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Magnetic-field induced dimensionality switch of charge density waves in strained 2H-NbSe₂ surface

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Thinning van der Waals crystals to monolayers is crucial for nanoelectronic devices but often introduces strain, altering their electronic properties. This study explores how strain affects the charge density wave (CDW) in 2H niobium diselenide (2H-NbSe₂), focusing on a transition from a 2×2 to a 1Q CDW phase under weak magnetic fields (~ 30 mT), revealing high magnetic sensitivity. The strained 2H-NbSe₂ surface, prepared via vacuum and tape exfoliation, exhibits a 2×2 CDW phase observed using low-temperature (4.3 K) scanning tunneling microscopy and spectroscopy (STM/STS) combined with scanning electron microscopy (SEM) and cross-sectional transmission electron microscopy (TEM) under ultrahigh vacuum (UHV) conditions. STS maps show the 2×2 CDW around ± 100 meV from the Fermi level. Upon applying a magnetic field, a localized 1Q stripe CDW pattern emerges near ± 40 meV. These results highlight the influence of strain and magnetic fields on CDW behavior in 2D materials.

Layered transition metal dichalcogenides (TMDs) exhibit a variety of correlated phases, including charge density waves (CDW)^{1,2}, superconductivity, and magnetic orders³. Bulk 2H-NbSe₂ (2H niobium diselenide) is one of the most extensively investigated TMDs, demonstrating superconductivity with a critical temperature (T_c) of approximately 7.2 K⁴ and a triangular incommensurate CDW with a $\sim 3a$ period in real space (3×3 , $T_{CDW} \sim 33$ K)^{5–8} (see also Fig. S1).

Recently, bulk-like 2H-NbSe₂ with thicknesses on the order of tens of nanometers has been explored as a promising material for supercurrent diodes and advanced charge- or spin-transfer electronics, capitalizing on its strong electron correlations. Electric and magnetic fields have been employed to manipulate spatial or time-reversal symmetry, while the CDW in 2H-NbSe₂ remains robust even under large magnetic fields on the order of tens of Tesla^{9–12}, with magnetic vortices observed under 600 mT¹³.

However, magnetic-field-sensitive CDWs have been reported in few-layer NbSe₂¹⁴, where a weak magnetic field of approximately 30 mT can induce an electronic phase transition within the thin film, leading to the manifestation of a supercurrent diode effect¹⁵. In monolayer NbSe₂, surface or interface effects can break spatial inversion symmetry, and an external magnetic field can disrupt time-reversal symmetry, resulting in substantial modifications to the electronic band structure^{16,17}. Monolayer NbSe₂ exhibits remarkable elasticity, with the ability to withstand large in-plane strains ($>10\%$)¹⁸, making it an ideal platform for designing topological phases and

facilitating strain-induced switching of many-body ground states^{19,20}. Thus, tuning electronic or magnetic properties via strain is critical for developing 2D material-based nanoelectronics²¹. A notable phenomenon in the CDW of NbSe₂ is the transition between the 2H phase with 3×3 charge ordering, typically driven by distortions within the Nb layer. 2H-NbSe₂ exhibits pronounced layer-dependent properties²², with monolayers hosting enhanced $3a$ -period triangular (3Q) CDW ordering ($T_{CDW} \sim 145$ K)^{23,24} and diminished superconductivity ($T_c \sim 1.9$ K), potentially showcasing exotic Ising pairing^{25–27}.

From an applied perspective, NbSe₂ monolayer films may experience significant strain during the attachment process to a substrate or during the bonding of nanowires. Therefore, it is critical to understand how strain influences the CDW patterns in 2H-NbSe₂ and also CDW phase switching under weak magnetic fields.

This study investigates the strained 2H-NbSe₂, fabricated via vacuum exfoliation, exhibiting the 2×2 CDW phase. We employ low-temperature (4.3 K) scanning tunneling microscopy and spectroscopy (STM/STS) under ultrahigh vacuum (UHV) conditions. The STS maps reveal the 2×2 CDW patterns below and above the Fermi energy within a 100 meV range. However, applying an out-of-plane magnetic field of approximately 30 mT induces a dramatic transformation, causing a transition from the 2×2 CDW to a 1Q CDW pattern with electronic band localization around ± 40 meV relative to the Fermi energy. Additionally, the 1Q stripes are not

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perfectly aligned with the atomic lattice, shifting approximately 10 degrees from the Q_{Bragg} direction.

Results

Magnetic field-induced phase switching in CDW Pattern

Figure 1a presents an atomically resolved STM topographic image of the 2H-NbSe₂ surface, prepared in UHV using the tape-cleaving method (“2 × 2 CDW in electronic maps” and Fig. S2). The image reveals a regular pattern, with its periodicity illustrated by the FFT

map inset in Fig. 1a. The FFT map displays two sets of spots: the outer six spots, arranged in hexagonal symmetry, correspond to the p(1 × 1) atomic lattice of Nb and Se atoms on the 2H-NbSe₂ surface, while an additional six spots appear within the p(1 × 1) spots, indicating the presence of the CDW pattern.

The height profile along the arrow in Fig. 1a shows regular CDW corrugations of approximately ±20 pm (black line in Fig. 1c). Additionally, the profile reveals that the surface is not atomically flat but exhibits a winding topography, with a height variation of roughly 200 pm over a

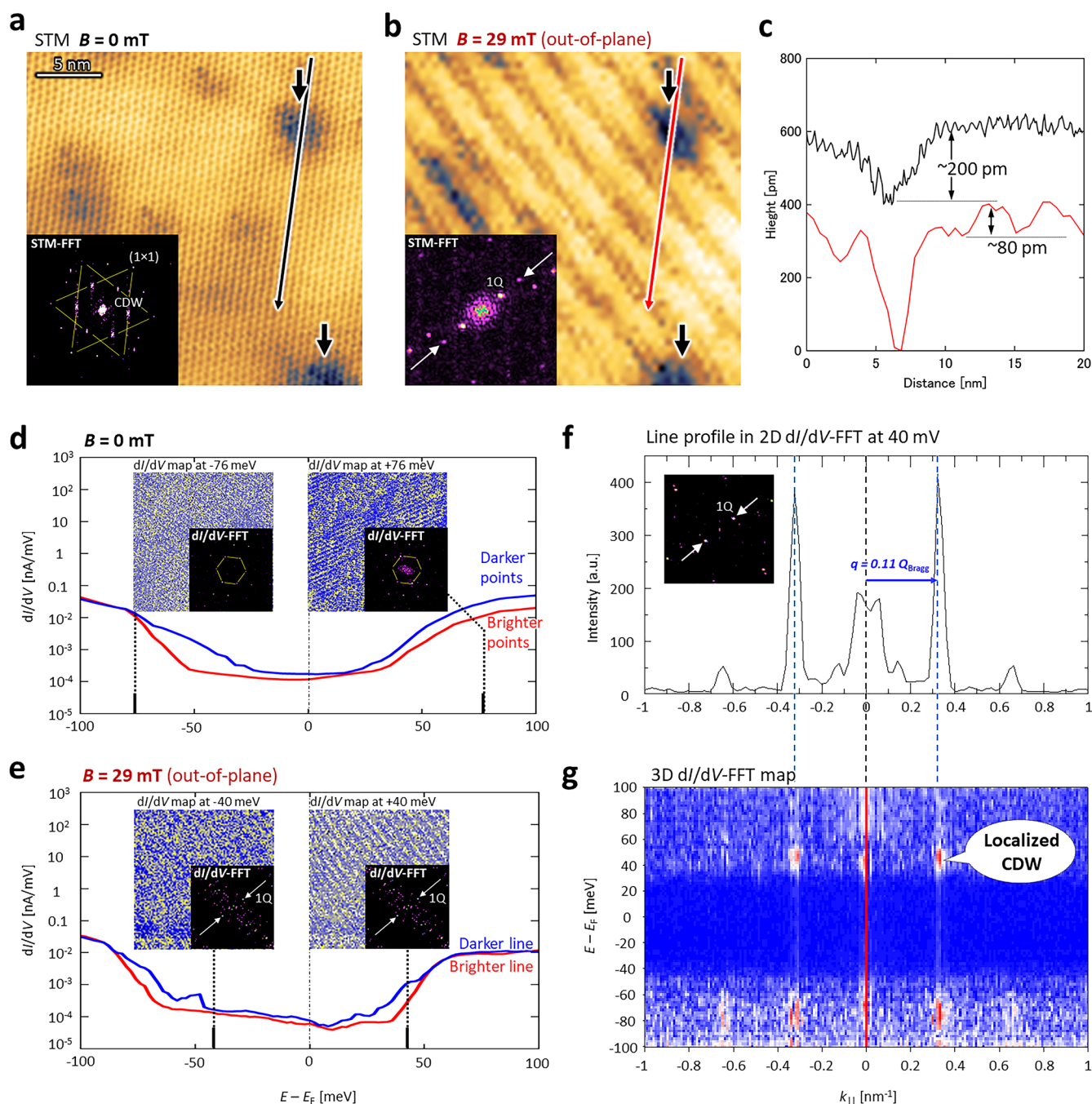


Fig. 1 | Magnetic field-induced CDW phase switching. STM topographic images obtained on the identical 2H-NbSe₂ surface (a) before and (b) after the out-of-plane magnetic field application. **a** $V_s = -100$ mV, $I_t = 500$ pA, 26.4×26.4 nm²; **b** $V_s = -100$ mV, $I_t = 300$ pA, $B = 29$ mT, 26.4×26.4 nm². Insets denote these FFT maps. (c) Height profiles obtained from the same line marked by black and red arrows in **a** and **b**, respectively. **d** dI/dV curves obtained from brighter (red line) and darker points (blue

line) in the CDW pattern in **a**. Both dI/dV maps at -76 and $+76$ meV and these FFT maps reveal the same CDW order. **e** dI/dV curves obtained from brighter, darker lines in **b**. Both dI/dV maps at -40 and $+40$ meV and the insets denote these FFT maps reveal the 1Q-CDW order. (f) Line profile across the dI/dV -FFT map at $+40$ mV shown in the inset in **f**. **g** FFT dI/dV intensity map (z -axis) as a function of wave number: $k_{||}$ [nm⁻¹] (x -axis) and energy: $E - E_F$ [meV] (y -axis), where red dots indicate localized 1Q-CDW.

20 nm in-plane displacement (see a wide-area STM topographic image displayed in 3D view mode in Fig. S12).

Figure 1b displays an STM topographic image of the same region as Fig. 1a, while an out-of-plane magnetic field of 29 mT was applied. Two marked bumps, indicated by arrows, confirm that the locations in Fig. 1a, b are identical. Notably, a dramatic transformation was observed between the images. Specifically, additional stripe patterns emerge under the influence of the magnetic field in Fig. 1b. This 1Q stripe pattern has not been previously reported in the bulk 2H-NbSe₂ crystal under magnetic field application. Generally, the 3 × 3 CDW is stable under a magnetic field^{9,13}. The strong electron-electron interactions inherent in the NbSe₂ system are likely responsible for this behavior. The inset in Fig. 1b displays an FFT map derived from the topographic image in Fig. 1b. The stripe pattern gives rise to C₂ symmetric spots, marked by two arrows, which are shifted by approximately 10 degrees from the Γ -M direction.

The red curve in Fig. 1c shows the height profiles along the arrows in Fig. 1b, corresponding to the same locations as in Fig. 1a. Comparing the height profiles measured along the same line before (black line) and after (red line) the application of the magnetic field in Fig. 1c clearly shows the drastic change in the CDW periodicity, which corrugation has an approximately 80 pm. We have extracted line profiles along one of the 2 × 2 CDW pattern directions and compared the FFT-derived line profiles before and after applying the magnetic field (see Figure S11). A comparison of the line profiles extracted from the FFT maps in Fig. 1a, b reveals a significant change in periodicity. Specifically, the 1Q CDW stripe pattern exhibits a periodicity of $k = 0.32 \text{ nm}^{-1}$, whereas in the absence of a magnetic field, the $p(1 \times 1)$ peak is located at 3.58 nm^{-1} . This indicates that the periodicity of the 1Q CDW is $11.2a$, corresponding to $1/k = 1/(0.32 \text{ nm}^{-1}) = 3.125 \text{ nm} \sim 3 \text{ nm}$. This starkly contrasts with the conventional 3 × 3 phase, indicating the emergence of a non-trivial phase on the surface. The observed 1Q-CDW periodicity of $\sim 3 \text{ nm}$ is significantly larger than the atomic lattice of $\sim 0.34 \text{ nm}$. This suggests that the 1Q-CDW pattern observed under applying a magnetic field likely originates from different factors, such as strain, with the magnetic field potentially inducing a different CDW order.

To investigate the CDW pattern further before and after applying the magnetic field, we conducted scanning tunneling spectroscopy (STS) measurements (see Methods, “Strained 2H-NbSe₂ Surface Due to Tape Cleavage”). At each pixel position on the surfaces shown in Fig. 1a, b, the tunneling current was measured as a function of the sample bias voltage. The numerical differentiation of this data yielded the differential conductance dI/dV curves (Fig. 1d, e). Thus, dI/dV maps at each energy were obtained (Fig. S3–S6).

Figure 1d presents dI/dV curves measured in Fig. 1a ($B = 0 \text{ mT}$), where the blue and red lines correspond to measurements taken at the brighter and darker regions of the topographic image in Fig. 1a. This surface exhibits a significant decay of approximately 50 meV around the Fermi energy, which may suggest the presence of a bandgap. However, as shown in Fig. 1d, log-scale dI/dV curves reveal that the 2 × 2 CDW surface retains an LDOS near the Fermi energy, preserving its metallic nature. Nevertheless, its LDOS characteristics differ from those of the conventional metallic 3 × 3 CDW surface, which exhibits LDOS peaks at $E - E_F = -0.8, -0.2, -0.035, +0.035$, and $+0.5 \text{ eV}$ (E_F representing the Fermi energy)²⁸. This indicates that the surface might possess an electronic structure distinct from that of the normal 2H phase. Compared to the 1 × 1 atomic position (Fig. S1), the brighter and darker spots in the STM image correspond to the Nb and Se positions, respectively. Two insets correspond to the dI/dV maps at -76 and $+76 \text{ meV}$ and their FFT maps, where the CDW patterns are visible and resemble those observed in Fig. 1a.

Figure 1e shows dI/dV curves measured in Fig. 1b ($B = 29 \text{ mT}$), with the blue and red lines corresponding to measurements taken at the brighter and darker regions of the stripe patterns in the STM topographic image in Fig. 1b. An important observation is that the stripe pattern alters the original CDW configuration in Fig. 1a from a hexagonal to a two-fold symmetry. Under the influence of the magnetic field, the hexagonal CDW patterns vanish, giving way to 1Q CDW stripe patterns. The dI/dV maps in Fig. 1e

were acquired simultaneously with Fig. 1b in the same area. The 1Q spots were observed in their dI/dV -FFT maps from the valence and conduction bands ($+40 \text{ mV}$ and -40 mV) throughout the entire surface (see Fig. 1e and Figs. S5, S6). Both the topographic image and the dI/dV maps exhibit the same stripe pattern associated with the 1Q CDW.

We performed a line profile between two arrows in the dI/dV -FFT map obtained from the dI/dV map at $+40 \text{ mV}$ above the Fermi energy (Fig. 1f), revealing that the stripe peaks occur at approximately $\pm 0.35 \text{ nm}^{-1}$ in k -space, corresponding to $q = 0.11 Q_{\text{Bragg}}$. The 3D plot in Fig. 1g, obtained along the line between two arrows in the dI/dV FFT map, represents the energy spectrum E versus wavevector k within the energy window of $\pm 100 \text{ meV}$ near the Fermi energy. Here, the stripe CDW is localized in energy around $\pm 40 \text{ meV}$.

These experimental findings in Fig. 1 are pivotal for preparing the 2H-NbSe₂ crystal surface, particularly for applications in nanoelectronics, which involve thinning the material to monolayer thicknesses from bulk crystals. In recent years, 2H-NbSe₂ crystals have been widely utilized, for instance, in superconductor diodes, where a drastic resistance change has been observed around 30 mT ¹⁵, which corresponds to the field applied in this study. Consequently, it would be intriguing to explore why the NbSe₂ surface, cleaved in UHV, exhibits such an unusual phase transition upon applying an external field. Specifically, applying a relatively weak magnetic field of approximately 29 mT , perpendicular to the surface, induces a profound transition in the phase to 1Q charge ordering.

2 × 2 CDW in electronic maps

Although the 2H-NbSe₂ crystals were cleaved in UHV at 300 K using blue tape (see Methods), we consistently observed CDW patterns as depicted in Fig. 1. Spectroscopic mappings performed on this surface revealed a magnetic field dependence that deviates from the conventional 3 × 3 CDW pattern (Figure S1), suggesting the emergence of a distinct phase on the surface. Consequently, we meticulously analyzed the CDW pattern presented in Fig. 1.

Figure 2a displays an enlarged STM topographic image obtained without applying a magnetic field, in which bright spots align in a hexagonal symmetry. This observation contrasts with the periodic triangular pattern characteristic of the conventional 2H-phase CDW (Fig. S1)²⁸. Figure 2b shows a dI/dV map at 0 eV , corresponding to the Fermi energy acquired from the same area as Fig. 2a. The periodicity is resolvable in the FFT map presented in Fig. 2c. In this map, six-fold symmetric spots, indicated by red circles, correspond to the surface Se atomic distance of 0.34 nm , matching the $p(1 \times 1)$ scattering vector: Q_{Bragg} .

Notably, additional spots, marked by blue circles in the FFT map, reveal a 2 × 2 charge order rather than the expected 3 × 3 pattern. These spots are situated at the edges of the Brillouin zone, where the Γ , K , and M points are marked in reciprocal lattice space (k -space). Comparing the periodicity between the 2 × 2 CDW and the 1 × 1 atomic regularity aligned on the surface (Fig. S1d) suggests that the Nb atom positions (dark spots in the CDW pattern) could align with the CDW spots, as the Nb atoms occupy the three-fold hollow site positions on the Se layer.

A line profile between two arrows, parallel to the Γ -M direction in the FFT map of Fig. 2c, is shown in Fig. 2d. This profile identifies the CDW peak position as occurring precisely at half of the Bragg peak positions ($q = 0.5 Q_{\text{Bragg}}$), confirming that the observed CDW in Fig. 1 is not the conventional 3 × 3 phase but a non-trivial 2 × 2 CDW pattern.

A plausible origin for the appearance of this 2 × 2 CDW pattern may lie in significant strain^{29–31}. Strain-induced phase formation has been previously demonstrated through mismatches in thermal expansion coefficients, where the NbSe₂ crystal was bonded not to a conventional metal substrate but to silica, followed by cooling from room temperature to 4 K . STM imaging of this strained NbSe₂ surface revealed unidirectional stripe ordering with a periodicity of $4a$ and a triangular arrangement with a $2a$ periodicity (2 × 2 CDW)²⁹. A similar unexpected 2 × 2 phase was observed on a heavily electron-doped 2H-NbSe₂ surface³⁰.

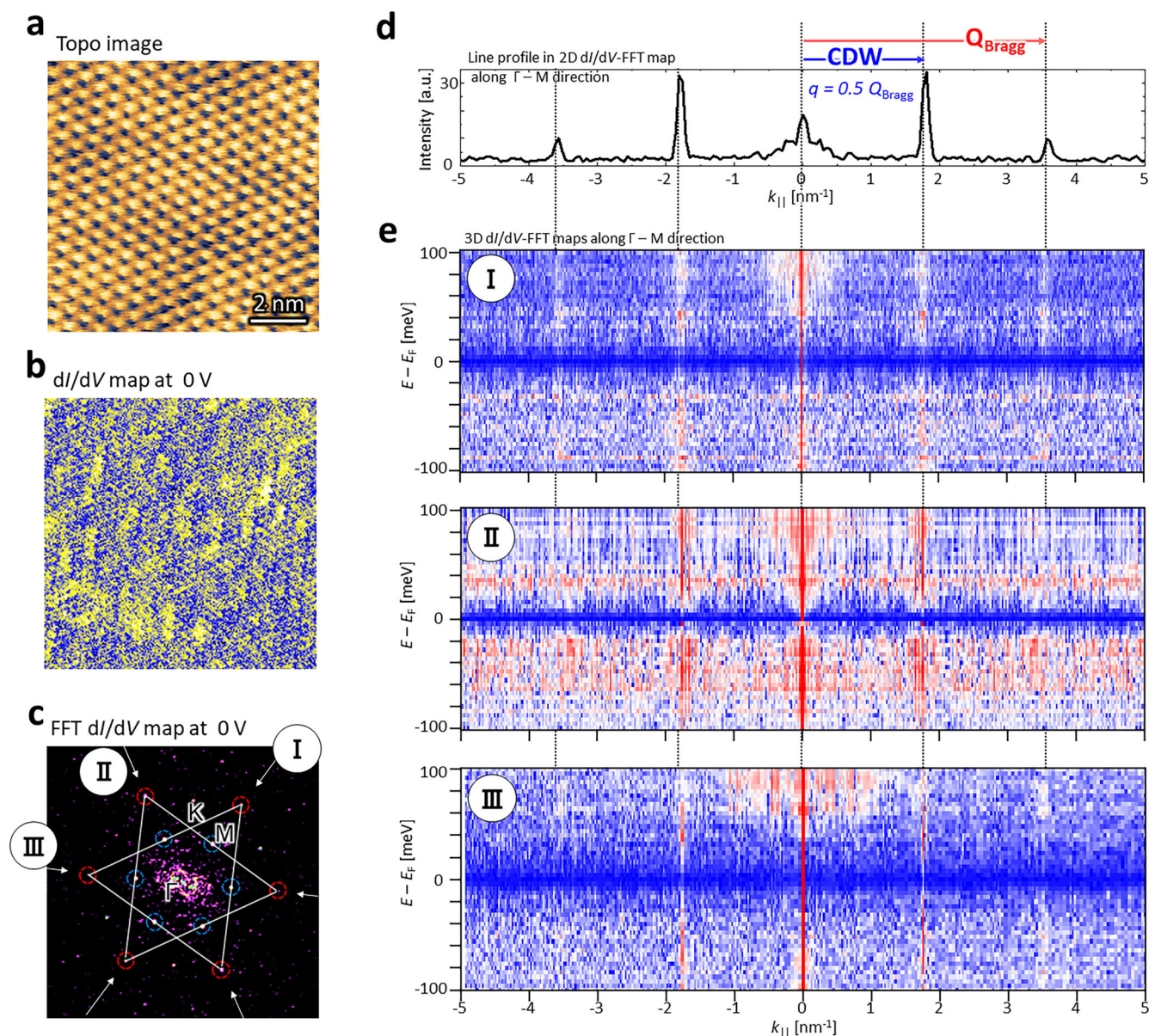


Fig. 2 | Non-trivial CDW phase. **a** STM topographic image obtained on the NbSe₂ surface, magnified from Fig. 1a: $V_s = -100$ mV, $I_t = 500$ pA, 10×10 nm². **b** dI/dV map at 0 eV, corresponding to the Fermi energy, obtained from the same area as **a**. **c** FFT dI/dV map obtained from **b**, representing six-fold $p(1 \times 1)$ symmetry spots, marked by red circles, with additional six spots marked by blue circles, located at the

first Brillouin zone, along the Γ -M direction. **d** Line profile between two white arrows in **c** along the I direction. **e** FFT dI/dV intensity map (z-axis) as a function of wave number: $k_{\parallel}$ [nm⁻¹] (x-axis) and energy: $E - E_F$ [meV] (y-axis), where red lines indicate localized CDW, along I, II, and III directions in **c**.

As shown in Fig. 1c, the height variation is approximately 200 pm over a 20 nm in-plane displacement, which is about one-third of the unit height of bulk 2H-NbSe₂ (~600 pm, Fig. S10). This indicates that the cleaved 2H-NbSe₂ surface in UHV is not atomically flat but rather undulating. Estimating the exact strain present in the lattice from STM images is challenging. However, theoretical studies suggest that a 2% strain is required to induce a transition from the 3×3 to the 2×2 phase in monolayer NbSe₂³¹. Furthermore, we have carefully examined whether strain affects the $p(1 \times 1)$ lattice, as shown in Fig. 2. This strain may explain the relatively broad peak observed in the FFT line profile in Fig. 2d, which is significantly wider than the 2×2 CDW peak. This observation suggests that the surface atomic arrangement is not perfectly uniform, providing potential experimental evidence of strain-induced lattice distortion.

To further investigate the CDW with respect to energy, Fig. 2e presents three-dimensional (3D) dI/dV FFT intensity plots across the dI/dV FFT

map obtained along the three symmetric directions I, II, and III (marked between two arrows in Fig. 2c) as a function of energy. The x-axis represents the wave number $k_{\parallel}$ [nm⁻¹], the y-axis denotes energy relative to the Fermi level ($E - E_F$), and the z-axis corresponds to the normalized dI/dV FFT intensity (in arbitrary units), with the red-blue scale indicating higher-lower values.

The energy spectra E versus wavenumber $k_{\parallel}$ within the energy window of ± 100 meV near the Fermi energy, presented in Fig. 2e, exhibit 2×2 CDW peaks around ± 1.7 nm⁻¹ in k -space across the entire energy range. However, intensity variations are observable between these regions, with the I, II, and III directions remaining identical in k -space, aligned parallel to the Γ -M direction. This suggests the presence of anisotropic electronic structures within the 2×2 CDW pattern.

DFT calculations suggested that strain-induced instabilities in NbSe₂ could be responsible for these substantial changes³¹, where in-plane biaxial

tensile strain shifts the soft phonon mode of the unmodulated structure from momentum $q_{\text{CDW}} \sim 2/3 \Gamma\text{M}$ to $q_{\text{CDW}} \sim \Gamma\text{M}$. This instability leads to a structural reconstruction corresponding to a triangular $2a$ charge order. Consequently, the monolayer 2H-NbSe_2 can transition from a 3×3 to a 2×2 CDW phase. The 3×3 phase competes with the 2×2 phase when strain is between 0–2%, whereas the 2×2 phase becomes dominant when strain exceeds 2%³¹.

Strained 2H-NbSe_2 surface due to tape cleavage

Due to the weak van der Waals interactions, all Se-Se interfaces can be separated when the tape, adhered to the top layer of the NbSe_2 crystal, pulls the crystal upwards. In contrast, typically, only a single interface is initially separated, as the force required to overcome the van der Waals interaction at that interface is sufficient to initiate cleavage. The remaining interfaces, however, may relax without strain, preserving the original symmetry of the 2H phase stacking due to the van der Waals interaction. Consequently, after cleavage, the conventional 3×3 CDW pattern is usually observed on the surface (Fig. S1)^{8,22}. However, this outcome highly depends on the method of cleaving the 2H-NbSe_2 crystal. To identify the source of strain on the NbSe_2 surface, we investigated the surface and interfaces of cleaved 2H-NbSe_2 crystals using scanning electron microscopy (SEM) and

transmission electron microscopy (TEM) with chemical identification. The results are presented in Fig. 3.

Figure 3a displays an SEM image of the 2H-NbSe_2 crystal surface following tape cleavage in UHV (Fig. S2), where several NbSe_2 layers are overturned; many are floating and winding, failing to maintain stable contact with the NbSe_2 crystal substrate. This indicates that the cleaved surfaces consist of multiple NbSe_2 thin films of varying thicknesses.

Figure 3b, c present cross-sectional TEM images, combined with chemical identification of the NbSe_2 crystals: (b) near the surface and (c) in the bulk, where Se and Nb atoms are depicted in green and red, respectively. The TEM lamella thickness is approximately 50 nm, and we focus on scanning only the topmost surface region. From the TEM image in Fig. 3b, the monolayer NbSe_2 film near the surface is not flat but exhibits winding (indicated by the box), leading to a variable Se-Se interface distance compared to the bulk interface, which suggests significant strain in the surface layers. Although different crystals were used for the STM and TEM measurements, and no direct comparison was made, the key point is that cleavage in UHV can reproducibly produce a winding surface, resulting in significant stress on the surface monolayer film.

In contrast, in bulk (Fig. 3c), approximately five monolayers beneath the surface, the atomic Se-Nb-Se stacking remains constant, with a thickness of approximately 0.6 nm—the position of the Nb atom shifts between odd

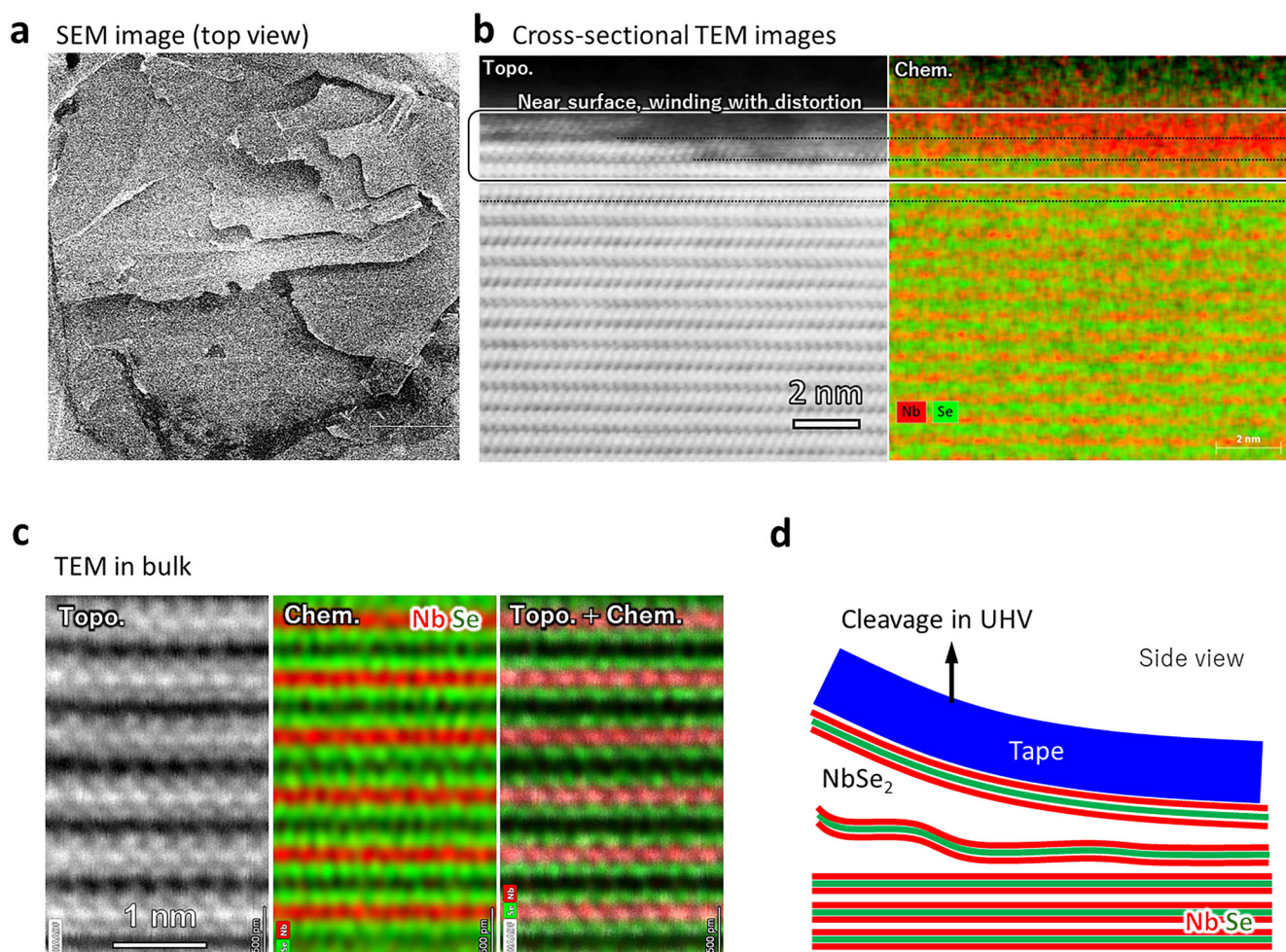


Fig. 3 | Strained surface due to tape cleavage. **a** SEM image (top view, $3 \times 3 \text{ nm}^2$) obtained from the cleaved surface of NbSe_2 in vacuum. **b** Cross-sectional TEM images near the surface (side view, $12 \times 12 \text{ nm}^2$). The left and right images show topographic and chemically identified images, where Nb and Se atoms are colored

red and green, respectively. **c** Cross-sectional TEM images (side view, $2.4 \times 3.9 \text{ nm}^2$) obtained from the bulk NbSe_2 crystal. Topographic (HAADF-STEM), chemical identification, and merged images are shown from left to right. **d** Schematic side view model during the vacuum cleavage on the NbSe_2 surface using the tape.

and even stacking layers within the 2H phase. The chemically identified maps obtained simultaneously show the Se and Nb distributions, highlighted in green and red, forming an ordered array in bulk, with atomic flatness maintained and the Se-Se interfaces parallel to the substrate.

Figure 3d summarizes a cross-sectional model based on the SEM and TEM data, illustrating that the surface top monolayers may be wound, leading to significant strain that produces a non-trivial 2×2 CDW pattern. This strain is sensitive to magnetic field application, causing a transition from the 2×2 CDW to a 1Q-CDW pattern, as shown in Fig. 1. The results presented in Fig. 3 provide essential insights for fabricating thin films of 2H-NbSe₂ for nanodevices. Specifically, thinning to an atomically thin film and bonding to a substrate surface during nanoelectronics fabrication can induce substantial strain in the atomically thin 2H-NbSe₂ film.

Bulk 2H-NbSe₂ crystals, with thicknesses of tens of nanometers—corresponding to several hundred monolayers—are widely used for fabricating nanojunctions in conductance measurements. These crystals are well known for exhibiting superconductivity below their critical temperature and forming vortex arrays under Tesla-range magnetic fields^{9–13}. Therefore, conventional 2H-NbSe₂ crystals are generally not expected to show significant magnetic field dependence. However, upon applying a weak magnetic field, we unexpectedly observed a striking transition from the 2×2 CDW pattern to 1Q.

Our experimental findings, presented in Figs. 1–3, suggest that this 2×2 CDW pattern originates from strain in the top surface layer, while its magnetic field dependence implies the presence of a local minimum in the 2×2 CDW phase. The subtle Zeeman splitting induced by the weak magnetic field suggests that strained NbSe₂ may host multiple phases within a narrow energy range. Theoretically, monolayer NbSe₂ is predicted to transition from a 3×3 to a 2×2 CDW phase when the strain exceeds 2%³¹. Under spin-orbit coupling and periodic lattice distortion, this 2×2 phase could acquire a nontrivial topological character. Since even a weak magnetic field can break time-reversal symmetry, the drastic phase transition from 2×2 to 1Q CDW observed in Fig. 1 may be attributed to this symmetry breaking.

Discussion

We have demonstrated that thin, surface monolayer films of 2H-NbSe₂ can be readily distorted by external forces, leading to the winding or bending of the film and an enhancement of strain, as observed through UHV-STM/STS at 4.3 K combined with SEM/TEM measurements. This investigation reveals that strained surface films predominantly exhibit a 2×2 CDW order, unlike the conventional 3×3 CDW charge order typically seen on the 2H-NbSe₂ surface after vacuum tape cleavage. Unlike the conventional case, this 2×2 CDW order is highly sensitive to external fields, undergoing a transition to a 1Q configuration as the CDW is compressed in energy. These experimental findings provide critical insights for the fabrication of nanodevices utilizing ultrathin NbSe₂ films, as thinning or wire-bonding processes can induce significant strain, thereby altering the intrinsic electronic properties and enhancing sensitivity to magnetic fields.

Methods

Home-built low-temperature UHV STM setup

STM measurements were conducted using a custom-built UHV-STM system^{32–35}, which comprises three main components: an STM analytical chamber equipped with a UHV cryostat (CryoVAC) to cool the STM setup, a preparation chamber for tip cleaning, and an introduction chamber for the vacuum cleaving of 2H-NbSe₂ crystals (HQ graphene). The base pressures of the chambers were below 1.0×10^{-8} Pa, 2.0×10^{-8} Pa, and 1.0×10^{-7} Pa, respectively. The cryostat features inner and outer tanks filled with liquid helium and nitrogen, enabling over 40 h of STM/STS measurements at 4.3 K. Samples and STM tips were transferred between chambers using transfer rods, maintaining UHV conditions. Gate valves separated each

chamber. We employed sharp tungsten tips as STM probes, utilizing conventional chemical etching^{36,37} and flame etching techniques^{38,39}.

Sample preparation: UHV 2H-NbSe₂ cleavage

We used 2H-NbSe₂ crystals (HQ graphene, purity 99.995%) with typical dimensions of 2–3 mm in size and 0.1–1.0 mm in thickness. These TMD crystals were typically adhered to a metal substrate; in this case, we used a Mo sample plate with a conductive epoxy (H20E). Care must be taken to ensure the adhesive does not extend beyond the bottom of the crystal. Suppose the glue comes into contact with the sides of the crystal. In that case, silver atoms from the adhesive can diffuse into the crystals during thermal treatment, potentially altering their properties (Scanning electron microscopy with energy dispersive X-ray spectroscopy: SEM-EDX, JEOL JSM-6510A, Fig. S8).

SEM-EDX measurements shown in Fig. S8 revealed that Ag nanoclusters could diffuse into the 2H-NbSe₂ crystals during the process of fixing the 2H-NbSe₂ crystal onto the Mo sample plate using Epoxy H20E and Ag glue for UHV conditions. Although the Ag glue was applied only to the bottom of the crystal, the Ag nanoclusters diffused onto the surface after heating in air at 400 K for 1 h. The large-area STM image in Fig. S10 shows these nanoparticles on the surface.

Although van der Waals materials can provide atomically flat and clean surfaces through tape cleaving in air, our preliminary STM tests on such surfaces revealed impurity adsorption from the air, which could damage and modify the material's intrinsic properties (Fig. S1). To mitigate this, we introduced the sample from the air through a load lock chamber. We performed the cleavage in the UHV introduction chamber, transferring the sample into the STM while maintaining UHV conditions.

The 2H-NbSe₂ single crystal was cleaved using blue tape (Nitro ELP-BT-150E-CM), which was affixed to the apex of the transfer rod. First, the tape was gently pressed against the surface of the 2H-NbSe₂ crystal; then, the sample was moved laterally while simultaneously pulling out the rod, thereby achieving the peeling operation (Fig. S2).

STM/STS measurements

Our custom-built STM was controlled using the Nanonis SPM controller BP4. STM topographic images were acquired in constant current mode and analyzed using WSxM 5.0 Develop 10.2 software and Gwyddion 2.56. For STS measurements, dI/dV data were collected at each pixel position in the STM topographic image. During these measurements, the STM tip position was fixed with the feedback disabled, allowing us to measure the tunneling current as a function of the sample bias voltage (I - V curve). The differential conductivity (dI/dV) was numerically obtained, as it is proportional to the sample's local density of states (LDOS). By repeating the STS measurements across all pixel positions ($256 \text{ points} \times 200 \times 200 \text{ pixels}$), we generated dI/dV maps at each energy level on the NbSe₂ surface, which were then fast Fourier transformed (FFT) to produce 2D k -space maps at each energy level using our Python Spyder code.

Additionally, we developed another Python code to create a 3D dI/dV plot as a function of the sample bias voltage along a line profile on the k -space map, excluding the tunneling background in the dI/dV curve to highlight the Q_{Bragg} and CDW peaks. The original 2D- dI/dV map data were converted from ASCII row format to a 200×200 matrix format, followed by 2D Fourier transformation. This FFT data was then converted back to ASCII, allowing us to produce 256 FFT dI/dV maps corresponding to the electron intensity map in reciprocal lattice space at each energy level. In this study, we covered 256 energy levels within $\pm 100 \text{ meV}$, and our code generated 1D intensity plots along the line profile drawn on the desired position in the 2D-FFT dI/dV map.

Magnetic field system

A magnetic field was generated using custom-built Helmholtz-type superconducting (SC) coils made from fine-insulated NbTi wire (Supercon Inc. 54S43, $\phi = 0.299 \text{ mm}$). Two coils were positioned above and below the STM, aligned along the central axis, providing an out-of-plane magnetic field to the sample surface. Both coils were directly connected to the bottom of the

inner helium tank. The current was controlled by a Mercury IPS power supply (Oxford Instruments), with a copper mesh wire connecting the power supply outside the UHV environment to the inside of the UHV cryostat through a feedthrough. Inside the UHV chamber, the copper mesh wire connected to the bottom of the outer liquid nitrogen tank and contacted a high-Tc BISCCO wire supported by indium. This BISCCO wire extended through the inner helium tank, contacting the NbTi coils at the bottom of the helium tank.

TEM measurements

The high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) observations were conducted using an FEI Titan G2 80-200 microscope equipped with a probe corrector, operating at an accelerating voltage of 200 kV. Samples for TEM analysis were prepared via the FIB lift-out technique using an FEI Helios Nanolab 650. To prevent damage during ion-beam milling, the Ni films were coated. Energy-dispersive X-ray spectroscopy (EDX) was carried out using an FEI Super-X detector, and the data were analyzed using Bruker Esprit version 1.9.

Data availability

No datasets were generated or analysed during the current study.

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Author contributions

T. K. Y. conceived and designed the project. R. I. and T. K. Y. performed all STM / STS experiments. E. I. and R. I. developed a Python-based analysis program. Y. K. T. performed all TEM measurements. R. I. wrote the first draft, and T. K. Y. corrected and added a discussion to the manuscript. All authors discussed the results and commented on the manuscript.

Competing interests

The authors declare no competing interests.

Additional information

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