Two-Dimensional Transition Metal Dichalcogenides and Their Advanced Transistors

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Abstract. With the found of graphene, people got great interest in its properties. But as no band gap exists in graphene, it's not easy to be used in semiconductor production. Inspired by its disjuncture, transition metal dichalcogenides (TMDs) are developed which have many fascinating properties. Meanwhile, silicon gradually reaches its physical limits. As the feature size of silicon transistors gets smaller, silicon devices are becoming more complicated and their cost and energy consumption keeps rising. Finding a new material to take silicon's place puts on the agenda TMDs show potential in producing high-frequency devices and have lower energy consumption. Using TMDs in high-speed devices makes great hope to keep Moore's law. It also can be used in other areas like photodetection. This article gives a full and concise review of TMDs from what TMD is, its mechanism and properties, how to produce it, devices made by TMDs to problems they face.

Keywords: Transition metal dichalcogenides; semiconductors; transistor; integrated circuit.

1. Introduction

Transition metal dichalcogenides (TMDs or TMDCs) have a long history. Its structure was first found in 1923 by Linus Pauling [1]. There is a format to be determined before the 60s and when graphene was found in 2004, people got new interests in layer-structure materials which led to a new research wave for TMDs as well. There has already been much research in TMDs presentive materials, MoS_2 and WSe_2 [1,2].

With the structure of silicon transistors getting smaller and smaller, Moore's law is facing great challenges. TMDs have high electron mobility and their 2d structure makes it easy to be controlled by applied electric field. Thus, it has good potential to keep Moore's law running.

TMD is a kind of chemical compound's general name. Its chemical general formula is MX_2. M is a transition metal element and X is a chalcogenide element. Their place in the tuple periodic table is shown in Fig 1.

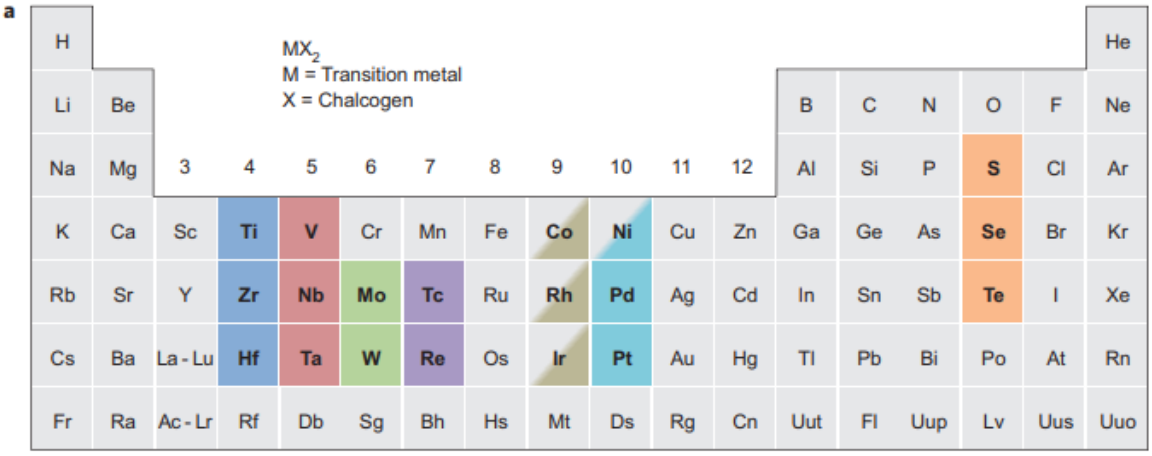


Fig. 1 Elements constructing TMDs [3]

TMDs' lattice structure forms like a sandwich, atom placed like graphene in every atom layer, and one metal layer M placed in two chalcogen atoms X [1]. These layers are placed in ABC or ABA two types to form a TMD lattice (Fig. 2a). Scientists already observed 5 lattice phases of TMDs: 2h, 3r,

1t, 1t' and $1t_d$ type (Fig. 2b) [4]. Usually, the t phase will act like metals and the h phase will show semiconduction properties. Since the t phase is metastable, it can be changed into the h phase in proper condition [2].

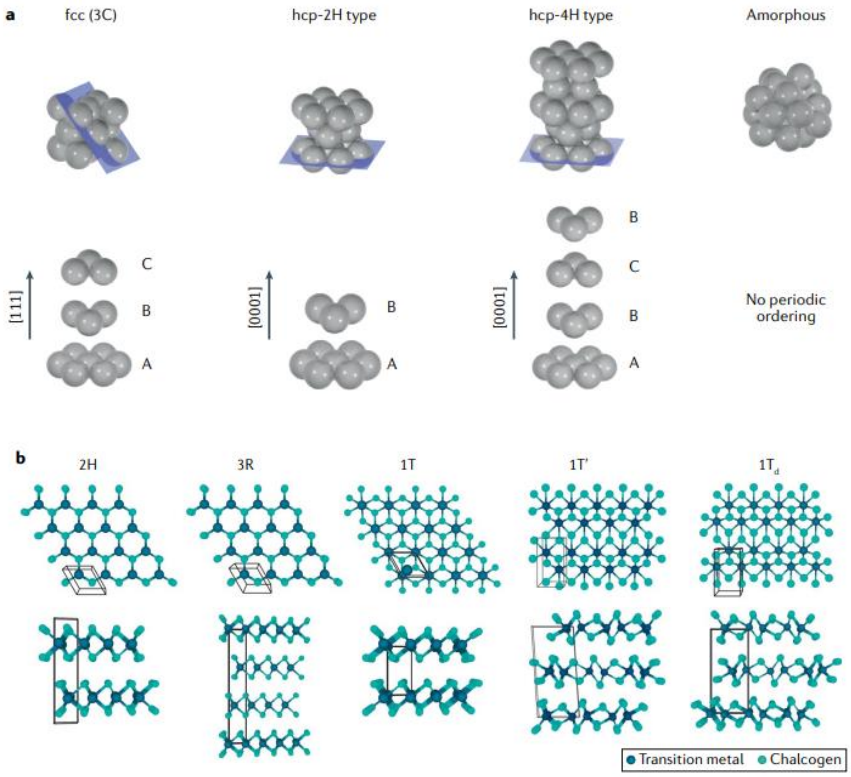


Fig. 2 Schematic models of different phases of metals and TMDs [4].

2. Transport Mechanism of TMDs

Like other crystals, TMDs' electronics are infected by acoustic scattering, optical phonon scattering, and Coulomb scattering. But as a 2d material surface interface phonon scattering and roughness scattering also strongly influence its electronics transport.

At low temperatures, transport is mainly controlled by optical phonon scattering. With temperature getting higher, acoustic scattering will become more important. Under 100 K optical phonon scattering takes main place. Coulomb scattering comes into effect at ~5×10^{11} cm^{-2} which is heavy doping [5].

Interface phonon scattering and roughness scattering take an important place in TMDs' electronics transportation, and they are so easy to be influenced that even placing on another material can change its phonon condition [5]. This property gives more potential for TMDs to make unique devices.

3. Characteristic of TMDs

TMDs have many unique properties. Like other 2d materials, its small volume and flexibility fit today's wearable devices very well [6]. The big specific surface area makes it sensitive to atoms and numerators absorbed on its surface, which can be used in making gas or liquid sensors. And some more interesting properties will be introduced in detail that TMDs have.

Van der Waals combined. Combining with another TMD layer or with other materials, they combined not by atomic or ionic bonds but by Van der Waals. This gives many advantages to TMDs. First, junctions can be made by putting TMD layer by layer manually with a microscope. And its different parts like electrodes can be made separately and assembled when needed. This gives great advantages in junctions' lab research in that researchers can have materials from high-quality

factories and don't have to get crystal generation equipment in their labs. Second, since TMD transistors are formed by Van Der Waals force, it means that no need to consider the lattice mismatch problem when combining two different materials [6]. This lets TMDs can be combined with many other materials to make heterojunctions.

Photoelectric properties. Transition metal disulfide semiconductor materials have a strong absorption of visible light and near-infrared light. Through the grid to its Fermi surface, TMDs can switch the ratio, to achieve a wide range of light detection. Similarly, transition metal disulfides have high electron-hole separation efficiency and show excellent properties of high light responsiveness and sensitivity.

Adjustable band gap. Different from graphene, transition metal sulfide has the characteristic of an adjustable band gap. It is convenient for us to study the wavelength of transition metal sulfide light-emitting devices. TMDs are direct bandgap material, and their bandgap can change with the number of layers from 0.88 to 1.71 eV. With one single layer, its bandgap is around 1.71 eV to 1.81 eV and is good at detecting visible and infrared rays [6].

No hanging bonds [6]. Not like silicon or other crystals, there is no hanging bond on the TMD surface. That means less electron trap and can lead to higher mobility. It is a great advantage in making high-speed devices.

TMD material also showed unique properties in the Quantum area [7]. Its hexagonal lattice structure and valleys of energy-momentum structure made it show the quantum control of valley pseudospin, which makes it a possible material in quantum counting [1].

4. TMDs' Production

To make TMDs, there are a lot of ways: CVD, PVD, Mechanical Cleavage, Liquid-phase exfoliation, etc. It can be roughly divided into three kinds: mechanical, liquid environment, and gas environment.

Mechanical is the cheapest way of making TMD material. TMDs can be produced by using a tape and stick it down from crystals [1]. However, this method can't control how the number of layers made, and it can't be used in making big-scale TMDs. Researchers are trying to improve its effectiveness by changing sticker material or growing TMDs on new substrates to help in making big-scale TMDs [8].

Liquid environment has many subdivisions. First is separating layers by ultrasonic. The second is producing high liquid velocity to separate layers. The third is the electrochemistry way., by placing ions into the gap between layers, expanding their distance, and weakening the force between them [5].

The gas environment has lots of ways to produce TMDs, for example, CVD and PVD. CVD can precisely control how many layers to get and only needs a Tube Furnace [1,3]. How to get a big scale is the main problem for the CVD method. Researchers are working by changing reactant composition, air flow velocity, and other conditions to solve this. The PVD method is making TMDs first then heating them in a Tube Furnace, making them into gas and regrowth on substrate prefabricated. There are also PLD, ALD, SPUTTER, and other ways to produce TMDs in air condition [8].

5. Devices Made by TMDs

Because TMDs have so many unique properties, they can be used in making many sorts of devices.

5.1. Junctions

Theoretically, MoS_2 electron mobility changes with the number of layers. Though the specific relation between some layers and electron mobility is not clear, single layer MoS_2 got the electron mobility at ~10–20 $cm^2\ V^{-1}\ s^{-1}$ [9]. Luckily combining it with graphene which has the highest electron mobility will give some improvement [1]. What's more, with a thicker width and smaller

dielectric constant than silicon, it can have higher frequency and lower power-hungry. B. Radisavljevic's team proved that MoS_2 can be used in making logic gates and their imitation also showed MoS_2 's great potential in making high-speed devices [10,11].

5.2. Photodetectors

TMDs' band gap will change with its lattice layer. When only one layer remains, MoS_2's band gap will change into a direct band gap at 1.8–1.9 eV, which gives it have potential to make new photosensitive devices. Its main response area is at visible lights and the silicon device is at infrared rays. There have been reports showing that devices made by MoS_2 light responsivity reached 7.5 mA/W, and the following reports show its light responsivity reached 880 A/W, which can be compared with silicon devices. It can also make up for graphene's no band gap property, make it to be used as a photosensitive device, and has an operating point under 1 V. Here are some photodetectors' light responsivity made by MoS_2 shown in Table 1.

Table 1. MoS_2 Device Light Responsivity

Material	MoS_2	MoS_2/ Graphene,	MoS_2/ $PdSe_2$	MoS_2/ CuO-NW
Light responsivity	880 A/W	45.5 A/W	2.7 A/W	2500 A/W

*At their best response wavelength

5.3. Memory Device

T phase MoS_2 has memristive behavior which can be used in making Ideal Memristor [12,13]. Ideal Memristor can nonvolatile memory storage, neuromorphic computing, digital logic, and analog circuits into the next step. In Peifu Cheng's research, they build a Memristor with 2 nanosheets MoS_2. Hong-Sub Lee and his team's reach introduced the MoS_2 device into neuromorphic devices and used it to enable gate-tunable learning and efficient integration

5.4. Energy Storage

Like graphene, TMDs have a web structure and gaps between layers making it useful in storage ion. However, a low average voltage and energy density limit their potential. Confining with graphene will strongly improve its properties. With Mo: C at a 1:2 ratio, it has a capacity of ~1,100 mAh g^{-1} at a current of 100 mA g^{-1} [3].

6. Problems TMDs Facing

TMDs fantastic properties give us great hope in making new devices with it. With silicon gradually reaching its physical limits, TMDs also show great potential in keeping Moore's Law running. Its good quality in visible light responsivity makes it a strong competitor in new type photodetector producing.

But like other 2d and recently developed materials, its shortcoming in manufacturing with low cost and big scale making gets in its way to real use. Even though researchers have studied TMDs' properties and mechanisms for decades, there are still so many problems and mysteries for scientists to solve to discover laws lying behind TMDs' unique properties. It is difficult to understand the TMDs mechanism for solving it needs crystallography and quantum mechanics had more development or raised highly efficient math methods to simulate it. However, TMDs great potential and rewards lying behind these efforts.

Once factory production of TMDs is solved, photocatalysis of Hydrogen will be put into real use and energy problems can have a relief. The door to quantum computing can be opened and scientists can have a good observation about quantum mechanics. Wearable electronic devices will reach a new revolution that can change people's lives.

7. Conclusion

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