Direct Growth of van der Waals Tin Diiodide Monolayers

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Two-dimensional (2D) van der Waals (vdW) materials have garnered considerable attention for their unique properties and potentials in a wide range of fields, which include nano-electronics/optoelectronics, solar energy, and catalysis. Meanwhile, challenges in the approaches toward achieving high-performance devices still inspire the search for new 2D vdW materials with precious properties. In this study, via molecular beam epitaxy, for the first time, the vdW SnI₂ monolayer is successfully fabricated with a new structure. Scanning tunneling microscopy/spectroscopy characterization, as corroborated by the density functional theory calculation, indicates that this SnI₂ monolayer exhibits a band gap of \( \approx 2.9 \) eV in the visible purple range, and an indirect- to direct-band gap transition occurs in the SnI₂ bilayer. This study provides a new semiconducting 2D material that is promising as a building block in future electronics/optoelectronics.

1. Introduction

The success of mechanically exfoliated graphene has sparked blowout research interests in two-dimensional (2D) van der Waals (vdW) materials,[1–23] with substantial attention paid to the graphene family,[2–7] transition metal dichalcogenides (TMDs),[8–10] 2D metal carbides/nitrides (MXenes),[11–16] and black phosphorene.[17–21] In contrast to the bulk counterparts, these materials at the 2D limit exhibit a diverse range of intriguing properties.[24–27] Yet, challenges still exist in respect of applications for the currently explored 2D materials, such as the gapless band structure of graphene, [4] relatively low carrier mobility of TMDs,[28] and the poor air stability of black phosphorene.[29–31] Therefore, it is crucially important to develop new types of 2D layered materials that exhibit new properties complementary to the current 2D material families.

The group IVA metal dihalide has been extensively explored regarding to their superior properties such as the visible-range band gap and the thickness-dependent band structure,[32–35] as well as the potential applications in semiconductor optical devices and perovskite solar cells.[36–41] However, on one hand, the layered 2H-PbI₂, as one of the most widely studied materials, is unfriendly to the environment. On the other hand, the bulk SnI₂ hosts a rather different three-dimensional (3D) crystal structure,[42] and its vdW monolayer has never been experimentally realized.

In this work, for the first time, we successfully grew the vdW monolayers of SnI₂ via molecular beam epitaxy (MBE) technique. The growth takes a 2D mode, and the thickness is well controllable at the monolayer precision. Scanning tunneling microscopy/spectroscopy (STM/STS) measurements, with the aid of first principle density functional theory (DFT) calculations, confirm that the grown SnI₂ monolayer hosts a new structure of the layered 2H-PbI₂ type. The SnI₂ monolayer possesses an appreciable indirect band gap of \( \approx 2.9 \) eV, and an indirect–direct band gap transition occurs as the thickness increases to above two layers. Such transition is opposite to the MoS₂ monolayers that exhibit a direct-indirect band gap transition as the thickness increases.[8]
We emphasize that the high-quality SnI$_2$ monolayer can be directly grown on the substrate kept at room temperature ($\approx$20–22 °C), without further annealing. The reflection high-energy electron diffraction (RHEED) pattern was in situ measured to monitor the morphology of SnI$_2$ monolayers. As displayed in Figure 1b, the streaks in the RHEED pattern indicate the 2D growth mode of SnI$_2$ on the Td-WTe$_2$ substrate. Quantitatively, the streak spacing for the SnI$_2$ film ($d$) is $\approx$1.27 times that of the Td-WTe$_2$ substrate ($ds$). The surface morphology of $\approx$0.5 monolayer (ML) SnI$_2$ deposited on the Td-WTe$_2$ substrate (Figure 1c) verifies the formation of atomically flat and hexagonal-shaped SnI$_2$ islands. The step height of the SnI$_2$ islands, as obtained through the line-scan profile (inset to Figure 1c) is $\approx$0.7 nm high. Atomically resolved STM images (Figure 1d,e), together with the corresponding fast Fourier transformation (FFT), clearly evidence the hexagonal lattice symmetry. The lattice parameter is determined to be $a = b = 4.48$ Å, in accordance with the quantitative analysis of the RHEED data. Besides, the FFT result (inset to Figure 1d) also exhibits extra dots, which originated from the Moiré pattern formed between the SnI$_2$ monolayer and Td-WTe$_2$ substrate, and can also be clearly observed in the STM image in Figure 1d (marked in black). It is noteworthy that the grown SnI$_2$ monolayer is in a new structural phase, which is completely different from its bulk counterpart. As previously reported,[42] the bulk SnI$_2$ crystallizes in the 3D monoclinic structure with the space group of C2/m. Randomly distributed defects are observed on the SnI$_2$ islands, particularly on the SnI$_2$ monolayer (Figure 1c). More STM data indicate that three different defects can be identified, among which the type A is the majority, and types B and C are occasionally observed (see Figure S5, Supporting Information). In combination with DFT simulation, we ascribe the type A defect as the extra I atom at the bottom of SnI$_2$ monolayer, and types B and C as the extra Sn atom at the bottom and I vacancy on the top, respectively.

Figure 1. Epitaxial growth, structural, and electronic characterizations of vdW SnI$_2$ monolayers grown on Td-WTe$_2$. a) Schematic illustration of the growth of hexagonal SnI$_2$ monolayer on Td-WTe$_2$. b) RHEED patterns of epitaxial SnI$_2$ film and Td-WTe$_2$ substrate. c) Large-scale STM image of SnI$_2$ monolayer (size: 100 × 100 nm$^2$, $U = +2$ V, $I = 100$ pA). Inset: height profile of line scan across the step indicated by the green arrowed line. d) High-resolution STM image taken on the SnI$_2$ monolayer (size: 20 × 20 nm$^2$, $U = −700$ mV, $I = 100$ pA). The surface unit cells of SnI$_2$ monolayer and the Moiré pattern are marked in blue and black, respectively. Inset: the corresponding FFT pattern with the blue and red circles marked the reciprocal lattice peaks of SnI$_2$-(1×1) and the Moiré pattern respectively. e) Atomic resolution of monolayer SnI$_2$. The blue rhombus represents the unit cell (size: 6 × 6 nm$^2$, $U = −1$ V, $I = 100$ pA). It indicates the hexagonal lattice of $a = b = 4.48$ Å. f) Typical $dV$/d$V$ spectra taken on monolayer SnI$_2$ ($U = +2.2$ V, $I = 100$ pA, modulation: 40 mV). The black lines indicate the band edges.
Figure 2. Van der Waals growth of vDW multilayer of SnI₂ on Td-WTe₂. a) Large-scale STM topographic image of multilayered SnI₂ films with thickness varying from 1L to 3L (size: 100 × 100 nm², U = −2 V, I = 100 pA). b–d) Atomic resolutions (20 × 20 nm²) obtained on 2L, 3L, and 6L, respectively (U = −1.5 V, I = 50 pA). Inset: the corresponding FFT images. e) Line scan profile across from 3L to 1L along the green allowed line in (a). f) dI/dV spectra taken on SnI₂ with different thicknesses ranging from 1L to 6L.

the boundary structure (Figure S4b,c, Supporting Information). Even though the two adjacent domains exhibit different lattice orientations, the growth at the boundary is seamless.

To further explore the electronic structure of the SnI₂ monolayer, differential conductance (dI/dV) spectra, which reflect the local density of states, were measured. Figure 1f presents the typical dI/dV spectrum taken on the SnI₂ monolayer away from defects (more data can be found in Figure S1, Supporting Information). The semiconducting nature of the SnI₂ monolayer is revealed, and a wide band gap of ≈2.9 eV is determined, within the range of visual purple spectrum. The valence band maximum (VBM) and conduction band minimum (CBM) are also identified at ≈−1.6 eV (below Fermi energy) and ≈+1.3 eV (above Fermi energy).

Multilayered films can also be epitaxially grown with a monolayer precision. Figure 2a shows the surface of the multilayered SnI₂ films with thicknesses varied from monolayer (1L) to three layers (3L). Atomically resolved STM images, Figure 2b–d, demonstrate that the layered hexagonal lattices are maintained in these SnI₂ multilayers, and no structural transition to the bulk phase is observed (more data can be found in Figure S2, Supporting Information). It is noteworthy that the defect concentrations in SnI₂ bilayer or multilayers, typically the extra I atoms at the bottom, are significantly lower than the monolayer, which can be attributed to the different adsorption and diffusion of I atoms at the SnI₂ interlayer from SnI₂/WTe₂ interface. We further calculated the formation energies of the extra iodine defect at the SnI₂/WTe₂ and SnI₂/SnI₂ interfaces. Our calculation results indicate that the extra iodine defect formed at the SnI₂/WTe₂ interface is more stable than at the SnI₂/SnI₂ interface by ≈0.3 eV. Interestingly, the interlayer spacing for the multilayered SnI₂ (Figure 2e) keeps a near constant of ≈0.7 nm, the same as the step height for the monolayer, indicating no identifiable layer-dependent interlayer coupling. All of these results collectively suggest that such hexagonal vDW structure can be stabilized in the 2D limit, although it does not exist in the bulk.

The dI/dV spectra (Figure 2f) taken on the SnI₂ monolayers indicate that the width of gap keeps nearly the same for the thickness up to six layers (6L) (The spatial uniformity of the STS spectra are verified by the STS line scans, as shown in Figure S1, Supporting Information). This differs from most of the other TMD vDWs materials hosting the electronic structures sensitive to the number of layers.[24,41–50] The locations of CBM and VBM can be extracted from the dI/dV data in the logarithmic form (see Figure S6b, Supporting Information). As the thickness is decreased to monolayer, the Fermi energy (E_F) gradually shifts upwards with respect to the band edges, which may be due to the electron doping effect from the intrinsic defects or the substrate. Such doping effect becomes prominent in the proximity of interface, similar to what was reported for GaSe/graphene heterostructures.[50]

To investigate the chemical stoichiometry of the grown SnI₂ monolayers, X-ray photoelectron spectroscopy (XPS) measurements were ex situ performed after exposure in air. Figure 3a,b displays the XPS spectra of Sn 3d and I 3d core levels, respectively. The binding energy of Sn 3d5/2 (486.4 eV), Sn 3d3/2 (494.8 eV),
I 3d5/2 (619 eV), and I3d3/2 (630 eV) reflects the valence states of Sn (+2) and I (−1) for the SnI₂ compound. The chemical stoichiometry for SnI₂ is quantitatively determined to be ≈1:2, consistent with the ideal SnI₂ compound. Moreover, there is no oxidation state of SnI₂ detected within the instrumental resolution. Thus, it is concluded that the as-grown SnI₂ monolayers is significantly inert to air.

The DFT optimized atomic models of the SnI₂ mono- and multi-layers are constructed. The monolayer structure is shown in Figure 4a. It adopts the 2H-PdI₂ type (space group: P3m1)
structure. Each monolayer comprises three atomic planes covalently bonded in the sequence of I-Sn-I with the in-plane lattice of \(a = b = 4.53 \, \text{Å}\). In multilayers, the separation between adjacent layers governed by vdW interactions is \(\approx 0.32 \, \text{nm}\). Both theoretical atomic structures and lattice constants agree well with the experimental results. Moreover, the calculated band structure indicates that monolayer SnI\(_2\) has an indirect semiconducting gap of \(\approx 3.25 \, \text{eV}\), as shown in Figure 4d. Even though there still exists a minor discrepancy between the calculated and experimentally observed gap value (\(\approx 2.9 \, \text{eV}\)), the DFT + GW calculation method we applied corrects the usual underestimation of energy gap by DFT method. The corresponding calculated DOS based on the proposed crystal structure (Figure 4c) agrees well with the experimental \(dI/dV\) spectra, further demonstrating the as-grown SnI\(_2\) monolayer to be a new 2D layered semiconductor. The calculated band structure of SnI\(_2\) (Figure 4d–f) shows that the monolayer and bilayer host the indirect-gap, and a transition to direct-gap occurs on the trilayer SnI\(_2\), opposite to hexagonal 2H-phase MoS\(_2\) (2H-MoS\(_2\)) whose direct band gap only exists in monolayer.\(^{[42]}\) We also considered the other possible stacking, the common structure for semiconducting TMDs, such as MoS\(_2\). However, the calculated energy is significantly higher, and the energy difference is \(\approx 0.56 \, \text{eV per unit cell}\). Please note that a nomenclature inconsistency exists between 2H-PbI\(_2\) and TMDs. In fact, the crystal structure of 2H-PbI\(_2\) corresponds to the 1\(\text{st}\) structure, as referred to in TMD compounds, which is different from the common structure of 2H-MoS\(_2\).

This substrate-assisted growth of the 2D hexagonal SnI\(_2\) monolayer is universal, regardless of the lattice symmetry and lattice constants of the substrate. As shown in Figure S3, Supporting Information, the SnI\(_2\) monolayer with the hexagonal lattice can also be successfully grown on the bilayer graphene (BLG)/SiC substrates at room temperature (\(\approx 20–22^\circ\text{C}\)). The SnI\(_2\) monolayer grown on the graphene/SiC substrate exhibits an irregular shape, which differs from the equilateral triangular SnI\(_2\) grown on the Td-WTe\(_2\) substrate. This is probably due to the pinning effect triggered by the native defects on the graphene/SiC surface (see Figure S7, Supporting Information). We also find that both its structural and electronic properties are similar to the SnI\(_2\) monolayers on the Td-WTe\(_2\) substrate. Particularly, their similar properties include the atomic structure and in-/out-plane lattice parameters, 2D vdW growth mode as manifested by the streaky RHEED patterns, air stability as suggested by the XPS spectra, and semiconducting nature with a comparable energy gap of \(\approx 2.9 \, \text{eV}\). In view of the distinct atomic structures of hexagonal graphene and orthorhombic Td-WTe\(_2\), these results show that the growth of semiconducting SnI\(_2\) with layered hexagonal lattice is barely influenced by the different lattice symmetry of substrates.

3. Discussions

The bulk SnI\(_2\) is a monoclinic structure with \(a = 14.17 \, \text{Å}, b = 4.535 \, \text{Å}, c = 10.87 \, \text{Å}\) (space group: \(\text{C2/m}\)).\(^{[42]}\) The DFT calculated free energy per unit volume of the bulk monoclinic SnI\(_2\) is \(\approx 6.7 \, \text{meV}\) lower than that of the layered hexagonal SnI\(_2\), suggesting that the layered phase is less stable. However, in the 2D limit, the formation of monolayer or few layers of the bulk phase requires the interlayer bonds of monoclinic SnI\(_2\) to be broken; consequently, the energy needed will be higher than that in the 2D hexagonal phase. Therefore, the hexagonal phase of SnI\(_2\) in the monolayer limit is more stable, which is consistent with our experimental results. We also addressed the kinetic issue for the growth of 2D hexagonal phase. We calculated the adsorption energies of the SnI\(_2\) layer on the WTe\(_2\) substrate and another SnI\(_2\) layer, respectively. The calculation results show that the adsorption energy of the SnI\(_2\) on WTe\(_2\) is higher than that on another SnI\(_2\) layer by \(\approx 75 \, \text{meV per unit cell}\). Therefore, the SnI\(_2\) prefers to adsorb on the WTe\(_2\) substrate, instead of another SnI\(_2\) layer, which favors the 2D growth. The hexagonal monolayer becomes kinetically trapped in the 2D limit, owing to the lower surface energy.

4. Conclusion

In summary, we have successfully fabricated vdW SnI\(_2\) monolayers. The substrates with different lattice symmetries, such as the orthorhombic Td-WTe\(_2\) and hexagonal graphene, are both feasible to the epitaxy of vdW SnI\(_2\) monolayer. XPS data manifested its stability in air. The grown SnI\(_2\) monolayer is found to be a new layered vdW semiconductor with an appreciable band gap of \(\approx 2.9 \, \text{eV}\). The SnI\(_2\) monolayer also exhibits thickness-dependent properties, for example, the indirect- to direct-band gap transition. The experimental realization of SnI\(_2\) monolayers, a new 2D semiconductor with thickness-dependent properties, provides an optimal material candidate for applications in electronics and optoelectronics.

5. Experimental Section

MBE Growth of SnI\(_2\) Films: The SnI\(_2\) monolayers were grown on the Td-WTe\(_2\) and BLG/SiC substrates using the MBE. The Td-WTe\(_2\) substrates were obtained via in situ cleaving the Td-WTe\(_2\) single crystal in ultrahigh vacuum (UHV), and the BLG/SiC substrates were obtained by repeatedly flashing the SiC single crystal for more than three times in UHV with base pressure lower than \(1 \times 10^{-10} \, \text{Torr}\). Prior to the SnI\(_2\) growth, the surface qualities of Td-WTe\(_2\) and BLG/SiC substrates were checked via STM characterization. Anhydrous SnI\(_2\) powder (Alfa Aesar, 99.999%) was loaded in a Knudsen diffusion cells as the evaporation source. The growth morphology was in situ monitored by RHEED. During the growth, the SnI\(_2\) source was heated to \(\approx 280 \, ^\circ \text{C}\), and the substrates were kept at room temperature (\(\approx 20–22^\circ\text{C}\)).

Scanning Tunneling Microscopy Characterization: The STM measurements were in situ carried out with a commercial low-temperature UHV-STM system (Unisoku, USM1500). The base pressure was lower than \(1 \times 10^{-11} \, \text{Torr}\). A mechanically polished Pt-Ir tip was used for scanning under the constant-current mode. The \(dI/dV\) spectra were collected using the lock-in amplifying technique with an AC modulation of \(\approx 10 \, \text{mV}\) at a frequency of \(879 \, \text{Hz}\).

Density Functional Theory Calculation: The DFT calculations in this work were performed using the projected augmented wave method\(^{[52]}\) as implemented in the Vienna ab initio simulation package.\(^{[53]}\) The exchange correlation potential was described by the generalized gradient approximation of Perdew–Burke–Ernzerhof type.\(^{[54]}\) An energy cutoff of 250 eV was used, which was converged in the authors’ test. The Brillouin zone was sampled by a \(16 \times 16 \times 1\) \(k\)-point mesh. To accurately describe the interlayer interactions, the D2 vdW correction method presented by Grimme was adopted.\(^{[55]}\) In all the slab models, the vacuum distances were larger than 15 Å. This distance was large enough to avoid the interaction between the two nearest slabs. The atomic structures were carefully relaxed until the forces on each atom were less than 0.01 eV Å\(^{-1}\).
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.

Author Contributions

Q.-Q.Y. and F.Z. contributed equally to this work. S.-C.L. conceived the project. Q.-Q.Y. grew the SnI$_2$ monolayers and carried out STM experiments with the assistance of Z.-Q.S. and Q.-Y.L. F.Z. and P.Z. carried out the DFT and GW theoretical calculations. Y.-Y.L. and Y.C. grew the single-crystal WTe$_2$ substrates. Q.-Q.Y. and S.-C.L. wrote the manuscript with the input from F.Z and P.Z. All authors discussed the results and commented on the manuscript.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

density functional theory, molecular beam epitaxy, scanning tunneling microscopy, SnI$_2$, van der Waals monolayers

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