces has an impact on all diffraction spots in such a way that their width periodically varies between sharp and diffuse appearance, particularly with observation of streaks, with increasing electron energy. Otherwise, the LEED pattern, which shows some integral order spots split into doublets, indicates terraces on the surface that have a single orientation, regular spacing and height. Besides, all spots might appear alternately as doublets and single spots with changes in electron energy. It is obvious that spacing of the doublets depends on the terrace width and the doublets direction is normal to the step direction.

Typical LEED patterns recorded from the GaTe cleavage surfaces, which concern the above common considerations, are shown in Figs. 4, *b*, *c*. Figure 4, *b* shows very prominent threefold streaks along the $[1\bar{1}0]$, [010] and [100] directions, and Fig. 4, *c* exposes clear doublets associated with the spots of hexagonal structure. As already mentioned, the streaks in Fig. 4, *b* are caused by random distributed terraces, while the spot splitting demonstrated in Fig. 4, *c* is caused by regular arranged step arrays. The observed characteristic spot splitting is about 8.55% of BZ (Brillouin zone) that corresponds to the width of about 48 Å (6 single packet distances in hexagonal structure).

The possibility of structural transformations on GaTe cleavage surfaces as a result of thermal heating up to 500–600°C has also been investigated by LEED, considering the known results on the hexagonal/monoclinic transformations in GaTe polycrystalline thin films [2] at elevated temperatures. The characteristic hexagonal reflections, which were observed directly after the cleavage at room temperature, never disappeared also after consecutive heating at 200, 300, 400°C up to 500–600°C. However, diffraction spots of monoclinic structure were not observed in the LEED pattern even after the heating, thus, one could not state about the reconstruction of the cleavage surface, at least on macroscale.

4. CONCLUSIONS

The results of the combined scanning probe and electron diffraction study of the GaTe cleavage surface indicate the presence of different structures: hexagonal one on macroscale and local monoclinic one randomly distributed at the nanoscale. Furthermore, it is found that the surface structure is not perfectly flat, but is characterized by a well-developed staircase structure that is formed by cleavage. All this confirms the possibility of partial hexagonal/monoclinic surface reconstruction after the cleavage, when the local stepped structures on the surface appear as thick as one Te–Ga–Ga–Te packet.

We believe that such reconstruction, generally atypical of layered crystals, is determined by the presence of double Te–Ga–Ga–Te packets in the structure of the unit cell and from the corresponding anisotropy, which is higher for GaTe than for similar structures of GaS, GaSe, and InSe layered crystals. The possibility of partial on-nanoscale reconstruction of the basic hexagonal structure towards a monoclinic one is directly related to the number of surface defects, such as the loosely distributed steps, which are as high as a single Te–Ga–Ga–Te packet. This helps to understand why the structural monoclinic phase cannot be detected in LEED patterns, namely, the cause is the randomness and incoherence of the above-mentioned stepped areas that are formed on the surface due to cleavage.

Data of this study might be directly applied to explain experimentally obtained results such as those of paper [3], for the GaTe hexagonal-to-monoclinic structural transformations upon grinding due to the increase of the surface-to-bulk ratio in the powder.

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