The Reduction of Substrate-induced Strain of Monolayer MoS₂ Grown on a Nonplanar Sapphire Substrate

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Abstract

Two-dimensional (2D) transition metal dichalcogenides (TMDCs) owns the excellent optical properties for photoelectron devices. We demonstrated that the monolayer MoS₂ 2D material was directly grown on the nonplanar substrate with three dimensional (3D) structure. The monolayer MoS₂ grown on a cone-shaped sapphire substrate effectively reduces the substrateinduced tensile strain due to decrease the thermal expansion mismatch between a 2-D materials. The monolayer MoS₂ grown on a nonplanar substrate also increases the light extraction efficiency by scattering effect. In the future, a large-area and strain-less of monolayer 2D material grown on a nonplanar substrate can be used to realize future ultra-thin optoelectronic integrated systems.

1. Introduction

The two-dimensional (2D) transition metal dichalcogenides (TMDCs) have attracted wide attention to develop the atomically thin light emitters [1]. The atomically thin and bendable membrance and of TMDCs is a potential candidate for developed the novel light emitter devices on the nonplanar micro or nano-structures. At present, many research groups used the CVD-grown or exfoliated TMDCs on flat substrate to transfer onto target substrates [2,3]. However, the material and optical properties of TMDCs are easily affected by changes in the number of stacked layers and strain. The electrical band structure of TMDCs will be changed from a direct energy gap to an indirect energy gap with increasing the number of layers and tensile strain [4]. The CVD-grown or exfoliated TMDCs are placed on a nonplanar substrate with nanostructure. It could cause the formation of locally large strain or cannot achieve the large area of monolayer TMDCs 2D material [5].

In this study, we demonstrated that the large-area of monolayer molybdenum disulphide (MoS_2) were directly grown on a three-dimensional (3-D) substrate by using chemical vapor deposition (CVD). The substrate-induced strain effect and the optical properties of a monolayer MoS_2 grown on a nonplanar substrate are investigated. In the future, the development of large-area monolayer 2-D material grown on a 3-D substrate with micro or nano-tructures to realize the ultra-thin optoelectronic integrated

systems.

2. Results and Discussion

The monolayer MoS₂ were grown on c-plain FSS and PSS by using CVD. First, the 1 nm of Mo metal was deposited on the substrates by using an RF sputtering system. Then, the metal contacted with air to form natural oxidized MoO₃ on substrates. After Mo deposition, the samples are placed in the center of a furnace tube under the pressure of 5×10^{-3} torr with rising the temperature from 25°C to 750 °C during the 40 minutes. The MoO₃ on the sapphire substrates will be sulfurized at the 750 °C of growth temperature and under the 0.7 torr of furnace pressure. The thermal evaporation of S powder at 120 °C is placed on the upstream of the Ar gas flow of 130 sccm. Finally, the monolayer MoS₂ on the FSS and PSS were formed during the sulfurization process. Fig. 1 (a) and (b) show the cross-sectional scanning electron microscopy (SEM) image and cross-sectional view of transmission electron microscopy (TEM) image of a monolayer MoS₂ grown on a patter sapphire substrate (PSS). The height (H), diameter (D), and period (P) of the hexagonal lattice of the micro-cone of the PSS are approximately 1.56 µm, 2.6µm, and 3µm, respectively. The slant angle of the



cone of the PSS was approximately 60°.

Fig. 1 (a) The cross-sectional SEM image of a monolayer MoS_2 grown on a patter sapphire substrate (PSS) (b) The cross-sectional TEM image of monolayer MoS_2 grown on the cone of the PSS.

Fig. 2(a) shows the Raman spectrum of monolayer MoS₂ grown on the FSS and PSS. The Raman spectrum of MoS₂ on sapphire substrate have three Raman shift peaks at 385.5×405.3 and 417 cm^{-1} . The 385.5 and 405.3 cm^{-1} of Raman shift peaks are the E^{l}_{2g} vibrational mode and the A_{lg} vibrational mode of the monolayer MoS₂, respectively.

The E_{2g}^{I} and A_{1g} modes of the Raman shift peak for the monolayer MoS₂ grown on PSS exhibits significant blue shift compared with the monolayer MoS₂ grown on FSS. It implies that the monolayer MoS₂ grown on the PSS diminishes the tensile strain, resulted in the Raman blue shift. The tensile strain of the monolayer MoS₂ grown on the FSS and PSS were estimated to be approximately 0.18%, and 0.03%, respectively as shown in Fig. 2 (b). The substrate-induced strain in the monolayer MoS₂ is from the thermal expansion coefficient mismatch between the 2D material and the substrate. Fig. 2 (c) presents the schematic of the lattice constant (a) of the monolayer MoS₂ grown on the FSS and an inclined surface of the cone of the PSS while cooling down from 750 °C to 25 °C. By assuming, the monolayer MoS_2 does not have strain at the 750 °C. After cooling down to room temperature, the different the lattice reduction between the 2D material (a_{MoS_2}) and the substrate $(a_{Al_2O_3})$, resulted in the substrate-induced strain of the monolayer MoS₂. The strain-less of the monolayer MoS₂ grown on the cone of PSS can be obtained due to decrease in the thermal expansion mismatch.



Fig. 2 (a) Raman spectra of the monolayer MoS_2 grown on the FSS and PSS. (b) The strain of the monolayer MoS_2 grown on the FSS and PSS. (c) Schematic of lattice compression with decreasing the temperature from 750 °C to 25°C for the monolayer MoS_2 grown on the c-plane of FSS and PSS.

Fig. 3(a) shows the PL spectrum of the monolayer MoS₂ grown on FSS and PSS by continue-wave 532 nm laser excitation. The PL peaks of the monolayer MoS₂ grown on the PSS also exhibited a significant blueshift. This results were agreed well to the results of Raman spectrum due to reduce the tensile strain. Besides, the PL intensity of the monolayer MoS₂ grown on the PSS was enhanced 3 times. In order to explain the enhancement factor of the PL intensity, the light extraction efficiencies of the monolayer MoS₂ grown on the FSS and PSS were simulated using finite-element method (FEM) as shown in Fig. 3 (c). Based on the light emission of MoS₂ from the FSS, the integrated optical powers of the far fields for MoS₂ on the FSS

exhibits a 3.3-fold enhance. It can be believe that the light emission of monolayer MoS_2 on a PSS to increases the light extraction efficiency.

Fig. (a) PL spectrum of the monolayer MoS₂ grown on the *c*-planes



of the FSS and PSS. The simulated light emission distribution of the monolayer MoS_2 grown on (b) the FSS and (c) the PSS.

3. Conclusions

We investigated the substrate-induced strain and optical properties of monolayer MoS₂ grown on a nonplanar sapphire substrate. The monolayer MoS₂ grown on the PSS could reduce the substrate-induced tensile strain due to the reduction in the thermal expansion coefficient mismatch between the material and the substrate. In addition, the growing monolayer MoS₂ on PSS increased the light extraction efficiency. The PL intensities of the monolayer MoS₂ grown on the PSS exhibited 3-fold enhancement, compared with the monolayer MoS₂ grown on the FSS. In the future, this method can be used to design novel light-emitting devices by using 2D materials to facilitate the growth of large-area and strain-less of 2D materials on nonplanar sapphire substrates. The development of large-area monolayer 2-D material grown on a 3-D substrate with micro or nanotructures to realize the ultra-thin optoelectronic integrated systems.

Acknowledgements

The authors would like thank for the Center for Nano Science and Technology in National Chiao Tung University (NCTU) to provide the fabrication facilities support. This work was supported by the Academia Sinica in Taiwan and the Ministry of Science and Technology (MOST) in Taiwan under Contract Nos. No. 105-2112-M-001-011-MY3.

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