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Study of titanium disulfide with layered structure for carbon capture

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Abstract: CO_2 adsorption is an effective way to reduce carbon emissions. Many researchers have investigated the CO_2 adsorption performance of titanium-based materials. Mesoporous titanium disulfide (TiS_2) with layered structure was prepared by solid state reaction method under different temperatures. Then the synthesized samples were characterized by X-ray powder diffraction (XRD), scanning electron microscope (SEM), and nitrogen physical adsorption. CO_2 adsorption isotherms between 0-1.1 bar were measured at 0 ℃ and 20 ℃. It confirmed that CO_2 adsorption mechanism was physical adsorption determined by pore volume. Dependence of the amount of CO_2 adsorbed on the pore volume was analysed and proved again the importance of pore volume to physical adsorption. Absorption/regeneration cycle on TiS_2-700 was also performed. The CO_2 adsorption capacity decreased slightly over 4 cycles. Mesoporous TiS_2 with layered structure displayed an excellent CO_2 adsorption property.

1. Introduction

Postcombustion capture is probably the first technology that will be applied in CO_2 removal because existing combustion technologies could still be used without radical changes on them [1]. Among the various separation technologies such as absorption, adsorption and membrane, adsorption may be regarded as a promising method [2]. Its major advantage is the ease of the adsorbent regeneration and low-cost CO_2 capture [3]. The application of adsorption requires easily regenerable and durable adsorbents with a high CO_2 adsorption capacity.

Seayad A. M. et al. [4] found that mesoporous Ti oxides may serve as hosts for hydrogen storage. These materials possess high surface areas, tunable pore sizes, the capacity for coordinative unsaturation and variable oxidation states of the Ti center [5-6], which are not present in other materials such as MOFs, zeolites and porous carbon. Therefore, titanium-based materials show exciting prospects for gas adsorption [7].

Many researchers have investigated the CO_2 adsorption performance of titanium-based materials, including potassium-based TiO_2 sorbents [8], TiO_2-doped K_2CO_3/Al_2O_3 [9] and MEA modified TiO_2 nanoparticles [10]. All of them showed excellent CO_2 adsorption capacity and good

regenerability because the CO_2 adsorption mainly relies on the weak chemisorption provided by amino groups, which can be regenerated efficiently.

Similar to graphite, titanium disulfide (TiS_2) have a layered (X-M-X) structure. Atoms within S-Ti-S sheets are bound by strong covalent interactions. Bonding between the layers is determined by weak Van der Waals forces [11]. In recent years, TiS_2 and their intercalation compounds have attracted considerable theoretical and experimental interests because of their interesting layer structure and anisotropic physical properties as well as owing to their potential applications [12-13]. For example, TiS_2 exhibits metallic electronic conductivity at all temperature with an unusual T_2 temperature relationship due to the high density of free carriers in this layered material, which can be regarded as a kind of 2D solid [14]. TiS_2 has been used as the cathode material in high energy-density lithium batteries [15].

TiS_2 shows excellent hydrogen storage performance, since foreign atoms can be easily intercalated in between the S-Ti-S layers that are held by van der Waals interactions. Chen et al. have synthesized tubular TiS_2 with uniform open-ended structure with reversible hydrogen storage of 2.5wt % at 25 ℃ and 4 MPa. Among them, chemical and physical adsorbed hydrogen are 40% and 60% respectively [16].

Inspired by the studies mentioned above, mesoporous TiS_2 with layered structure was prapared by solid state reaction method for CO_2 capture. The structure and CO_2 adsorption performance of layered TiS_2 was investigated. CO_2 adsorption mechanism was deduced. Absorption/regeneration cycle was also performed.

2. Experimental

2.1. Preparation of layered TiS_2

Mesoporous TiS_2 with layered structure was prepared by solid state reaction method. 2.4 g Ti and 3.2 g S powder (Ti: S mole ratio =1: 2) were mixed evenly in a ceramic combustion boat, in which iodine was added as the transport agent. The boat was transferred into a tubular reactor and evacuated for 30 min. After heating at 600 ℃ for 48 h, the powder was washed with ethanol and dried at 100 ℃. The obtained sample was denoted as TiS_2-600. TiS_2-700 and TiS_2-800 were prepared by the similar method.

2.2. Characterization

The power X-ray diffraction (XRD) (Beijing Purkinje General Instrument Co., Ltd., China) pattern were recorded using nickel-filtered Cu Kα radiation at 36kV and 40mA (2θ ranging from 5°to 80°, λ=0.15418nm and 0.02°step size). The morphologies of samples were observed on the FEI Quanta 250F microscope (Quantachrome Instrument, American). The BET surface areas (SBET) and pore volumes (Vpore) of given samples were determined by surface area and pore porosimetry analyzer (V-Sorb 2800P).

CO_2 adsorption isotherms were measured using a surface area and pore porosimetry analyzer (V-Sorb 2800P) under low pressure (0-1.1 bar). The experiments were conducted at 0 ℃ and 20 ℃ by the dewar flask using ice water or circulated water in which the sample tube was immersed. Prior to each adsorption experiment, the samples were degassed at 120 ℃ overnight. The reversibility of the CO_2 adsorption process on the samples studied was tested by multiple CO_2 adsorption cycles. The corresponding adsorption isotherms have been acquired after heating at 120 ℃ for 12 h in vacuum in sequence.

3. Results and discussion

X-ray diffraction patterns of the synthesized adsorbents are presented in Figure 1. The diffraction of TiS_2-600 shows the presence of peaks at 2θ = 15.2°, 33.9°, 43.6° and 53° corresponding to (001), (101), (102), and (110) planes of TiS_2, respectively (JCPDS No. 15-0853) [17]. The peak at 27.3 °is attributed to the (110) plane of rutile-phase TiO_2 [18]. The major peaks of TiS_2-600 are almost replicated by TiS_2-700 with an intensity increase and peak shifts. In addition, new peaks were observed at 2θ of 36.8 ° and 41 °, corresponding to (101) and (111) reflections of crystalline anatase phase [19]. When the synthesis temperature increased to 800 ℃, the intensity of characteristics diffraction peak for TiS_2 decreased and other peaks disappeared, while the intensity of rutile-phase TiO_2 increased dramatically. In conclusion, the synthesized material changed from TiS_2 to rutile-phase TiO_2 with the increase of synthesis temperature.

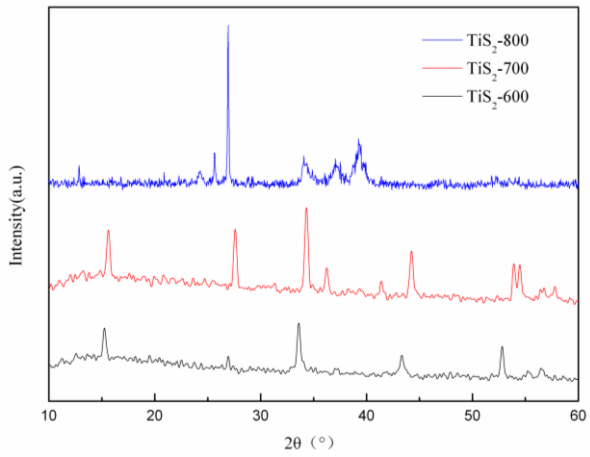

Figure 1: XRD patterns of layered TiS_2 prepared under different temperatures.

Scanning electron images of synthesized materials are given in Fig. 2. Figure 2A displays that the TiS_2-600 consists of irregular lumps with part of layered structures. In Figure 2B, TiS_2-700 is composed of layered structures almost completely. When the synthesis temperature increased to 800 ℃, cracks could be observed on the surface of material in Figure 2C.

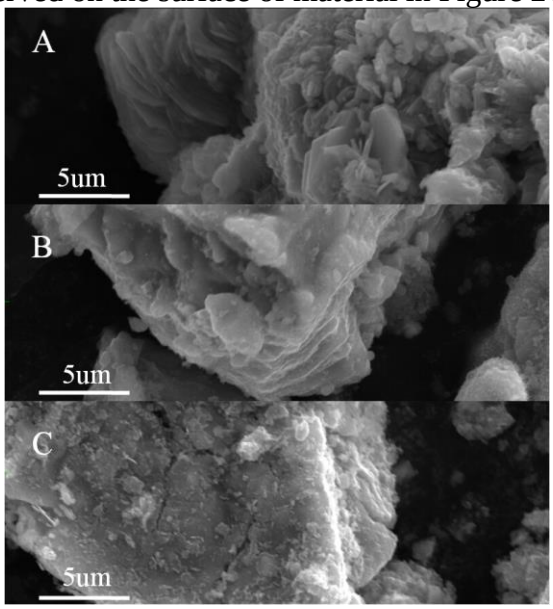

Figure 2: SEM of TiS_2-600 (A), TiS_2-700 (B) and TiS_2-800 (C).

The N_2 adsorption-desorption isotherms of the synthesized materials are collected in Figure 3(a). All isotherms of the samples reveal typical type-IV behavior with hysteresis loops of type H2, indicating that the adsorbents contained mesoporous structures (2-50 nm) with ink-bottle pore [20].The BJH pore size distributions were shown in Figure 3(b). It could be seen that pore size of all the three samples distributes in the range of 2-18 nm, with different average pore diameter of 7.4nm, 8.6nm and 8.3nm respectively. The physical properties of the materials are presented in Table 1. The surface area and pore volume of three samples is in the order of TiS_2-700 > TiS_2-800 > TiS_2-600.

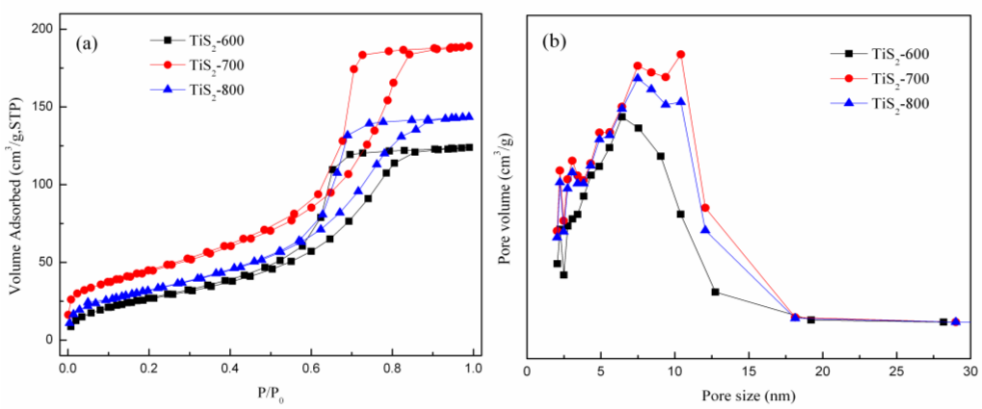

Figure 3: N_2 adsorption-desorption isotherms (a) and pore size distributions (b) of TiS_2 prepared under different temperatures.

Table 1: Physicochemical characteristics of TiS_2 prepared under different temperatures.

Samples	Surface area (BET)(m^2/g)	Pore volume (cm^3/g)	Pore diameter (BJH)(nm)
TiS_2-600	113	0.19	6.93
TiS_2-700	179	0.34	8.38
TiS_2-800	138	0.25	9.27

Figure 4 show the CO_2 adsorption isotherms on the synthesized materials at 0 ℃ and 20 ℃ in the pressure range from 0 to 1.1 bar. The CO_2 adsorption capacities at 1 bar are collected in Table 2. The order of the CO_2 adsorption uptakes on the two samples studied at two temperatures follows the trend found at dynamic conditions [21]. The CO_2 uptake at 0 ℃ is almost 1.5 times of that 20 ℃. At the same temperature, CO_2 uptake of the three samples follows the trend of TiS_2-700 > TiS_2-800> TiS_2-600, which is consistent with that of surface area and pore volume. Therefore, the CO_2 adsorption on the synthesized adsorbents is mainly dependent on van der Waals interaction determined by the surface area. In addition, the layered structure of TiS_2 is combined by electrostatic interaction, which also enhances the CO_2 uptake enormously. Both van der Waals interaction and electrostatic interaction could be attributed to physisorption.

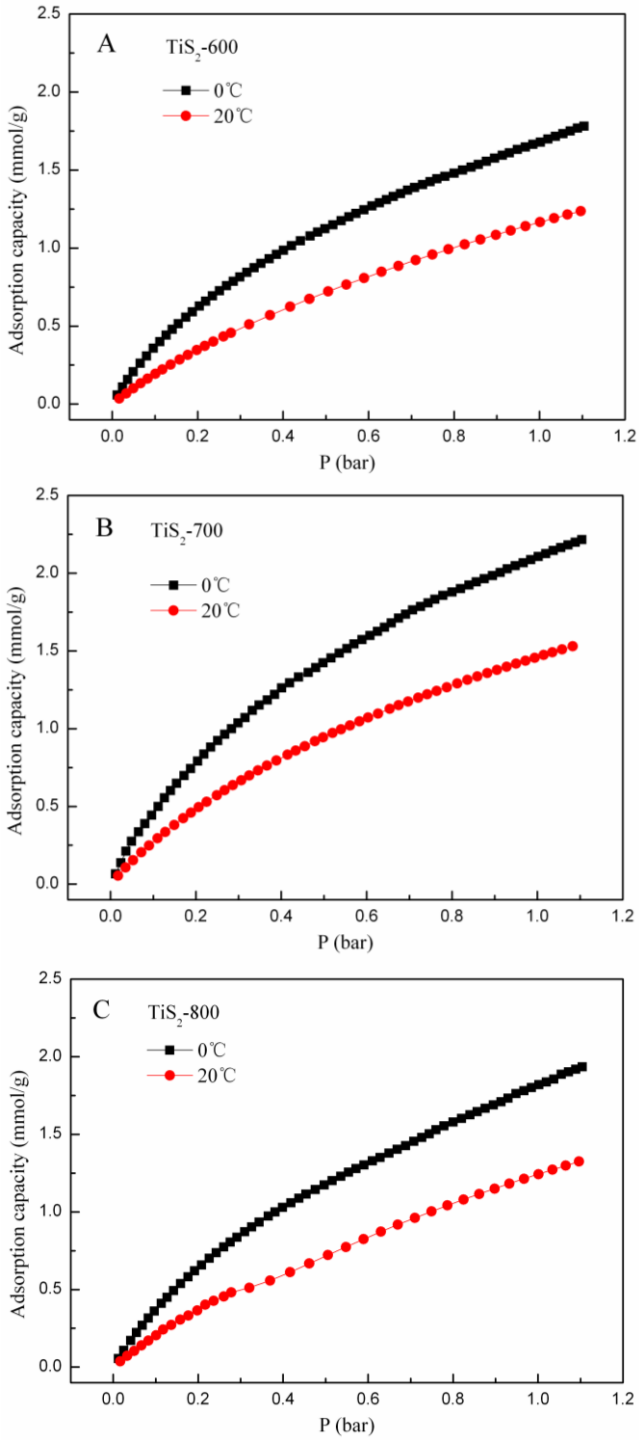

Figure 4: CO_2 adsorption isotherms on the synthesized TiS_2 at 0 ℃ and 20 ℃.

Table 2: Amount of CO_2 adsorbed at 0 ℃ and 20 ℃ under 1 bar.

Samples	Amount of CO_2 adsorbed (mmol/g)	
	0 ℃	20 ℃
TiS_2-600	1.68	1.17
TiS_2-700	2.11	1.47
TiS_2-800	1.82	1.24

To visualize the importance of pore volume on the CO_2 uptake, the dependence of CO_2 adsorption capacity at 0 ℃ and 20 ℃ on the pore volume was analysed. As seen in Figure 5, CO_2 uptake increases linearly with the increase of pore volume at both 0 ℃ and 20 ℃. Good linear correlation validates the hypotheses on the physical adsorption as the main mechanism of CO_2 adsorption on the synthesized materials.

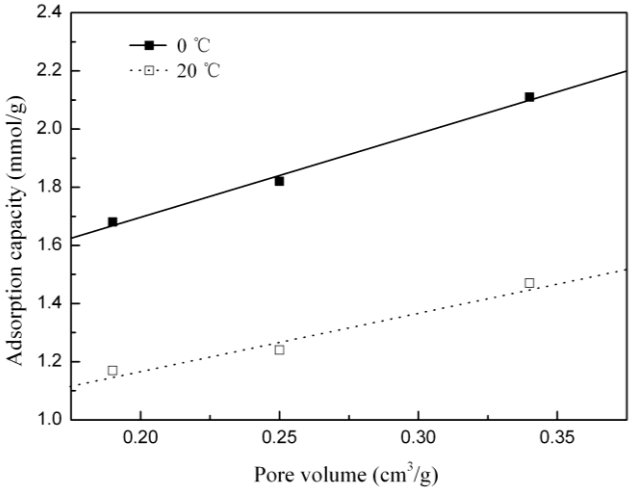

Figure 5: Dependence of the amount of CO_2 adsorbed on the pore volume

The mechanism of CO_2 adsorption on the synthesized materials is deduced in Figure 6. As mentioned above, the order of CO_2 uptake of the three samples is consistent with that of pore volume. It confirmed that CO_2 adsorption on the synthesized adsorbents is dependent on van der Waals interaction determined by the pore volume to a great degree. In addition, the layered structure of TiS_2 is combined by electrostatic interaction, which also enhances the CO_2 uptake enormously [22]. Both van der Waals interaction and electrostatic interaction could be attributed to physisorption.

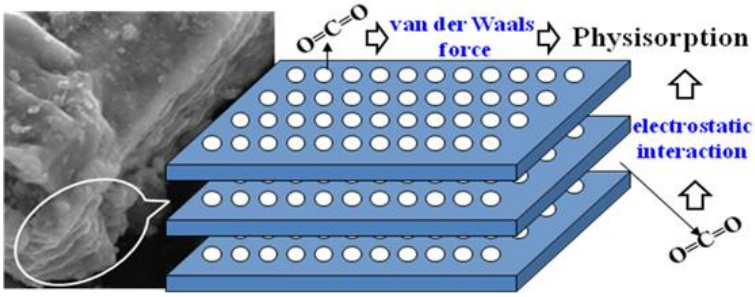

Figure 6: The mechanism of CO_2 adsorption on mesoporous TiS_2 with layered structure.

Figure 7 depicts the reversibility of the CO_2 adsorption on TiS_2-700 at 0 ℃ and 20 ℃. The regeneration was performed at 120 ℃ in vacuum in sequence. The absorption/regeneration cycle was repeated for a total of 4 cycles. The cyclic CO_2 adsorption capacities at 1 bar are collected. CO_2 uptake at 0 ℃ and 20 ℃ are 2.11 and 2.03 mmol/g, which decrease by 3.8 % and 4.1 % over 4 adsorption/desorption cycles.

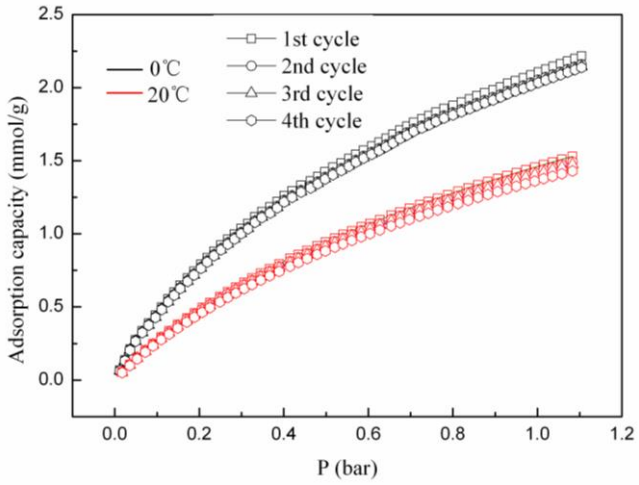

Figure 7: CO_2 adsorption/desorption isotherm cycle on TiS_2-700 measured at 0 ℃ and 20 ℃

4. Conclusions

TiS_2 was prepared by solid state reaction method under different temperatures for CO_2 capture. SEM showed that TiS_2 consisted of layered structures. Nitrogen physical adsorption indicated that the adsorbents contained mesoporous structures (2-50 nm) with ink-bottle pore. CO_2 adsorption isotherms between 0-1.1 bar were measured at 0 ℃ and 20 ℃. It confirmed that CO_2 adsorption mechanism was physical adsorption determined by pore volume. In addition, the layered structure of TiS_2 is combined by electrostatic interaction, which also enhances the CO_2 uptake enormously. Both van der Waals interaction and electrostatic interaction could be attributed to physisorption.

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