Improving electron mobility in MoS$_2$ field-effect transistors by optimizing the interface contact and enhancing the channel conductance through local structural phase transition$^\dagger$

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The microscale structural phase transition in TMDs from 2H to 1T or 1T$^0$ phases offers a distinct approach for modulating the electronic properties of these materials. Although phase engineering for contacts has been partially investigated, the effect of embedding 1T domains in the semiconductor channel on electronic transport has rarely been studied. Here, we investigate the electronic performance of few-layer MoS$_2$ FETs with a local 1T structural phase transition. Through a mild oxygen plasma treatment, we successfully incorporated the 1T phase into the 2H-MoS$_2$ host and observed a significant improvement in the electron mobility of the MoS$_2$ FETs. On the contact side, the local 1T domain serves as a conductive bridge connecting the Au electrode and MoS$_2$ channel, which substantially improves the carrier-injection efficiency. On the channel side, 1T embedded 2H-MoS$_2$ can effectively tailor the electronic structure of the MoS$_2$ channel, significantly increasing channel conductivity. Compared with that before the oxygen plasma treatment, the MoS$_2$ FET demonstrated a higher maximum electron mobility of about two orders of magnitude (up to $237 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$). This study could further promote the development of advanced two-dimensional electronic devices with improved performances.

Introduction

Two-dimensional (2D) transition metal dichalcogenides (TMDs), in particular molybdenum disulfide (MoS$_2$), have attracted great interest in extending Moore's law beyond silicon.$^\text{1-3}$ Such materials exhibit a unique combination of atomic-scale thickness, dangling-bond-free surfaces and tunable band structures, which offers the potential to inhibit the short channel effect of transistors as device dimensions shrink.$^\text{4,5}$ In spite of the great promise as a channel material, the reported electronic performance of field-effect transistors (FETs) based on single- or few-layer MoS$_2$, such as carrier mobility, is still substantially lower than the theoretically predicted phonon-limited values, that is, $410 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at room temperature.$^\text{6}$ It is found that the lower experimental mobility arises from two intrinsic challenges: (i) metal–semiconductor interface contacts, where the presence of defect-induced gap states can suppress the carrier-injection efficiency, leading to both Fermi level pinning and Schottky barriers.$^\text{7-9}$ (ii) electron transport in semiconductor channels, mainly influenced by Coulomb impurities near the semiconductor-dielectric interface, charge traps, defects, etc.$^\text{10-12}$ Therefore, further electronic performance optimization of MoS$_2$ devices by reducing contact resistance, enhancing carrier transport, and improving the mobility is the central task to tackle the application challenges of transistors.

It has been demonstrated that the microscale structural phase transition in TMDs, which occurs from trigonal prismatic (2H) to distorted octahedral (1T) or dimerized (1T$^0$) phases, presents a novel approach to modulate the electronic properties of these materials.$^\text{13-15}$ 2H-TMDs inherently exhibit semiconductor behavior, which can be attributed to the complete filling up of the d-orbitals of transition metals (TM$^{4+}$). In contrast, the TMDs with an octahedral coordination or T structure have rearranged the energy splitting of the d-orbitals of transition metals. The partial electronic states of the TM$^{4+}$ d-orbitals are filled, which provide unoccupied states available near the Fermi level, resulting in the metallic conductivity of the material. Based on this conductive characteristic, 1T$^0$-TMDs have been used as contact electrodes and demonstrated to effectively
reduce contact resistances in transistors. Kapper et al. first fabricated MoS 2 FETs with 1T-MoS 2 electrodes, exhibiting excellent performance with a remarkably low contact resistance of 200–300  Ω μm under zero gate bias conditions. The authors demonstrated seamless contacts by converting the MoS 2 of the contact area to the 1T phase while preserving the MoS 2 of the channel as the 2H phase. Density functional theory (DFT) simulations by Wang et al. predicted that the edge bands at the 1T-2H contact interface connect the conductive band and valence band near the Fermi surface, which indicates fine connection conditions and preferable orbital structures for carrier transport. However, we note that the 1T phase is commonly used as the electrode for improving device contact, and the effect of embedding 1T domains in the semiconductor channel on electronic transport has rarely been studied.

Tuning the electronic structure of semiconductor channels is of great importance for further improving their mobility. It is important to note that when the 1T phase is incorporated into the host structure of 2H-TMDs, it leads to a unique electronic transport behavior that cannot be simply classified as a secondary phase. For instance, the 1T phase incorporated into the 2H-TMDs results in a significant enhancement in the electron carrier concentration and the emergence of a distinctive bandgap energy state characterized by Mo 4+ d-orbitals. These changes are presumably attributable to electronic interactions between Mo 4+ ions in the 1T and 2H phases. Moreover, at the 1T-2H coplanar phase boundary, the electronic states of the 1T phase can penetrate the boundary and extend into the 2H phase by approximately two unit-cells, according to the atomically resolved STEM-EELS analysis. In addition, the band gaps and carrier transmission probabilities are subjected to the concentration of the 1T phase, which strongly influences the electronic properties of the material. Inspired by the insights from the above discussion, we anticipate that embedding the 1T phase within 2H-TMD could prove to be a promising strategy for improving channel transport in TMD-based transistors.

In this work, we investigate the electronic transport of few-layer MoS 2 FETs with a local 1T structure phase transition. Through a mild oxygen plasma treatment, the 1T-MoS 2 domains were success-fully embedded into the matrix of 2H-MoS 2, and a significant increase in the electron mobility of MoS 2 FETs was observed. On the one hand, in the contact region, the local 1T region serves as a conducting bridge between the metallic electrode and MoS 2, which substantially improves the electron-injection efficiency at vdW interfaces. On the other hand, 1T phase embedded 2H-MoS 2 can effectively modify the band structure of MoS 2 and increase the electron concentration in the channel, which significantly increases channel conductivity. Benefiting from the embedding of the 1T phase with an optimal concentration, high mobilities (up to 237 cm 2 V -1 s -1 in few-layer MoS 2) were obtained at room temperature in MoS 2 FETs, with the accomplishment of ohmic contact.

Experimental

Material preparation and characterization

High-quality MoS 2 channels were mechanically exfoliated from bulk crystals onto 285 nm SiO 2/Si substrates using the scotch-tape method. The first step involved sonication of the SiO 2/Si substrates in acetone and ultra-pure water. This helped to clean the substrates and remove any impurities or contaminants. Next, the substrates were treated with O 2 plasma to improve the adhesion between MoS 2 and the substrate surface. Once the substrates were prepared, the adhesive tape carrying high-quality MoS 2 layers was carefully pressed onto the substrate to ensure proper alignment and minimal wrinkles or folds. After applying pressure to the tape to enhance the adhesion between MoS 2 and the substrate, the tape was slowly peeled off from the substrate, leaving behind the MoS 2 layers.

MoS 2 films were analyzed by optical microscopy, Raman and PL spectroscopy, X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM) and Lorenz transmission electron microscopy (TEM). Optical microscopy analysis utilizing a Nikon LV150 microscope was conducted to determine the morphological characteristics and size of the MoS 2 samples. Confocal micro-Raman and PL (Horiba Jobin Yvon LabRAM) spectroscopy were used to identify the composition and quality of the MoS 2 samples. A laser excitation wavelength of 532 nm with an intensity of 25 mW was used. XPS was conducted using a Thermo Fisher ESCALAB Xi+ setup equipped with a monochromatic Al K α X-ray source. XPS was used to probe the surface chemistry and determine the elemental compositions of the samples. AFM (Icon AFM, Bruker) was used to accurately probe the thickness of few-layer MoS 2. The TEM images were obtained using a Talsos-F200X operated at an accelerating voltage of 200 kV.

Device fabrication

The metal electrodes were patterned using standard photolithography. First, 285 nm SiO 2 with p-type heavily doped Si (p + Si) was used as the device substrate. The two sites were etched on SiO 2 using inductively coupled plasma-reactive ion etching (ICP-RIE 5000). Following the etching process, chromium (Cr) with a thickness of 5 nm and gold (Au) with a thickness of 80 nm were sequentially evaporated onto the sites, serving as the source and drain electrodes respectively. As a result, a narrow gap of approximately 5 nm was created between the sample and electrode, enabling easy access for subsequent oxygen plasma entry.

The PPC polymer was used to transfer MoS 2 for device fabrication and TEM characterization. First, the mechanically exfoliated MoS 2 flakes with the desired size and thickness were spin-coated with a PPC solution at 2000 rpm for 60 s. After being baked at 70 °C for 1 min, the polymer stamp, carrying the MoS 2 flakes, was carefully peeled off from the growth substrate using tweezers or a roller. Subsequently, the polymer stamp was transferred to the electrodes or TEM grid by utilizing the electrostatic force by the location transfer technique. Finally, the polymer was dissolved in deionized water at 60 °C for 20 min.

O 2 plasma treatment

The MoS 2 and devices were subjected to O 2 plasma treatment for various durations (ranging from 1 to 25 s) using a Harrick
Plasma Cleaner (EQ-PDC-001), an inductively coupled plasma (ICP) system operating at a low power of 13.56 MHz RF source. High purity oxygen (99.999%) was introduced into the plasma cavity to excite the oxygen ions. The excitation power was set to 7.2 W (with 10 mA DC), while the pressure was maintained at 5 mTorr at room temperature.

Device measurements

The DC \( I_d-V_d \) and \( I_d-V_g \) characteristics were measured using a Keithley 2612A sourcemeter. The contact resistance was determined by calculating the resistance difference between two- and four-probe measurements. The mobility of the device is calculated using the equation, 
\[
\mu = \frac{L}{W C_i V_d} \times \left( \frac{d I_d}{d V_g} \right),
\]
where \( L \) and \( W \) are the channel length and width, respectively, \( I_d, V_g \) and \( V_d \) are the drain current, back-gate voltage, and drain voltage, respectively. \( C_i \), which can be expressed as \( C_i = C_{di}/d \), is the capacitance per unit area between the channel and back gate, where \( e_0 \) is the permittivity of free space, \( e_r \) is the permittivity of SiO\(_2\) and \( d \) is the thickness of SiO\(_2\). In this work, \( C_i = 1.21 \times 10^{-4} \text{ F m}^{-2} \).

Results and discussion

To achieve 1T phase embedding in 2H-MoS\(_2\), we fabricated the vdW FETs based on few-layer MoS\(_2\) using the polypropylene carbonate (PPC) dry transfer method, as illustrated in the Methods section and ESI,† Fig. S1. The fabrication process closely resembled our previous work on SeS\(_2\) devices. Briefly, prepatterned Au electrodes were initially fabricated on a SiO\(_2\) (285 nm)/Si (P++) substrate in an electron-beam evaporator system. Subsequently, the MoS\(_2\) flakes with a few layers (see Fig. S2 in the ESI†) were carefully aligned and attached to the source and drain electrodes using the dry transfer method, forming vdW contact interfaces. To achieve a clean interface between the bottom contacts and top MoS\(_2\), the Au electrodes were plasma-cleaned in hydrogen and oxygen atmospheres respectively, and the target sample was quickly transferred to the electrodes after cleaning. Compared with conventional metal deposition techniques, the vdW metal–MoS\(_2\) interface effectively avoids the associated chemical disorder and defect-induced gap states. Sequentially, we chose oxygen plasma to trigger a metallic 1T phase transition on the entire MoS\(_2\), as shown in Fig. 1(a). When exposed to oxygen plasma, the MoS\(_2\) surface is bombarded with energetic oxygen atoms, leading to the substitution of oxygen atoms for some of the S atoms. Theoretical simulations reveal that a single oxygen atom is predicted to be the energetically most favorable substitution for individual S atoms. Moreover, the bond length between atoms is closely related to the covalent radius of atoms. According to the periodic table of elements, the covalent radius of the oxygen atom is 0.73 Å, while that of the S atom is 1.02 Å. Therefore, the Mo–O bond length (2.29 Å) formed by...
oxygen atoms with a small covalent radius should be shorter than the Mo–S bond length (2.41 Å) formed by S atoms with a slightly longer covalent radius. The change in the bond length produces local stress after oxygen doping, resulting in an increase in the bond angle to form the 1T phase nanostructure. It is worth emphasizing that, to avoid generating defects in MoS2, a soft-landing method was adopted during the oxygen plasma treatment, which involves reducing the oxygen concentration in the vacuum cavity, as well as decreasing the input power and processing time.

To elucidate the atomic mechanisms that drive the 2H-to-1T phase transition in MoS2, comprehensive HR-TEM characterization was carried out. The HR-TEM images of MoS2 that have undergone the phase-transition treatment are shown in Fig. 1(b) and (c). In order to precisely monitor the phase transition, MoS2 is placed in a vacuum tank following the O2 plasma treatment to enable prompt characterization. The atomically resolved image reveals the presence of two distinct lattice regions within the MoS2 nanosheets. One region displays a hexagonal lattice structure with a lattice spacing of 0.281 nm, which corresponds to the (100) facet of 2H MoS2. Another region exhibits a trigonal lattice structure with a lattice fringe spacing of 0.280 nm, associating with the (100) planes of 1T MoS2. Remarkably, the phase boundary between the 1T and 2H phases is atomically sharp without any visible defects, indicating the formation of a seamless stitched interface. Here, it is difficult to distinguish the oxygen substitution atoms due to their similarity in atomic number to the sulfur atoms. XPS analysis further determined the substitutional doping of oxygen in the MoS2 lattice, and a detailed analysis is presented later.

Raman and photoluminescence (PL) spectroscopy analyses were carried out to further clarify the structural phase transition in MoS2 following plasma treatment. Fig. 1(d) shows the Raman spectra of MoS2 prior to and after exposure to the O2 plasma. In the case of pristine 2H-MoS2, the Raman spectra exhibited two prominent Raman features at ~386 cm⁻¹ (E1g phonon mode) and ~406 cm⁻¹ (A1g phonon mode). In contrast, three additional distinctive peaks, namely J1 (~149 cm⁻¹), J2 (~188 cm⁻¹) and J3 (~328 cm⁻¹) appear in the Raman spectra of plasma-treated MoS2 (inset of Fig. 1(d)), indicating the presence of mixture phases of MoS2. The corresponding PL spectra are shown in Fig. 1(e). The pristine 2H-MoS2 exhibits an experimental band gap of ~1.83 eV, which is equivalent to a wavelength of 677.5 nm. With the O2 plasma treatment, the optical bandgap decreases to 1.81 eV (683.7 nm), revealing a modulation of the bandgap by 1T phase doping. Moreover, in contrast to 2H-MoS2, we can clearly observe a gradual decrease in the PL intensity after plasma treatment, which indicates an increase in the proportion of the metallic 1T-phase. When MoS2 is completely metallized, the complete quenching occurs. Interestingly, we found that under the same plasma treatment time, the 1T phase transition of MoS2 occurs in the region in contact with the Au electrodes first, as shown in Fig. S3 in the ESI. This phenomenon may be attributed to the catalytic effect of Au nanoparticles, in which Au provides free electrons in the plasma process, which can accelerate the kinetic process of the oxidation reaction, thus

![Fig. 2](image-url)  
**Fig. 2**  
Electrical properties of MoS2 vdW FETs device with and without local 1T structure phase transition. (a) The schematic and micrograph of typical MoS2 vdW FET. (b) and (c) Transfer curves of the MoS2 transistors measured at Vds = 0.5 V for untreated, after vacuum annealing (b) and local 1T structure phase transition (c), respectively. The channel width was 9 μm and the length was 3 μm. (d)–(f) Output curves corresponding to the MoS2 FETs up to Vds = 1 V and Vg ranging from -50 V to 50 V, showing Schottky contact for pristine devices (d) and after vacuum annealing (e) and ohmic contact for devices with local 1T structure phase transition (f).
reducing the reaction energy barrier of oxygen doping.\textsuperscript{30} Atomic force microscopy (AFM) was performed to further verify the effect of oxygen plasma on the surface morphology of MoS\textsubscript{2}, as shown in Fig. S4 in the ESI.\textsuperscript{†} After soft oxygen plasma treatment, the MoS\textsubscript{2} samples exhibited uniform and flat surfaces without significant thinning or surface etching.

Owing to the unique structural feature of the 1T phase seamlessly embedded into 2H-MoS\textsubscript{2}, MoS\textsubscript{2} FETs exhibit high electrical performance. Fig. 2 shows the $I$–$V$ characteristic curves of the MoS\textsubscript{2} transistor measured in air with and without the local 1T structure phase transition. Fig. 2(a) shows a schematic and micrograph of a typical MoS\textsubscript{2} vdW FET. The $I_d$–$V_g$ transfer curves of the MoS\textsubscript{2} FETs for untreated, after vacuum annealing and the local 1T structure phase transition, are shown in Fig. 2(b) and (c). It is immediately evident that the device with the local 1T phase transition shows a drastic increase in the saturation current (on/off ratio $\approx 10^4$), which is approximately two orders of magnitude greater than that of the pristine MoS\textsubscript{2}. Here, the high Off current is due to the limitation of the instrument (Keithley 2612A source meter) accuracy rather than gate leakage. We measured the leakage currents through the S or D electrodes and back gate, as shown in Fig. S5 in the ESI,\textsuperscript{†} and observed no conduction was observed between the two. Moreover, the fluctuation range of the leakage current is $\pm 0.1\ \mu\text{A}$, which is close to the magnitude of the Off current, which supports the above statements. The transconductance values ($g_m$) of the device with the local structural phase transition is $\sim 4.3\ \mu\text{A V}^{-1}$ when $V_g$ is 0.5 V. In comparison, 0.1 $\mu$A V$^{-1}$ and 0.6 $\mu$A V$^{-1}$ were achieved for devices with pristine MoS\textsubscript{2} and after vacuum annealing. The electron mobility ($\mu$) of the device was calculated according to the $I_d$–$V_g$ transfer curves, as described in the Methods section. Here, the channel length ($L$) and width ($W$) were 3 $\mu$m and 9 $\mu$m, respectively. In the absence of an encapsulation layer, the FET properties of MoS\textsubscript{2} with local 1T phase transition exhibit a large gate modulation of the channel. The field-effect mobility value was $\sim 237\ \text{cm}^2\ \text{V}^{-1}\ \text{s}^{-1}$, as compared to $7$–$43\ \text{cm}^2\ \text{V}^{-1}\ \text{s}^{-1}$ for pristine 2H-MoS\textsubscript{2}. Multiple devices were measured after plasma exposure for 5–10 s, and a similar trend of significant improvement in the electronic performance was observed, as shown in Fig. S6 and S7 in the ESI.\textsuperscript{†} Here, the differences in the plasma treatment times may be due to slight variations in the MoS\textsubscript{2} thickness between the samples.

Based on a comparison of the transfer characteristic curves of MoS\textsubscript{2} FETs before and after oxygen plasma exposure, we attribute the improved electron mobility to the oxygen-substitution-induced local structural phase transition of MoS\textsubscript{2}, which plays an important role in promoting both interface contact and channel conductance.

First, the local 1T domain serves as a conducting bridge connecting the metal electrode and MoS\textsubscript{2} channel, thereby enhancing electron transport from the metal Fermi level to

![Fig. 3](image-url) Contact resistance and conductivity of MoS\textsubscript{2} vdW FETs with a local 1T structure phase transition. (a) and (b) Comparison of the contact resistances ($R_{\text{contact}}$) of the MoS\textsubscript{2} device under different gate voltages prior to and following exposure to oxygen plasma. Here, $R_{\text{contact}}$ was estimated by calculating the difference in the resistance between two- and four-probe measurements as a function of the gate voltage. It is observed that in both cases, $R_{\text{contact}}$ exhibits minimal dependence on back gating when $V_g > 20$ V. (c) Calculated channel conductivity of the MoS\textsubscript{2} device before and after embedding in the 1T structural phase. (d) Contact resistance versus channel conductivity of MoS\textsubscript{2} FETs from different studies reported in the literature; the related references are presented in the ESI.\textsuperscript{†}
the conduction band edge of MoS$_2$. Moreover, the “seamless” contact is formed between the 1T region and semiconducting sides, thus significantly elevating the carrier-injection efficiency at contact interfaces. Fig. 2(d)–(f) shows the $I_{ds}$–$V_{ds}$ output curves corresponding to the MoS$_2$ FETs for untreated, after vacuum annealing and local 1T structure phase transition. The device with the 1T phase transition shows linear $I$–$V$ curves under low bias, indicating Ohmic contacts. The contact resistance ($R_{\text{contact}}$) can be estimated by calculating the difference in the resistance between two- and four-probe measurements using the equation

$$R_{\text{contact}} = \frac{R_{2p} - (L_{\text{out}}/L_{\text{in}})R_{4p}}{W},$$

where $R_{2p}$ and $R_{4p}$ are the resistances measured with two- and four-probe configurations, and $L_{\text{out}}$ and $L_{\text{in}}$ represent the distances between the outer and inner probe pair in the four-probe setup, respectively. Here, the transfer length method (TLM), which is commonly used to analyze the contact resistance, is not suitable for our devices due to various concentrations of the 1T domain in the contact area. Fig. 3(a) and (b) compares the contact resistances of the MoS$_2$ device under different gate voltages prior to and following exposure to oxygen plasma. In both cases, it is observed that the contact resistance exhibits minimal dependence on the back gating once the device is fully turned on ($V_{bg} > 20 \text{ V}$). The contact resistance with local 1T contacts decreases by two orders of magnitude from 477.2 k$\Omega$ for 2H contacts to 4.0 k$\Omega$ at a 50 V back-gate voltage. An analysis of the literature reveals that our MoS$_2$ contacts provide device performance comparable to tunnelling contacts and have much lower resistances than the low-work-function metal contact resistance values (shown in Fig. 3(d) and Table S1 in the ESI†). Notably, for the vdW contacts between the metal electrodes and semiconductor channels, the existence of the vdW gap introduces an additional tunnel barrier and limits the charge injection. In this work, direct metallization of the contact region through microscale phase transformation significantly increases the carrier-injection efficiency at contact interfaces. Here, due to the low concentration of the 1T region (<20%) in the 2H-MoS$_2$ host (concentration analysis is shown in the XPS characterization in Fig. 4), our contact resistance is slightly lower than that of the pure 1T contacts, as shown in Fig. 3(d).

Second, the 1T MoS$_2$ embedded 2H MoS$_2$ can reduce the intrinsic bandgap, significantly increasing the channel conductance. During oxygen plasma exposure, sulfur atoms are partially substituted by oxygen atoms. Previous results have shown that a change in the bond length results in in-plane tensile strain and out-of-plane compressive strain, both of which contribute to a reduction in the bandgap. Theoretical study also shows that the incorporation of high electronegativity O atoms leads to charge transfer from Mo atoms to O atoms, which affects the electronic structure and reduces the bandgap. We compared the channel conductivity of the MoS$_2$ device before and after embedding in the 1T structural phase, as shown in Fig. 3(c). In the case of the pristine 2H channel, the conductivity is $0.7 \text{ S m}^{-1}$ with a 3 $\mu$m channel length. For the embedding of the 1T phase MoS$_2$ after plasma treatment, the conductivity significantly increased to $83.8 \text{ S m}^{-1}$, which

![Fig. 4](image-url)
matched well with the improvement in both the current and mobility of the MoS₂ FET. A comparison of the conductivities (shown in Fig. 3(d) and Table S1 in the ESI†) reveals that our 1T phase-incorporated 2H-MoS₂ channels have higher conductivities than those reported in the literature.

To further investigate the effect of 1T domain concentration on the electrical performance of the devices, we first performed X-ray photoemission spectroscopy (XPS) semiqualitative analysis of the structural phase components in MoS₂ with increasing plasma treatment time, as shown in Fig. 4(a) and (c) and Fig. S8, S9 (ESI†). In Fig. 4(a), the Mo 3d spectra exhibit two peaks centered at 230.2 and 233.3 eV, which are attributed to Mo⁴⁺ 3d₅/₂ and Mo⁴⁺ 3d₃/₂ of the pristine MoS₂ crystal, respectively.³ However, upon 2 s exposure of MoS₂ to the oxygen plasma, new distinct Mo-related peaks emerge, indicating the presence of Mo⁴⁺ 3d₅/₂ and Mo⁴⁺ 3d₃/₂ orbitals from the MoS₂ 1T phase, respectively (Fig. 4(b)). The shift in the binding energy signifies a movement of the Fermi level towards the valence band, providing strong evidence for p-type doping by substituting Mo with oxygen atoms.²⁷ The corresponding S 2p peaks also show a similar trend, as shown in Fig. S9 in the ESI.

Upon further increasing the plasma exposure time from 6 to 25 s, the 1T phase concentrations continued to increase up to 89% (Fig. S9 in the ESI†). Here, due to the high doping concentration of oxygen atoms in MoS₂, we can clearly observe the Mo–O peaks in the XPS spectra. The XPS analysis confirmed that controllable embedding of the 1T structural phase in the 2H-MoS₂ host can be achieved by adjusting the oxygen plasma exposure time. According to a previous study, however, when the exposure time of oxygen plasma exceeds 100s, many vacancies are generated, thereby reducing the electrical performance.³²

The corresponding output and transfer characteristics of our MoS₂ FETs with increasing oxygen plasma treatment time are shown in Fig. 4(d)–(f). Here, the total plasma exposure time of MoS₂ includes the cumulative exposure time of all preceding steps as well as the exposure time of the current step. The electron mobility of the device was calculated according to the \( \mu = \frac{\Delta I}{I_{DS} \cdot V_g} \) transfer curves, as described in the Methods section. We can see that the electron mobility of MoS₂ is enhanced from 7.1 cm² V⁻¹ s⁻¹ to 54.8 cm² V⁻¹ s⁻¹ when an 1T domain is incorporated into 2H MoS₂ (Fig. 4(d) and (e)). Typically, with further increasing the 1T domain concentration, the electron mobility of MoS₂ was greatly improved, up to 184.8 cm² V⁻¹ s⁻¹ (Fig. 4(f)). It is worth noting that when the 1T domain concentration in the device channel increases to the percolation threshold (oxygen plasma treatment time greater than 6 s), a percolation path of 1T structures is formed; thus, the device exhibits metallic properties (Fig. S10 in the ESI†). There is almost no effect on the drain source current with gate modulation, which shows that the Fermi level of 1T MoS₂ cannot be modulated.

From the discussions above, we can conclude that controllable embedding of the 1T domain with an optimal concentration (~17%) has been proved to be an effective approach for coordinately improving the interface contact and channel conductance (Fig. 5(a)–(f)). Compared with the before-1T phase transistors, the MoS₂ transistors exhibit robust ohmic behavior and high electronic transport properties at room temperature (Table S2 in the ESI†). Fig. 5(g) compares the mobility of our device with n-type MoS₂ FETs reported previously.²⁸,³³–⁵⁶ It is worth noting that the local 1T structural phase transition is an effective approach for coordinately improving both the intrinsic transport and contact properties to achieve high-speed and low-power MoS₂ FETs.
Conclusions

In summary, we investigated the effect of 1T phase transition in MoS2 on the interface contact and channel conductance to achieve MoS2 vdW FETs with high electrical performance. During soft oxygen plasma treatment, the sulfur atoms in MoS2 can be partially substituted by oxygen atoms. This substitution leads to spontaneous bond rearrangement, resulting in a structural phase transition from the 2H to 1T phase in MoS2. We demonstrate that the oxygen-substitution-induced local structural phase transition is an effective approach for coordinately improving (i) the carrier-injection efficiency at contact interfaces and (ii) the conductivity of MoS2 channels by inserting oxygen-substitution-induced strains. FETs tested at room temperature exhibit high mobility values of $\sim 237 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and on/off ratios of $\sim 10^4$. Our study could accelerate the development of atomic-scale surface modifications of 2D materials, which will be conducive to the functionalization and integrated application of 2D electronic devices.

Author contributions

Z. C. and M. X. proposed and supervised the project; Z. C. investigated and designed the experiments and curated measurement data; S. H. and X. Z. performed AFM, TEM and XPS measurements under the supervision of Z. C.; S. H. performed the Raman measurement; X. H. and Z. C. fabricated the MoS2 FETs and measured the I–V characteristic curves; L. C. performed mechanical peeling and plasma treatment of the MoS2 samples; Z. C. and S. D. performed the design and fabrication of Au electrodes; S. Z. assisted X. H. in I–V characteristic curve measurements; Z. C. analysed the data and wrote the manuscript; M. X. and Z. C. revised the manuscript, and all the authors discussed the results and commented on the manuscript.

Conflicts of interest

There are no conflicts to declare.

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Notes and references
