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Properties of Molybdenum Disulfide and Preparation Method

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ABSTRACT

Behind the development of integrated circuits to the current brilliant era is the contribution of Moore's Law, which has guided the development prospects of the industry for a long time. But as transistors continue to shrink in size and thickness, silicon itself approaches its own physical limits and Moore's Law no longer applies. Therefore, scientists are eager to solve this puzzle by introducing new materials, including two-dimensional materials. Molybdenum disulfide has attracted much attention because of its special properties, and the preparation method needs to be studied deeply for large-scale use of molybdenum disulfide. There are many factors that affect the synthesis of single layer molybdenum disulfide, such as the amount of reaction source, air pressure, substrate, reaction temperature of two sources, source heating rate, holding time, relative position between molybdenum source and sulfur source substrate, gas flow, etc. In short, these reaction conditions are summarized, which mainly affect the concentration and reaction speed of sulfur source and molybdenum source in the reaction substrate position. In this paper, the effects of CVD on the quality of single layer disulfide were summarized and its development trend was prospected.

KEYWORDS

New Materials; Molybdenum Disulfide; Preparation Method; CVD.

1. INTRODUCTION

Since the successful mechanical stripping and characterization of graphene, [1] there has been renewed interest in two-dimensional layered materials (2DLMs). In the case of graphene, its high inherent mobility, high current density, and bipolar electron hole symmetry all point to its potential in radio frequency (RF) applications. [2-7] Preliminary studies have shown that graphene-based Radio frequency field-effect transistors (RF FETs) have a transit frequency of more than 400 GHz. [2] However, the Dirac cone band structure of graphene results in a zero band gap, which limits current saturation in graphene devices, resulting in reduced voltage and power gain. [3] Therefore, the maximum oscillation frequency, f_{max} is much smaller than f_T in graphene devices, thereby reducing the performance of power amplifiers with a maximum operating frequency of f_{max}.

In addition to graphene, there is renewed interest in other 2DLMs. In 2DLMs, the transition metal dihalide (TMDs) family with the general formula MX_2 (M=metal, X= chalcogen) is of particular interest. Molybdenum disulfide (MoS_2) is one such TMD with thickness-dependent physical properties, which has opened up applications in optoelectronics, [8] flexible electronics, [9-10] spintronics, [11] and coupled mechatronics. [12]MoS_2 is a two-dimensional semiconductor with an overall indirect band gap of ~ 1.3 eV and a single layer direct band gap of ~1.8 eV. [13-15] Using high k media and substrate/top film engineering, [16-19] stripped monolayers of MoS_2 FETs have shown $I_{on}/I_{off} > 10^8$, the mobility exceeded 80 $cm^2/(V\ s)$. [20] In addition, stripped single-layer MoS_2 FETs exhibit current saturation, with a conduction current density of 300 μA/ μm and a transconductance of over 40 μS/μm. [20] Although MoS_2 has a lower mobility than graphene, the

intrinsic band gap of MoS_2 results in a voltage gain $A_v = g_m/g_{ds}$ greater than 30. [21] In addition, theoretical calculations predict electron saturation velocities greater than 3×10^6 cm/s, [22] sufficient to provide GHz transit frequencies at submicron channel lengths. These characteristics make MoS_2 an ideal candidate for RF applications.

At present, the chemical vapor deposition method is mainly used for the preparation of molybdenum disulfide materials at home and abroad, but it is still difficult to achieve large size and even wafer level growth of molybdenum disulfide by CVD method. Therefore, the relevant researchers have carried out a lot of research on the structure and properties of molybdenum disulfide in order to achieve the regulation of the structure and properties of molybdenum disulfide. Therefore, this paper reviews the research on molybdenum disulfide in recent years, puts forward the future development prospects of molybdenum disulfide, and provides new ideas and new methods for further regulating the growth of molybdenum disulfide.

2. STRUCTURE AND PROPERTIES OF MOLYBDENUM DISULFIDE

Molybdenum disulfide is a layered hexagonal crystal. Fused with a single layer of molybdenum disulfide, with a gap of 0.65 nanometers between each layer, a large number or multiple layers of molybdenum disulfide crystals can be produced using intermolecular interactions known as van der Waals forces. There are usually 1T, 2H, 3R three structures, Figure 1[23], because the 2H phase is the most stable structure of molybdenum disulfide, so it is more prone to this situation. During the 2H phase the stacking sequence is AbA BaB AbA, but during the 3R phase the stacking sequence is AbA BcB CaC AbA. Both types of polycrystals have a crystallographic distance of 2.41[24-26] angstrom between the molybdenum atom and its nearest S atom. The 2H-MOS_2 morphology is by far the most common, because the 2H phase MoS_2 cells are periodically arranged in two layers, and when the number of layers is odd, the 2H phase MoS_2 exhibits a spatially antisymmetric failure state, and when the number of layers is even, it exhibits a centrosymmetric arrangement. Therefore, the 2H-MoS_2 structure has received the greatest attention from scientists.

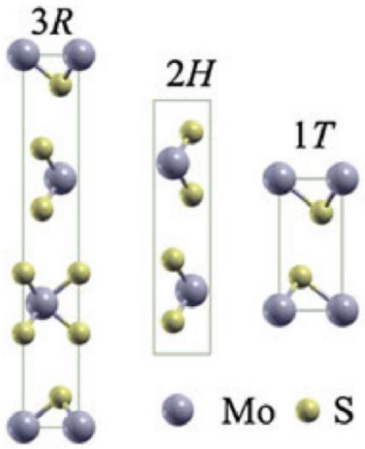


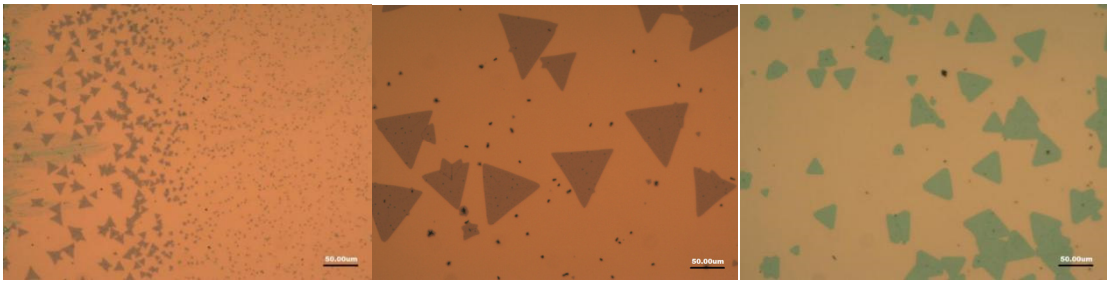
Fig 1. Side view of MoS_2 (cell) 3R, 2H and 1T phases [23]

3. PREPARATION OF MOLYBDENUM DISULFIDE

3.1. Effect of Temperature on Growth of Molybdenum Disulfide

As shown in Figure 2, the appearance of MoS_2 is different. At 700 ° C, the size of a single triangle is smaller; At 750 °C, the size of MoS_2 is larger; When the temperature rises to 800 degrees Celsius, although it is still dominated by triangles, the size of these triangles is reduced, and the edges are more rounded, which indicates that the growth conditions of MoS_2 are ideal at 750 degrees Celsius.

The different morphologies at different temperatures are caused by the different content ratio of Mo source vapor and S source vapor in the quartz tube. Since the temperature on the S side remains unchanged during growth, both being 180 ℃, the higher the temperature on the MoO_3 side, the more MoO_3 will be vaporized, and the ratio of Mo to S will increase. When the temperature is 700 ° C, the shape change is approximately dart-like, and the surrounding triangular edge phase is concave. This is because the lower temperature reduces the evaporation of MoO_3, resulting in a Mo:S ratio lower than the Mo:S ratio of 750 ° C, which makes the growth rate difference between the Mo terminal and the S terminal greater, and the edge growth of S cannot catch up with the edge growth of Mo. When the temperature is 800 ℃, the reaction degree is severe due to the high temperature, and the triangle shape becomes smooth and the size decreases. This is because at high temperatures, the high activity of the atoms at high temperatures promotes the reorganization of the atoms at the edge of the crystal, forming a smooth edge with lower energy and more stability, in addition to high temperatures, the edge of the MoS_2 crystal may be vaporized, especially in the late stage of the growth process. This evaporated material may recondense elsewhere, resulting in a reduction in the size of the original crystal and a smoother edge. Therefore, according to the growth situation, the optimal growth temperature of MoS_2 is 750 ℃

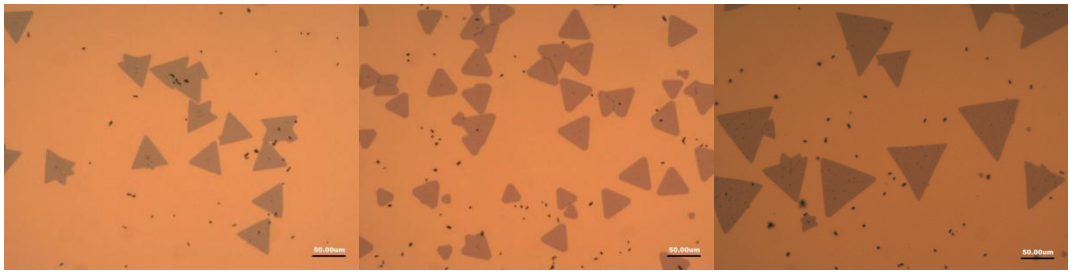


(a)700 ℃ (b)750 ℃ (c)800 ℃

Fig 2. Morphology of molybdenum disulfide at different temperatures

3.2. Effect of Heating Time on Growth of Molybdenum Disulfide

Figure 3,When the growth time is set to 20 min, MoS_2 on the substrate surface is very rare, and its size is only more than a few microns. This indicates that after MoS_2 crystal nuclei are formed and begin to expand, the growth process ends before it is completely completed, and this stage corresponds to the beginning of the temperature decline process. When the growth time is 25 min, the amount of MoS_2 coverage on the substrate increases, but the size does not change and the color is lighter. This showed that increasing the growth time did not have a significant effect on the transverse growth of MoS_2, and did not allow the island monolayer structure to grow into a larger area of MoS_2 monolayer film. This may mean that growth ends before expansion is complete after nucleation; With the growth time increased to 30 min, the color and size of the sample were significantly deepened. Therefore, according to the above analysis, it can be concluded that the ideal growth time of MoS_2 is about 30 min.

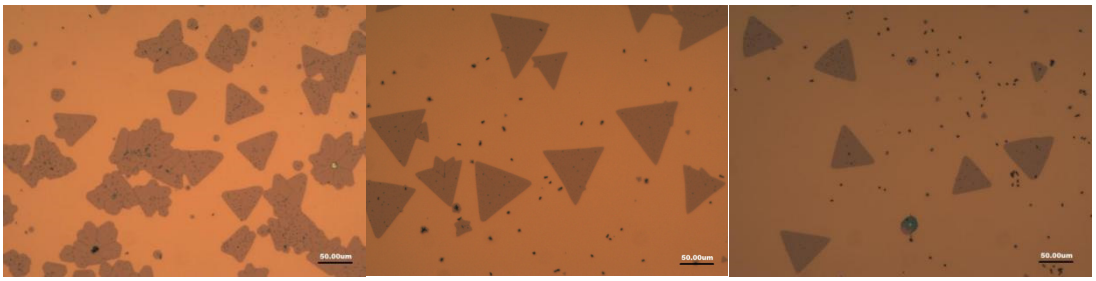


(a)20 min (b)25 min (c)30 min

Fig 3. Morphology of molybdenum disulfide under different heating time

3.3. Effect of Flow Velocity on Molybdenum Disulfide Growth

The growth of single layer MoS_2 also depends on the concentration of MoO_{3-x} and S precursors on the substrate surface, however, the distribution concentration of these two precursors on the substrate can be controlled by adjusting the flow rate of the carrier gas. The nucleation density is determined by the speed of gas flow when the substrate is inverted at the growth source. Under optimal growth conditions, three gas flow gradients were set, ranging from 5 sccm argon flow to 15 sccm argon flow, with intervals of 5 sccm. Too large or too small an air stream can result in a low concentration of precursors [27]. Lower gas flow rates are not sufficient to effectively deposit MoO_{3-x} and S on the substrate, while higher flow rates may blow away the precursor concentration below the substrate. Therefore, a moderate gas flow rate helps to form an ideal reactant concentration on the substrate surface. As observed in Figure 4 (a), a large number of nucleation points will appear on the substrate surface at low flow rates, and the growth will be disorderly. This is because at low airflow speeds, the mechanism controlling crystal growth changes from kinetic to thermodynamic. Therefore, at a higher growth temperature and a lower flow rate, the growth as shown in Figure 4 (a) will occur. In contrast, crystal growth is controlled kinetically at moderate airflow speeds, resulting in a uniform nucleation density on the substrate surface, as shown in Figure 4 (b). When the gas flow rate reaches 30 sccm, the nucleation point of MoS2 becomes thinner and the crystal size decreases, indicating that the high carrier gas flow rate causes the downstream S vapor to be displaced before reacting with the Mo source, which impedes growth, as shown in Figure 4 (c). Therefore, the gas flow rate set to 25 sccm is the ideal condition for MoS_2 growth.



(a)5 sccm (b)10 sccm (c) 15 sccm

Fig 4. Morphology of molybdenum disulfide at different flow rates

3.4. Influence of Other Conditions on Molybdenum Disulfide

In addition to the above conditions, the holding time will also affect the growth of molybdenum disulfide, in the case of sufficient supply of sulfur and molybdenum oxide atmosphere, the growth shape of the material under different holding time is consistent, only the size is different. However, when the atmosphere was insufficient, the growth situation was reversed, due to a change in the ratio between Mo and S atoms on the substrate surface when MoO_3 stopped heating growth. MoS_2 has two competing crystal faces, Mo and S, so the ratio between Mo and S atoms also affects the energy stability of the two growth directions. In addition, different sulfur sources will cause the lattice to receive different interstitial atomic interaction stresses, thus affecting the structure. Therefore, different sulfur sources will also affect MoS_2 growth.

4. SUMMARY

Molybdenum disulfide is a kind of two-dimensional transition metal sulfide. With the deepening of scientific and technological research, the single preparation technology of molybdenum disulfide cannot meet the needs of industrial production. As a result, the simultaneous use of many methodological systems is becoming an increasingly common research preparation strategy. In addition, due to the research carried out in the field of molybdenum disulfide over the past years,

molybdenum disulfide may one day replace silicon in the field of optoelectronics due to its better properties. Because people's understanding of molybdenum disulfide has not been systematically and thoroughly studied, there are still several important problems in its basic principle and special application. Most scholars need to make long-term, sustained efforts and seek new ways to solve these difficult problems. China is an important molybdenum mining country, which provides a resource guarantee for our future molybdenum research, but also requires us to make acceptable arrangements in the research process to use our molybdenum resources more effectively.

REFERENCES

[1] Novoselov, K.S;Geim, A.K;Morozov,S.V;Jiang,D;Zhang, Y.Dubonos, S.V; Grigorieva,I.V; Firsov,A. A Science 2004,306,666-669.

[2] Cheng,R; et al. Proc. Natl. Acad. Sci.U.S.A. 2012,109,11588-11592.

[3] Schwierz, F; et al. Proceedings of the IEEE 2013,101,1567-1584.

[4] Wu,Y;Jenkins,K;Valdes-Garcia,A;Farmer,D;Zhu,Y;Bol,A; Dimitrakopoulos,C; Zhu, W; Xia, F; Avouris, P; Lin,Y.-M. NanoLett. 2012,12,3062-3067.

[5] Lee,J.; Ha,T.-J;Li, H; Parrish,K; Holt, M; Dodabalapur, A;Ruoff, R; Akinwande,D.ACS Nano 2013,7,7744-7750.

[6] Ramon, M; Parrish, K; Chowdhury, S; Magnuson, C; Movva, H; Ruoff, R; Banerjee, S; Akinwande, D. IEEE Trans. Nanotechnol.2012,11,877-883.

[7] Han,S. J; Garcia,V. A; Oida,S; Jenkins,K. A; Haensch,W.Nat. Commun.2014,5,3086.

[8] Lopez-Sanchez, O; Lembke, D; Kayci, M; Radenovic, A; Kis, A.Nat. Nanotechnol.2013,8, 497-501.

[9] Akinwande,D; Petrone,N; Hone,J. Nat.Commun.2014,5,5678.

[10] Chang, H.-Y; Yang, S; Lee, J; Tao,L; Hwang, W.-S; Jena, D;Lu,N;Akinwande,D.ACS Nano 2013,7.5446-5452.

[11] Zeng, H; Dai, J; Yao,W; Xiao, D; Cui,X. Nat. Nanotechnol.2012,7,490-493.

[12] Nayak, A; Bhattacharyya, S; Zhu, J; Liu, J; Wu, X; Pandey, T;Jin,C; Singh,A; Akinwande,D; Lin,J.-F. Nat.Commun.2014,5,3731.

[13] Frey, G. L; Elani,S; Homyonfer,M; Feldman,Y; Tenne, R.Phys.Rev.B:Condens.Matter Mater.Phys. 1998,57,6666.

[14] Mak,K. F;Lee,C; Hone,J; Shan,J; Heinz,T.F. Phys. Rev.Lett.2010,10S,136805.

[15] Cao,T; et al. Nat.Commun.2012,3,887.

[16] Radisavljevic, B; Radenovic, A; Brivio,J; Giacometti,V; Kis,A.Nat.Nanotechnol.2011.6.147-150.

[17] Liu, H; Ye, P.D.D. IEEE Electron Device Lett.2012,33,546−548.

[18] Lin, M. W; Liu, L. Z; Lan,Q; Tan, X. B; Dhindsa,K. S; Zeng,P; Naik, V. M; Cheng, M.M.C; Zhou, Z.X. J.Phys. D: Appl. Phys.2012,4S,345102.

[19] Sanne,A; Ghosh, R; Rai,A; Movva, H.C. P; Sharma, A; Rao,R; Mathew,L; Banerjee,S. K. Appl. Phys. Lett. 2015, 106,062101.

[20] Krasnozhon,D; Lembke, D; Nyffeler, C; Leblebici,Y; Kis,A.Nano Lett.2014,14,5905-5911.

[21] Cheng, R; Jian,S; Chen,Y; Weiss, N; Cheng, H. C; Wu,H;Huang, Y; Duan,X.Nat. Commun. 2014, 5,5143.

[22] Li,X.;Mullen,J;Jin,Z.;Borysenko,K.;Nardelli,M.;Kim,K.Phys.Rev.B:Condens.MatterMater. Phys.2013,87,115418.

[23] Cheng Y, Schwingenschlogl U. MoSg: A First-Principles Perspective[A].see:Z.M. Wang. MoS2 [M]. Cham: Springer International Publishing, 2014,21: 103-128.

[24] G.A. Tsigdinos,W.W. Swanson, Ind Eng Chem Prod Rd,17(1978) 208-214.

[25] R.G. Dickinson,L. Pauling, J Am Chem Soc, 45 (1923) 1466-1471.

[26] F.Jellinek, G.Brauer, H. Muller, Nature, 185 (1960) 376-377.

[27] Zhou D, Shu H B, Hu C L, et al.Unveiling the growth mechanism of MoS2 with chemicalvapor deposition: From two-dimensional planar nucleation to self-seeding nucleation[J].Cryst Growth Des, 2018,18(2): 1012-1019.