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The Reduction of Substrate-induced Strain of Monolayer MoS_2 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 MoS_2 2D material was directly grown on the nonplanar substrate with three dimensional (3D) structure. The monolayer MoS_2 grown on a cone-shaped sapphire substrate effectively reduces the substrate-induced tensile strain due to decrease the thermal expansion mismatch between a 2-D materials. The monolayer MoS_2 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 MoS_2 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 MoO_3 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 MoO_3 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 MoS_2 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 MoS_2 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°.

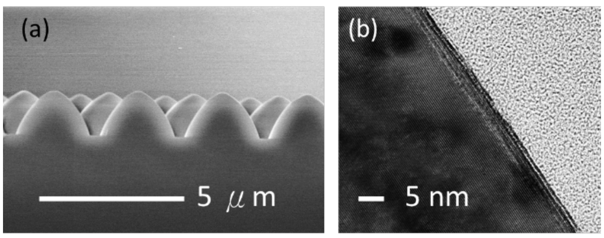


Fig. 1 (a) The cross-sectional SEM image of a monolayer MoS_2 grown on a patter sapphire substrate (PSS) (b) The cross-sectional TEM image of monolayer MoS_2 grown on the cone of the PSS.

Fig. 2(a) shows the Raman spectrum of monolayer MoS_2 grown on the FSS and PSS. The Raman spectrum of MoS_2 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^1_{2g} vibrational mode and the A_{1g} vibrational mode of the monolayer MoS_2, respectively.

The E^1_{2g} and A_{1g} modes of the Raman shift peak for the monolayer MoS_2 grown on PSS exhibits significant blue shift compared with the monolayer MoS_2 grown on FSS. It implies that the monolayer MoS_2 grown on the PSS diminishes the tensile strain, resulted in the Raman blue shift. The tensile strain of the monolayer MoS_2 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 MoS_2 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 MoS_2 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 MoS_2. The strain-less of the monolayer MoS_2 grown on the cone of PSS can be obtained due to decrease in the thermal expansion mismatch.

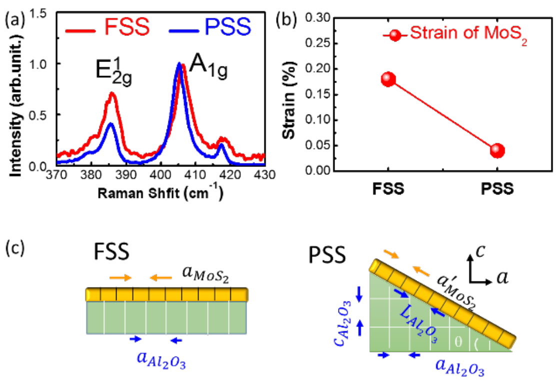
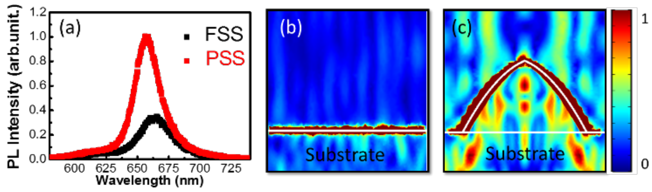


Fig. 2 (a) Raman spectra of the monolayer MoS_2 grown on the FSS and PSS. (b) The strain of the monolayer MoS_2 grown on the FSS and PSS. (c) Schematic of lattice compression with decreasing the temperature from 750 °C to 25°C for the monolayer MoS_2 grown on the c-plane of FSS and PSS.

Fig. 3(a) shows the PL spectrum of the monolayer MoS_2 grown on FSS and PSS by continue-wave 532 nm laser excitation. The PL peaks of the monolayer MoS_2 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 MoS_2 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 MoS_2 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 MoS_2 from the FSS, the integrated optical powers of the far fields for MoS_2 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 MoS_2 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 MoS_2 grown on a nonplanar sapphire substrate. The monolayer MoS_2 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 MoS_2 on PSS increased the light extraction efficiency. The PL intensities of the monolayer MoS_2 grown on the PSS exhibited 3-fold enhancement, compared with the monolayer MoS_2 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 nano-tructures to realize the ultra-thin optoelectronic integrated systems.

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