Correlation of Nanogap Formation and Strain Distribution in Single-Layer CVD MoS_2

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ABSTRACT

Molybdenum disulfide (MoS_2), a promising semiconducting material with high carrier mobility and atomic flatness, has shown potential in electronic applications. However, strain induced by the thermal expansion mismatch between MoS_2 and its growth substrate during the chemical vapor deposition (CVD) process can lead to nanogap formation, affecting its performance and functionality. In this study, the correlation between strain distribution and nanogap formation in single-layer CVD MoS_2 was investigated using photoluminescence (PL) mapping. We successfully imaged the strain distribution in MoS_2 flakes using PL mapping, and it was revealed that the adhesion between MoS_2 and substrate significantly affects strain distribution in MoS_2 flakes. In addition, we can conclude that the nanogap formation can partially release the growth-induced strain in MoS_2 flakes. The nanogap propagation mechanism was also revealed by comparing the strain distribution of two MoS_2 flakes with different nanogap structures.

KEY WORDS

Molybdenum disulfide (MoS_2), photoluminescence (PL) spectroscopy, strain, nanogap, chemical vapor deposition (CVD)

1. INTRODUCTION

Molybdenum disulfide (MoS_2) is a compromising semiconducting material due to its atomic flatness and high carrier mobility. In particular, chemical vapor deposition (CVD)-grown MoS_2 has been widely explored for electronic applications due to its high quality and scalability. However, the thermal expansion coefficient mismatch between MoS_2 and growth substrate induces strain in MoS_2 flakes, and the nanogap structure can be formed to release such growth-induced strain. Analyzing and controlling this unique nanogap structure is worthwhile since it can be an intriguing opportunity to explore new functional applications, such as nanogap electrodes, biosensing devices, and gas sensors. In this work, the correlation between the strain distribution and nanogap formation in single-layer CVD MoS_2 was investigated, which is necessary to reveal the nanogap formation mechanism and control the nanogap structure during synthesis. We successfully imaged the strain distribution in MoS_2 flakes using photoluminescence (PL) mapping, and it was revealed that the adhesion between MoS_2 and substrate significantly affects strain distribution in MoS_2 flakes. In addition, by comparing the strain distribution of the flakes with and without nanogap, it can be concluded that the formation of nanogap can partially release the growth-induced strain in MoS_2 flakes. The nanogap propagation mechanism was also revealed by comparing the strain distribution of two MoS_2 flakes with different nanogap structures.

2. RESULTS

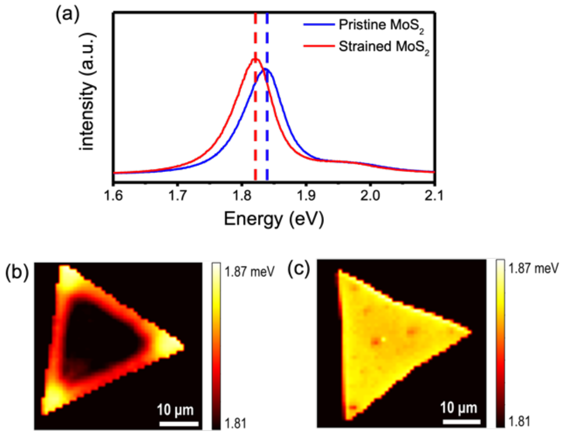

Figure 1. (a) Photoluminescence (PL) spectrum of the pristine (red line) and strained (blue line) single-layer MoS_2. PL mapping image of the single layer MoS_2 flake, which has (b) good and (c) bad adhesion with the growth substrate.

It is known that the PL peak position of single-layer MoS_2 shifts to the lower energy due to the strain in MoS_2, as shown in Figure 1(a). Therefore, a PL mapping image can visualize the strain distribution in MoS_2 flakes. Figure 1(b) and (c) are PL mapping images of the single-layer MoS_2 flake, which has good and bad adhesion with the substrate. Unlike the homogeneous signals in the bad adhesion sample, the good adhesion sample clearly shows the strain distribution. In the good adhesion sample, the relaxation of thermal strain induced in MoS_2 is retarded due to the relatively good adhesion between MoS_2 and the SiO_2 substrate during the cooling process. However, in the bad adhesion sample, the interface and edge bonding between the MoS_2 layer and the substrate are not sufficiently strong to retain the strain, resulting in the complete relaxation of thermal strain during the cooling process.

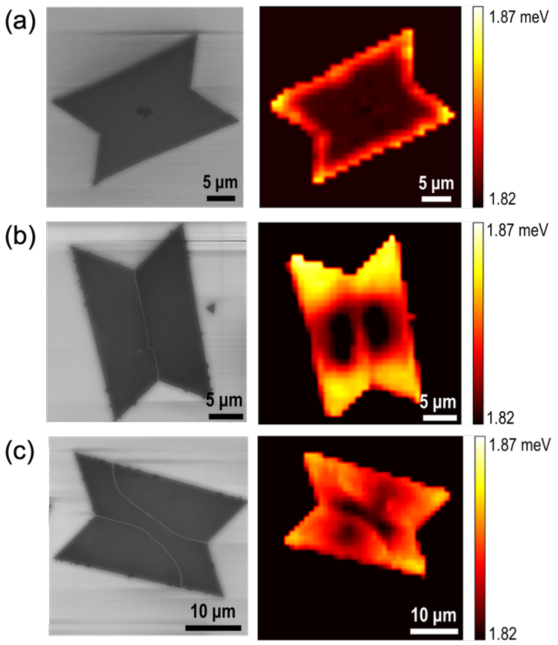

Figure 2. (a) Scanning electron microscopy (SEM) image (left) and PL mapping image of the polycrystalline MoS_2 flake without nanogap. (b) SEM image (left) and PL mapping image of the polycrystalline MoS_2 flake with nanogap following grain boundary. (c) SEM image (left) and PL mapping image of the polycrystalline MoS_2 flake with randomly oriented nanogap.

Figures 2(a), 2(b), and 2(c) are the scanning electron microscopy (SEM) (left) and PL mapping (right) images of the polycrystalline MoS_2 flakes without nanogap, with nanogap following grain boundary and randomly oriented nanogap, respectively. In the PL mapping image, the MoS_2 flake without nanogap shows a consistent peak position across the flake except for the edge area where partial strain release occurs (Figure 2(a)). In contrast, MoS_2 flakes with nanogap exhibit a peak position shift towards higher energies along the propagation direction of the nanogap, indicating a partial release of growth-induced strain along the path of the nanogap formation (Figures 2(b) and 2(c)). This result suggests that the thermal strain in MoS_2 flakes can be partially released by forming the nanogap structure. Moreover, the direction of nanogap propagation can also be related to the adhesion of MoS_2 and the substrate. Nanogap can be formed following the grain boundary of the polycrystalline MoS_2 flakes, as shown in Figure 2(b). However, nanogaps can be formed randomly, as shown in Figure 2(c). In 3 different samples that have different adhesion properties with the substrate, the ratio of the number of flakes with nanogap following the grain boundary and flakes with nanogap both following the grain boundary and random direction are calculated, and it was confirmed that the better the adhesion, the higher the ratio (47.8%, 36.3% and 12.1%). Due to the weak interaction with the underlying substrate, the bad adhesion sample can undergo higher mechanical deformation than the good adhesion sample. Therefore, in the bad adhesion sample, nanogap formation mainly occurred in random directions, starting from the edges of the grain boundary. However, in the good adhesion sample, sufficient interface bonding between the flakes and the substrate can make nanogap propagation occur at a relatively low speed, resulting in a higher ratio of nanogap formation along the grain boundary than in the case of the bad adhesion sample.

3. CONCLUSION

The strain distribution in various MoS_2 flakes was successfully measured using PL mapping. Adhesion between the MoS_2 layer and the substrate plays a key role in strain distributions of MoS2 flakes and the nanogap formation occurs to release the strain and the strain distribution can affect to resulting structure of the nanogap.

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REFERENCES

1. S. Luo, C. P. Cullen, G. Guo, J. Zhong, and G. S. Duesberg, "Investigation of growth-induced strain in monolayer MoS_2 grown by chemical vapor deposition," Applied Surface Science, vol. 508. Elsevier BV, p. 145126, Apr-2020.
2. Z. Liu et al., "Strain and structure heterogeneity in MoS_2 atomic layers grown by chemical vapour deposition," Nature Communications, vol. 5, no. 1. Springer Science and Business Media LLC, 18-Nov-2014.1 P. Sampras and A. Agassi, How to play successfully tennis (Int. Sports Press, Timbuktu, 1998).