High-Electric-Field-Induced Phase Transition and Electrical Breakdown of MoTe₂

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2D molybdenum ditelluride (MoTe₂) has recently received significant attention due to its unique phase transition and ambipolar behavior as well as thickness-dependent bandgap. The phase transition and electrical breakdown of various thickness MoTe₂ field-effect transistors observed under high electric fields are addressed. Interestingly, the MoTe₂ exhibits phase transition from a semiconducting 2H phase to a metallic 1T' almost simultaneously with electrical breakdown, and this is confirmed by a Raman peak of 1T'-MoTe₂ at 125 cm⁻¹. Using Raman mapping results of MoTe₂ FETs obtained after the breakdown, it is revealed that the phase transition is initiated from the metal contacting electrode regions of source and drain. All the Raman peaks of MoTe₂ shifted to low temperature with increasing drain voltage. Based on the Raman peak shifts, the temperature change in the MoTe₂ FETs while device operation is in progress is estimated. The maximum temperature and dissipated power of a tri-layer MoTe₂ device are found to reach 495 K and 5.85 mW, respectively, at an electric field of 6.5 V μm⁻¹. This research provides guidelines for circuit design toward the application of 2D semiconductor devices, related to the energy dissipation and electrical breakdown unique to 2D phase transitional materials.

1. Introduction

In recent years, 2D materials have been studied extensively for the applications in future field-effect transistors (FETs), memories, and microprocessors due to their unique optical, mechanical, magnetic, thermal, and electronic properties.[1–5] Especially, transition metal dichalcogenides (TMDCs) have been studied due to the availability of tunable bandgap and a variety of compounds consisting of transition metal and chalcogen atoms in the form of MX₂, for example, MoS₂, MoTe₂, and WSe₂.[6] As high performance and low power devices are more in need to meet the harsh requirements of the emerging mobile and Internet of Things (IoT) environment, it becomes clear that energy dissipation and electrical breakdown are formidable challenges, toward the realization of further miniaturization and functionalized integration of 2D electronics.[7–12] Power dissipation in 2D materials, including graphene, black phosphorus, and other TMDCs, has been studied by Raman spectroscopy under the high electrical fields applied to the FET structure.[13,14–16] To the best of our knowledge, the power dissipation and electrical breakdown of molybdenum ditelluride (MoTe₂) have not been studied intensively, although it is one of the most promising TMDCs that can be employed for future 2D device applications requiring ambipolar semiconducting properties.[17–20] MoTe₂ is known to have a 2H semiconducting phase with the thickness dependent band gap in the range from 0.83 to 1.1 eV.[21,22] Unlike other TMDCs, 2H-MoTe₂ exhibits controllable phase transition from semiconducting to metallic.[23] It is reported that the structural phase of semiconducting hexagonal 2H-MoTe₂ can be changed to metallic monoclinic 1T'-MoTe₂ by laser irradiation and electrostatic doping.[24–25] Raman spectroscopy is generally used to reveal the phonon properties, while in recent years it has been used effectively to determine the thickness of 2D materials.[26,27] It is also used to obtain the local temperature profile by analyzing Raman peak shifts, called Raman thermometry. The simultaneous measurement of electrical currents and Raman shifts on 2D materials enables to reveal the temperature profile of 2D materials induced by the Joule heating. It is obviously important to examine the energy dissipation of 2D electronics and the thermal state on their surface under electrical biasing.[11,13–16] In this work, we investigated the electrical breakdown and phase transition of MoTe₂, and examined the effects of voltage and temperature on Raman shifts from various thickness MoTe₂ transistors. Interestingly, MoTe₂ seems to show an unusual electrical breakdown, perhaps related to the phase transition. We observed that, just before the electrical breakdown the phase transition from 2H phase to 1T' phase of MoTe₂ occurred, and we confirmed this by Raman peaks representing 1T' phase MoTe₂. The Raman peak exhibited the red shift with increasing voltage, indicating the generation of the Joule heat. Based on the Raman thermometry, we estimated onset temperatures of electrical breakdown and phase transition for various thickness MoTe₂.

2. Results and Discussion

In order to investigate the voltage influence on the structural phase transition of MoTe₂, we applied drain voltage (V_D) and...
gate voltage ($V_G$), and increased $V_D$ up to breakdown voltage ($V_{BD}$) on 2H-MoTe$_2$ transistors, as shown in Figure 1. Note that electric field depends on $V_D$ and channel length. In order to apply high electric fields while avoiding the evaporation (removal) of metal electrodes, we used wide width but short length channels. The tested MoTe$_2$ field-effect transistor showed an ambipolar characteristic, as shown in Figure 2a. The 8 nm thick MoTe$_2$ transistor was composed of source and drain metal contacts with a channel length of 4 µm. The $V_D$ was applied in the range from 0 to 60 V at $V_G = −80$ V, as shown in Figure 2b. The current ($I_D$) increased with increasing the $V_D$ up to 56.5 V, where the phase transition and electrical breakdown were observed. The 8 nm thick MoTe$_2$ exhibits the maximum power and electrical field at 8.21 mW and 14.125 V µm$^{-1}$, respectively. The optical microscopic images of the 8 nm thick MoTe$_2$ before and after phase transition were exhibited in Figure 2c. It is clearly understood from Figure 2c that, when the voltage was applied, heat was generated firstly at the metal.
contacts and subsequently spread to the center of the channel. Also, electrical breakdown was understood to occur near drain contact due to high contact resistance. In order to verify the phase transition occurring in MoTe$_2$ transistors spatially, MoTe$_2$ was examined by using the Raman mapping method. Figure 2d presents the Raman mapping results of 2H-MoTe$_2$, 1T$'$-MoTe$_2$, and SiO$_2$ phases with peak positions of 231, 125, and 520 cm$^{-1}$, respectively. Interestingly, the Raman peak of 1T$'$-MoTe$_2$ was observed from electrode to the center of the channel, whereas that of 2H-MoTe$_2$ was observed at the edges of the channel. After electrical breakdown, the Raman peak of Si at $\approx 520$ cm$^{-1}$ was observed together with 1T$'$-MoTe$_2$, but no peak of Si with 2H-MoTe$_2$.

In order to clarify the thinning effect after phase transition, we performed AFM. It was reported that the phase transition occurs at the top layer of MoTe$_2$, and the thickness of MoTe$_2$ became thinner after the 1T$'$-MoTe$_2$ phase transition. The electrical breakdown and the phase transition of 2H- and 1T$'$-MoTe$_2$ give rise to change in thickness, as shown in Figure 3a. It was clearly observed from the optical microscopic image that the color of the 2H phase is different from the 1T$'$ phase. We took a live video to reveal the progress of the electrical breakdown. The phase transition and electrical breakdown occurred in very short time within 0.05 s. See the Video S1, Supporting Information and Figure S1, Supporting Information for the gradual phase change. Note that when high electric fields are applied, thin and narrow metal electrodes are evaporated (removed) before the breakdown of MoTe$_2$. Both the 1T$'$ and 2H phases were not detected after the evaporation of the electrodes. See Video S1, Supporting Information for comparison. The thickness was getting thinner while applying the voltage until the electrical breakdown, which occurred along with 1T$'$ phase of MoTe$_2$. Figure 3b shows the output curve obtained from a 26 nm thick MoTe$_2$ device with a maximum electric field of 9.5 V $\mu$m$^{-1}$. The Raman spectra of 1T$'$-MoTe$_2$ is presented in Figure 3c. The Raman peak of 1T$'$ phase of MoTe$_2$ was observed at the peak position of 120 cm$^{-1}$, while that of the 2H phase of MoTe$_2$ was no longer observed. The thickness of 2H and 1T$'$ phases of the MoTe$_2$ was investigated by AFM. The thickness of 2H-MoTe$_2$ phase decreased from 26 to 19 nm due to the 1T$'$-MoTe$_2$ phase transition, as shown in Figure 3d,e. Moreover, the surface of 1T$'$-MoTe$_2$ gets rougher than that of 2H-MoTe$_2$.

Figure 4 shows the electric power spent at the onset of the electrical breakdown of MoTe$_2$ with various thicknesses. It is found that the power and electric field required for electrical breakdown depends on the thickness of MoTe$_2$. Figure 4a,b presents the optical images of MoTe$_2$ taken before and after phase transition at various thicknesses, respectively. The effect of MoTe$_2$ channel thickness on power is shown in Figure 4c. Although the result seems obvious from the viewpoint of the volume effect, the power spent at the onset of the electrical breakdown increases with increasing thickness, indicating that thick MoTe$_2$ have higher thermal durability than thin MoTe$_2$.

In order to verify the phase transition related to the power dissipation, we applied voltages simultaneously while performing Raman spectroscopy. We examined the Raman peaks of the exfoliated MoTe$_2$ flakes of various thicknesses, as shown in Figure 5a. The thickness of MoTe$_2$ was estimated to be 1, 2, 3, 20, and 25 nm for monolayer, bilayer, tri-layer, multilayer, and bulk MoTe$_2$, respectively. Figure 5b shows the Raman spectra of MoTe$_2$ at the peak positions of $\approx 169$ cm$^{-1}$, $\approx 231$ cm$^{-1}$, and $\approx 287$ cm$^{-1}$, corresponding to the atomic vibration of out-of-plane $A_{1g}$, in-plane $E_{2g}^1$, and out-of-plane $B_{2g}$ modes, respectively.

![Figure 3](https://www.advancedsciencenews.com)  Figure 3. a) An OM image of a 26 nm thick MoTe$_2$ after phase transition. b) An output curve of MoTe$_2$ after applying $V_D$ from 0 to 20 V. The maximum electric field and power before the onset of breakdown are 9.5 V $\mu$m$^{-1}$ and 15.2 mW, respectively. c) Raman spectra of MoTe$_2$ 1T$'$ phase obtained at a peak position of 120 cm$^{-1}$. d) AFM image and e) AFM profile of 2H- and 1T$'$-MoTe$_2$. The thickness of 2H phase decreased from 26 to 19 nm (1T$'$ phase).
The Raman peak positions of all the MoTe$_2$ of different thicknesses were displayed in Table S1, Supporting Information. The $E_{2g}^1$ mode shifts to the lower frequencies, while the $A_{1g}$ mode shifts to the higher frequencies with increasing the number of layers. When the layer number increases, atomic vibration is reduced due to the van der Waals force exerting in the MoTe$_2$ interlayer and the dielectric screening arising from the long-range Coulombic interactions. However, the $B_{2g}^1$ peak disappears in monolayer, multilayers, and bulk MoTe$_2$ because of the breaking of translational symmetry. The intensity of the $B_{2g}^1$ mode becomes the highest at bilayers and decreases with increasing thickness.$^{[19,27,29]}$ The $A_{1g}$ active mode indicates an out-of-plane chalcogen atomic vibration between Te–Te in the Z-axis of a unit cell. The $E_{2g}^1$ active mode is an in-plane displacement of transition metal (Mo) and chalcogen (Te) atoms in the $x$–$y$ plane. The $B_{2g}^1$ inactive mode corresponds to an out-of-plane atomic vibration of Mo and Te.$^{[19]}$

In order to investigate power dissipation in MoTe$_2$, we used a tri-layer MoTe$_2$ flake, as thinner MoTe$_2$ can be damaged by Raman laser irradiation. We applied $V_D$ in the range from 0 to 15 V and $V_G$ at $-80$ V with a channel length of 2 $\mu$m. It can be observed that the Raman peaks of $A_{1g}$ and $E_{2g}^1$ modes shift.

Figure 4. a,b) OM images of MoTe$_2$ of various thicknesses taken before and after 1T' phase transition. c) Power applied at the onset of 1T'-MoTe$_2$ phase transition and electrical breakdown for various effective channel thicknesses.

Figure 5. a) An optical microscopic image of a MoTe$_2$ device. b) Raman spectra of different thickness MoTe$_2$ with the atomic vibrations of $A_{1g}$, $E_{2g}^1$, and $B_{2g}^1$ modes. c) Raman spectra of a tri-layer MoTe$_2$ obtained by applying $V_D$ in the range from 0 to 15 V at $V_G = -80$ V. d) Raman peaks of the tri-layer MoTe$_2$ obtained by applying various $V_D$. e) Raman peaks of 1T' phase MoTe$_2$ obtained at $V_D = 14$ and 15 V. f) Output curves of the tri-layer MoTe$_2$ obtained by applying $V_D$ in the range from 0 to 15 V and $V_G$ at $-80$, 0, and $+80$ V.
The relationship between \( V_D \) and Raman shifts can be seen clearly in Figure 5d. The tri-layer MoTe\(_2\) gave rise to the redshift of Raman peak of 1.7 cm\(^{-1}\) for \( A_{1g} \) mode and 3.0 cm\(^{-1}\) for \( E_{2g}^1 \) and \( B_{2g}^1 \) modes, more than at \( V_C \) of 0 and +80 V (Figure S3, Supporting Information), indicating that Joule heating is more effective at \( V_C = -80 \) V. The Raman peaks of MoTe\(_2\) redshift because \( V_D \) increases the temperature of MoTe\(_2\) by Joule heating.\(^{[11,14,27]}\) Interestingly, the tri-layer MoTe\(_2\) exhibited a higher intensity of three Raman peaks of 2H-MoTe\(_2\) phase at \( V_C = 14 \) V. After applying voltage (0 V), the pristine MoTe\(_2\) retained the trigonal 2H phase until \( V_D \) increased up to 14 V where the Raman peak of the 1T’-MoTe\(_2\) phase appeared. The intensity of three Raman peaks of 2H-MoTe\(_2\) phase at \( \approx 169 \) cm\(^{-1}\), \( \approx 231 \) cm\(^{-1}\), and \( \approx 287 \) cm\(^{-1}\) decreased when \( V_D \) increased, and the intensity of the 1T’-MoTe\(_2\) started to increase at \( V_D = 14 \) V. This implies that the phase of MoTe\(_2\) changed from semiconducting trigonal 2H to metallic octahedral 1T’ due to the electrically induced Joule heating. Figure 5f shows the output curve of the tri-layer MoTe\(_2\) device obtained with different \( V_C \).

Here, we confirmed that the electrical breakdown occurred together with 1T’ phase change of MoTe\(_2\) at \( V_D = 14 \) V. After the electrical breakdown, the Raman peaks of the \( A_{1g}^1 \), \( E_{2g}^1 \), and \( B_{2g}^1 \) in 2H-MoTe\(_2\) restore to the original position from 14 to 15 V because the Joule heating is no longer available. After undergoing the simultaneous measurements, MoTe\(_2\) was changed from 2H to 1T’ phase, but damaged by the Raman laser, as shown in Figure S10, Supporting Information.

Electrical breakdown is understood to be related to the generation of heat in semiconductor devices. Raman spectroscopy can also be used to investigate thermal properties of a semiconductor, called Raman thermometry. The correlation between temperatures and Raman peaks of \( A_{1g}^1 \), \( E_{2g}^1 \), and \( B_{2g}^1 \) modes can be found using the formula: \( \omega = \omega_0 + \chi T \), where \( \omega \) is the frequency at various temperature, \( \omega_0 \) is the frequency at room temperature, \( \chi \) is the first order temperature coefficient and \( T \) is the temperature (K). We investigated the temperature dependence using the first order temperature coefficient of \( \chi = -0.00919 \text{ cm}^{-1} \text{ K}^{-1} \) for \( A_{1g}^1 \), \( \chi = -0.01638 \text{ cm}^{-1} \text{ K}^{-1} \) for \( E_{2g}^1 \), and \( \chi = -0.01499 \text{ cm}^{-1} \text{ K}^{-1} \) for \( B_{2g}^1 \) according to the Zhang et al. research.\(^{[30]}\) The estimated temperatures and Raman shifts of the tri-layer, multilayer, and bulk MoTe\(_2\) at \( V_C = -80 \) V are plotted in Figure 6a–c, respectively. The Raman shift peaks of the \( A_{1g}^1 \), \( E_{2g}^1 \), and \( B_{2g}^1 \) modes decrease while the temperature increases. Figure 6a–f shows the relationship between \( V_D \) and temperature, which confirms that the temperature increases with the applied \( V_D \). The highest attained temperature of a multilayer MoTe\(_2\) is 534 K, which is higher compared with tri-layer (495 K) and bulk (511 K) MoTe\(_2\). See Figures S3–S9, Supporting Information for the details. The tri-layer MoTe\(_2\) exhibits the highest temperature at \( V_D = 13 \) V while the multilayer MoTe\(_2\) shows the highest temperature at \( V_D = 14 \) V before the electrical breakdown. This is because the bulk MoTe\(_2\) did not undergo electrical breakdown at high temperature at \( V_D = 15 \) V. The tri-layer, multilayer, and bulk MoTe\(_2\) showed the different highest temperatures.\(^{[10]}\) This clearly indicates that the bulk MoTe\(_2\) shows high resistivity for electrical breakdown and phase transition than multilayer and tri-layer MoTe\(_2\).

The phase transition of MoTe\(_2\) can occur by various inputs, for example, laser irradiation, electric field, and electrostatic doping.\(^{[18,23–25]}\) Wang et al. studied the phase transition from 2H-MoTe\(_2\) to 1T’ phase by electrostatic doping with an ionic liquid field-effect transistor.\(^{[25]}\) They found the reversible property of a monolayer MoTe\(_2\) from 1T’ to 2H phase. In addition, the laser irradiation also induced phase transition of MoTe\(_2\). Tan et al. reported the phase transition of MoTe\(_2\) from 2H to 1T’
phase under laser irradiation by using Raman spectroscopy.\(^2\)\(^,\)\(^3\) They used a laser power of 1 mW for measuring Raman spectra of a 9 nm thick MoTe\(_2\). For the comparison, we compared the requirement of the phase transition of MoTe\(_2\) in supporting Table S2, Supporting Information. Especially, in our research, the irreversible phase transition occurred almost simultaneously with electrical breakdown. The reason is that we applied the irreversible phase transition of MoTe\(_2\) cannot sustain the high fields due to its low electrical resistivity.

According to Raman thermometry, the highest temperatures obtained from tri-layer, multilayer, and bulk MoTe\(_2\) were found to be 495, 534, and 511 K respectively. Cho et al. reported that, when 2H-MoTe\(_2\) changed to 1T-MoTe\(_2\) with applying high electric fields, metallic 1T-MoTe\(_2\) cannot sustain the high fields due to its low electrical resistivity.

Supporting Information
Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest
The authors declare no conflict of interest.

Keywords
electrical breakdown, MoTe\(_2\), phase transition, power dissipation

4. Experimental Section

Preparation of MoTe\(_2\) Flake: A MoTe\(_2\) (supplied by HQ Graphene) was exfoliated by the mechanical exfoliation method onto a SiO\(_2\) substrate with a thickness of 285 nm. The SiO\(_2\) substrates were cleaned in acetone (C\(_2\)H\(_6\)O\(_2\), 99%) and isopropanol (C\(_3\)H\(_8\)O, 99%) solutions for 10 min by performing ultra-sonication. After that, the SiO\(_2\) substrates were cleaned using O\(_2\) plasma for 1 min at an O\(_2\) gas flow of 5.0 sccm and a power of 20 W. After the MoTe\(_2\) was exfoliated from bulk MoTe\(_2\) onto SiO\(_2\) substrate using a scotch tape, it was baked on hot plate at 373 K for 10 min. The morphology of MoTe\(_2\) was observed by optical microscopy. The thickness was measured using atomic force microscopy (AFM, Park system, XE-100).

Fabrication of MoTe\(_2\) FETs: The electrode pattern was formed by electron beam lithography (EBL) and the metal was deposited by an electron beam evaporator. Poly(methyl methacrylate) (950 PMMA, 6% concentration in Anisole) was deposited on MoTe\(_2\) by the spin coating method at 4000 rpm for 1 min. After that, MoTe\(_2\) was patterned to form electrical contacts, followed by the deposition and lift-off of chromium (Cr) 5 nm/gold (Au) 80 nm metal contacts.

Raman Spectroscopy with Applying Voltage: A 2400/300 grating and a 100x microscope objective lens (supplied by Olympus) was used for Raman spectroscopy. The laser source was employed with an excitation wavelength of 532 nm and an illuminating power of 0.15 mW with a 15% optical filter at room temperature. The diameter of laser beam is about 2 μm. That laser power was used because the phase of MoTe\(_2\) flakes was changed from 2H to 1T upon laser irradiation. Figure S2, Supporting Information shows a MoTe\(_2\) flake before and after laser irradiation. Before Raman measurement, MoTe\(_2\) was kept in vacuum to prevent the oxidation under ambient air. Raman shifts were measured while electrical voltages were applied.

3. Conclusion

We examined the effect of electric field on the phase transition of MoTe\(_2\). Interestingly, the phase transition from 2H phase to 1T phase was observed almost simultaneously with electrical breakdown. Furthermore, we investigated the effect of voltage and temperature on MoTe\(_2\) transistors by using Raman spectroscopy. It is observed that the Raman peaks of A\(_{1g}\), E\(_{2g}\), and B\(_{2g}\) modes shift to the lower frequency when increasing the voltage and temperature because of Joule heating. The electrical breakdown occurred also when the semiconducting 2H-MoTe\(_2\) phase transformed to the metallic 1T-MoTe\(_2\) phase because of the Joule heating induced by applying the voltage.

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