The Crystal Structure of Molybdenum Trioxide and its Main Applications

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Abstract

Molybdenum trioxide is a typical layered transition metal oxide and the most important intermediate compound in the production of molybdenum metal.MoO_3 has attracted more and more attention in many fields due to its unique two-dimensional layered structure and special physical properties.MoO_3 has 5 different crystal structures:α-MoO_3, h-MoO_3, β-MoO_3, β'-MoO_3 and MoO_3-II, among which there are three common phase structures: normal (α-MoO_3), monoclinic (MoO_3-II), and hexagonal (h-MoO_3).Molybdenum trioxide is widely used in many fields, such as gas sensors, lithium ion batteries, electrochromic, photochromic materials, catalytic materials, and raw materials for the synthesis of other materials.It can be seen from a large number of studies that layered MoO_3 has shown excellent performance in many fields and has attracted more and more attention.

Keywords

MoO_3, Layered transition metal oxide, Lithium ion batteries, Photochromic materials.

1. Introduction

Molybdenum trioxide is a typical layered transition metal oxide and the most important intermediate compound in the production of molybdenum metal.MoO_3 has attracted more and more attention in many fields due to its unique two-dimensional layered structure and special physical properties.

2. Organization of the Text

2.1 Structure of MoO_3

At present, there are 5 MoO_3 crystals with different structures, which are α-MoO_3, h-MoO_3, β-MoO_3, β'-MoO_3, and MoO_3-II, whose basic building units are MoO_6 octahedrons. However, molybdenum trioxide of different structures is due to the difference in the arrangement of octahedrons. Among them, there are three common phase structures: normal (α-MoO_3), monoclinic (MoO_3-II), and hexagonal (h-MoO_3).

2.1.1 Thermodynamically Stable Phase Structure

Steady-state α-MoO_3 crystal structure belongs to the orthogonal crystal system, it has a 2d layer structure, its layered structure perpendicular to the (1, 0, 0) surface accumulation , Within the plane, the distorted MoO_6 octahedron is joined by common edges in one direction to form a serrated chain. chain in another direction are connected to the common point between the chain, has formed a two-dimensional infinite extension of surface layer, and rely on van der Waals force between layer and layer, and the layers are arranged in a double wave along the direction of the a lattice, like this kind of layer structure in the metal oxide is rare.

2.1.2 Metastable Phase Structure

Monoclinic MoO_3 is a distorted ReO_3 structure, It is a solid structure formed by octahedral covertex Angle, Mo atoms distribution in MoO_3 cubic unit cell of eight corners, O atoms are distributed in every side, when heated to a certain temperature, MoO_6 octahedron will move, and the original yellow monocline will turn into the white orthorhombic phase α-MoO_3, In this process, the octahedron changes from being connected by vertices to being connected by common edges in one direction and by common vertices in the other direction, so it is called thermodynamic metastable phase.Because

of this particular distribution of Mo and O atoms, the monoclinal phase is a particularly empty structure, which facilitates the insertion and ejection of particles.

Hexahedral h-MoO_3 is connected by three octahedrons into a group of common vertices,forming a structural unit, which forms a chain form by common edges of each structural unit, and then the three-dimensional stacking of chains will form hexahedral h-MoO_3, which is very similar to the structure of ortho-intersection phase.There are many vacancies in the position of Mo in the hexagonal structure, which provides convenience for the movement of lithium ions in crystal holes. Therefore, h-MoO_3 as the cathode material of lithium ion battery [1], is a good choice.

2.2 Main applications of MoO_3

Due to its unique layered structure, molybdenum trioxide is widely used in many fields, mainly in the following aspects:

2.2.1 Gas Sensor

Semiconductor metal oxides are generally gas sensitive because of their stable structure, small size, low cost and high sensitivity.Among the numerous metal oxides, the octahedral elements in MoO_3 structure can form chain structure or special pore structure, so it is considered as an excellent gas sensitive material in the future in the detection of toxic and harmful gases. MoO_3 is highly sensitive to many gases, such as NO, NO_2, CO, H_2, NH_3, H_2S, HCOH, etc. However, compared with zinc oxide and titanium dioxide, molybdenum trioxide is still not competitive and has not been widely accepted as a gas sensor. It is hoped that a gas-sensitive material worthy of greater application can be developed. However, compared with traditional membrane MoO_3 materials, the special size of nanomaterials may give one-dimensional MoO_3 nanomaterials a more obvious advantage in the field of gas sensitivity, because the specific surface area of nanomaterials is larger than that of traditional membrane materials, which is crucial in the field of gas sensitivity [2].

2.2.2 Lithium Ion Battery

With the progress of The Times, science and technology are also growing rapidly, requiring electronic instruments and equipment to be smaller and smaller, resulting in a rapid increase in the demand for small, high-energy and highly reliable batteries. Lithium ion batteries are exactly the product of this era. Lithium battery is a kind of high efficiency battery, which is charged and discharged by the transfer of lithium ions between the positive and negative poles.Charging Li+ from the positive electrode through the electrolyte to the negative electrode, discharging the reverse, Li+ from the negative electrode through the electrolyte to the positive electrode. At the same time, the crystal structure of MoO_3 contains a lot of tetrahedral and octahedral holes, which are ideal embedding locations for some small ions such as Li+ and provide a wide channel for them. Moreover, the dissolution rate of MoO_3 in organic solvents is very low, and the polarization degree is also very small. Compared with other common cathode materials such as AgO, MoO_3 is cheaper and naturally rich than AgO, and it is more competitive than AgO due to its special layered structure, which makes molybdenum trioxide have great potential in the development of lithium batteries [3,4].

2.2.3 Electrochromic and Photochromic Materials

The performance of transition metal oxides in electrochromic and photochromic processes has attracted the attention of researchers.Electrochromic and photochromic film materials have been widely used in information storage, smart Windows, rear-view mirrors, self-developing holographic recording and some color changing devices. Electrochromism generally refers to the material under the action of external electric field, external ions inserted into the internal structure, resulting in the change of material transparency, color, and the process of color change is reversible, can change from color to transparent, also can change from transparent to color. When the color-changing glass is made of MoO_3 electrochromic film, it can change the color of the glass synchronously according to the outdoor light condition. This kind of glass can play the role of natural air conditioning, and when the energy saving efficiency is highest, it can save more than 50% of the energy required for building air conditioning. Similar to electrochromism, photochromism also changes the color of the irradiated material under the premise of light. However, this color change is also reversible. MoO_3 is an

electrochromic and photochromic material with low cost and good stability.However, because electrochromic devices do not require as much environmental factors as photochromic devices, they will be studied and applied by more people [1,5].

For metal oxides, photochromic changes are mainly due to impurities or crystal defects. Under light conditions, the charge in the crystal is transferred from the low energy state of oxygen to the high energy state of the metal.The MoO_3 we focus on has a relatively flat absorption curve in the visible light region, which can produce a better visual aesthetic effect. In addition, compared with other materials, the photochromic response time of MoO_3 films is shorter. But also has some limits in MoO_3 film, there is a big part of its light raw carrier in a relatively short time to compound, leading to a lower efficiency of MoO_3 film color, in order to avoid this shortcoming, can be covered on the surface of MoO_3 film precious metals to decorate, so on the MoO_3 and metal interface can form a Schottky barrier, this method reduces the light living carrier of composite risk, thus promoting the separation, greatly improve its efficiency.In addition, the photochromic properties of MoO_3 can also be improved by means of ion doping [6].

2.2.4 Catalytic Materials

In recent years, environmental pollution has become more and more serious, and how to control and govern it has become an important problem that needs to be solved urgently.Semiconductor materials have a broad prospect in photocatalytic application because of their unique properties. The photocatalytic oxidation-reduction reaction of semiconductor is also an effective new technology to control environmental pollution.The principle of photocatalysis is to use sunlight or other light as energy to completely oxidize organic pollutants to CO_2, H_2O and other harmless products through REDOX reaction at normal temperature and pressure, and the catalyst itself can be reused.When the semiconductor catalyst material is exposed to light, the internal electron transition phenomenon will occur, resulting in a large number of electrons and holes. When other materials touch the surface of the semiconductor catalyst, these electrons and holes will react with these materials, thus playing the role of photocatalysis.

At present, the catalytic properties of MoO_3 have attracted wide attention.MoO_3 is a wide-band gap semiconductor with a band gap width of about 3.0 eV, which can absorb visible light to a certain extent.When exposed to a certain wavelength of sunlight, MoO_3 is excited to produce conducting electrons and valence holes.The resulting cavity is a highly reactive oxide capable of breaking down common organic dyes.But light generated electrons and holes is easy to composite with electronic - hole on, in order to improve this, Huang [7] and others with g-C_3N_4 material covered on the surface of MoO_3, found that the g-C_3N_4 can help reduce MoO_3 electronic - hole on the composite time, through the degradation of methylene blue, the results show that the g-C_3N_4 under visible light is beneficial to improve the photocatalytic activity of MoO_3 and helpful to the heterogeneous barrier of the charge transfer. A. Chithambararaj[8] et al. successfully synthesized flower layered h-MoO_3 by using the advantage that h-MoO_3 band gap is located in the visible light region and is A suitable photocatalytic candidate material. Experimental observations have proved that h-MoO_3 completely degrades methylene blue (MB) in 120 minutes under visible light irradiation, showing excellent photocatalytic performance.Compared with bulk materials, catalytic performance of MoO_3 nanobelts is better, because nanobelts, small size, specific surface area is larger, so in many atoms on the surface of enhance the ability of the adsorption of organic catalytic materials, at the same time, the small size to make raw electron from the crystal light within a shorter time spread to the surface, nanobelts, this advantage greatly reduces the chances of electrons and holes in the compound and thus improve the catalytic efficiency.

2.2.5 Raw Materials for the Synthesis of Other Materials

As mentioned above, MoO_3 has many applications of its own. Besides, MoO_3 is also a raw material for synthesizing other substances.Helen a. teherese et al. [9] put MoO_3 in an environment full of H_2S gas and prepared fullerene-shaped MoS_2 and MoS_2 nanometer blocks by a simple and rapid synthesis

method.Bin Hu et al. [10] transformed MoO_3 nanoribbon into MoO_2 nanoribbon. They studied the mystery and explained its potential transformation mechanism.

3. Conclusion

At present, there are many literatures on the research of MoO_3 in various domestic and foreign journals.It can be seen from a large number of studies that layered MoO_3 has shown excellent performance in many fields and has attracted more and more attention.

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