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Realistic evaluation of the prospect of replacing silicon with other IC materials: Take molybdenum disulfide and graphene as examples

Zhexuan Chen

University of Electronic Science and Technology of China, Zhongshan Institute, Zhongshan,528402, China

1009866274@qq.com

Abstract. In recent decades, integrated circuits (IC) have played a more significant role in many areas of society, and silicon is one of the most commonly used materials in this industry. However, as times change and with the development of technology, silicon can only partially meet people's requirements for device performance. Hence, people need new materials to produce more effective IC equipment and devices like chips. Here I present two kinds of materials, molybdenum disulfide and graphene, to discuss their properties of them and the realistic assessment of the prospect that they replace silicon for IC.

Keywords: molybdenum disulfide, graphene, integrated circuit, silicon, new materials.

1. Introduction

IC is a technology that began to develop in the middle of the 20th century and has been created for several decades. IC has been inseparable from all aspects of people's lives in contemporary society. We can notice IC applications in plenty of places, like smartphones, computers, radios of cars, and chips of artificial intelligence. There is no doubt that IC has played an essential role in people's daily life and has a bright development prospect. With the increasing demand for high-performance IC devices and the progress of semiconductor theory, IC technology has become increasingly mature. One of the most noticeable features is that the number of transistors on an IC has exploded. In fact, at first, there were only a few transistors on a chip, but nowadays, the number of them has increased at a fantastic rate to more than one billion. There is also a well-known theory to explain this phenomenon. Moore's Law means that the number of integrated components of an IC doubles every 18-24 months, and every two months, when the price changes, the computer's performance will double; that is, every dollar can be bought. However, this increase seems to have gradually reached the limit because some problems will be encountered in the transistor's size reduction process, such as the short channel effect (SCE), which will make the transistor performance unstable. The current predicted limit channel length of the transistor made by silicon is 7nm, and it’s close to the actual situation. It seems that the silicon transistors have reached the limit of performance. Developing new semiconductor materials to replace silicon in the IC industry is necessary to meet people's higher requirements.

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Owing to the appropriate physical and chemical properties, 2D layered materials undoubtedly arouse people's interest. In this work, I will mainly talk about two this kind of materials, graphene, and MoS_2.

2. Physical and chemical properties

Two-dimensional materials are materials in which electrons (like nanoparticles, superlattices, and quantum wells) can only move freely in two dimensions (1-100 nanometers). In 2004, the Geim team at Manchester University successfully isolated a graphene layer to produce two-dimensional materials. Graphene has aroused great interest in theoretical research and application, and chewing gum is also called a "gold digger." Subsequently, molybdenum disulfide [MoS_2], boron nitrate [BN], tungsten disulfide [WS_2], and other two-dimensional materials were separated one after another. Recently, extensive research has been carried out in condensed matter physics. Two-dimensional materials show many strange properties. Because the vector migration and heat distribution are limited in a two-dimensional plane, their variable band gaps are widely used in field effect transistors, photovoltaic devices, thermal electronic devices, etc., to control their rotation and downstream degrees of freedom, which leads to depth.

Graphene is characterized by its single atomic layer thickness, high carrier mobility, linear performance spectrum, and high strength. Its high intrinsic conductivity makes it a semi-metallic material, especially the gate electrode, suitable for use in the IC area. MoS_2 is natural N doping, and its lower dielectric constant and greater electronic effective mass affect it less than the short channel effect. Therefore, MoS2 is also an ideal transistor channel material for the future.

2.1. Graphene

Graphene is a new type of material that is composed of carbon atoms in a single-layer sheet structure. It is a hexagonal planar thin film with a honeycomb lattice consisting of carbon atoms and a two-dimensional material with only one carbon atom thickness. Graphene has always been considered an imaginary structure and can't exist independently. It was not until 2004 that physicists Konstantin Novoselov and Andre Geim of the University of Manchester in the UK successfully separated graphene from graphite experiments.

It is the thinnest and stiffest nano-material. The global thermal conductivity is as high as 5,300 W/m·K, more elevated than carbon nanotubes and diamonds. It is almost entirely transparent, absorbing only 2.3% of light at room temperature, higher than carbon nanotubes or silicon crystals. Its resistance is about 10-6 Ω·cm, lower than copper or silver, which is what the world has learned. Faster conductive electronic components or transistors are also suitable for manufacturing optical panels, fine touch screens, and solar cells because images are excellent transparent conductors.

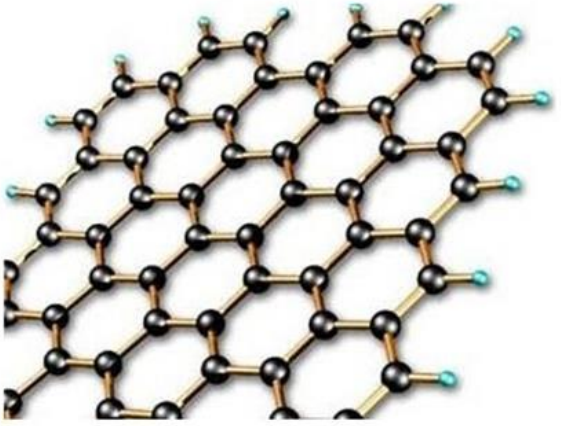

Figure 1. Structure of graphene.

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The arrangement of carbon atoms in graphene is the same as that of graphite monolayer, and it has the following characteristics: carbon atoms have four valence electrons, three of which produce sp2 bonds; that is, each carbon atom contributes a non-bond electron in the pz orbit, and the pz orbit of adjacent atoms is perpendicular to the plane to form π bonds, and the newly formed π bonds are in a semi-complementary state. The logarithm of carbon atoms is shown in Figure 3, in which the bond between two adjacent carbon atoms is 1.42 x 10^{-10}m, and the angle between the bonds is 120. Except for the cell layer structure of a hexagonal ring with other carbon atoms, each orbit pz of carbon can form a sizeable π bond perpendicular to the plane (similar to a benzene ring), and multiple bits pass through the whole layer, so it has excellent electrical conductivity and optical properties.

The mobility of graphene carriers at room temperature is about 15000cm2/(v·s), which is more than ten times that of silicon material and more than two times that of InSb. Depending on the conditions, the fluidity of the graphene carrier sometimes reaches 250,000 $cm^2/(v·s)$ at low temperatures and other requirements. Unlike many materials, the electron mobility of graphene is little affected by temperature changes. At any temperature of 50~50~500K, the electron mobility of single-layer graphene is about 15000$cm^2/(v·s)$. Therefore, the excellent electronic properties of graphene help replace silicon as an expected IC material.

2.2. Molybdenum disulfide

Under normal conditions, MoS_2, which looks like a leaden shiny powder, is black when synthesized artificially. Sublimation began at 450℃. Its melting point is 2375℃. It isn't enjoyable. MoS_2 is often used to make molybdenum compounds, lubricating additives, catalysts for hydrogenation, and isomerization. However, in the industrial production of integrated circuits, people often use single-layer MoS_2, that is, two-dimensional materials.

Two-dimensional molybdenum disulfide comprises a single layer or a few layers of molybdenum disulfide, a new two-dimensional layered material with similar structure and properties to graphene. In recent years, it has become a research hotspot in emerging materials because of its suitable physical, chemical, and photoelectric properties, so it has been expected in many fields, such as physics, chemistry, and materials, especially electronics. Its excellent electrical properties make transistors made of it have even better performance.

Two-dimensional layered molybdenum disulfide is a hexagonal structure generally composed of single-layer or multi-layer molybdenum disulfide. Single-layer molybdenum disulfide is composed of three atomic layers (see Figure 2) [1], the upper and lower layers are sulfur nuclear layers, and the middle layer is a molybdenum atomic layer, which just forms a layered structure like a sandwich biscuit. Molybdenum disulfide is similar to graphene, and there is a weak Van der Waals force between layers (which leads to their low friction coefficient and is widely used in solid lubrication). Multilayer Molybdenum disulfide consists of several single-layer disulfides, and the spacing between each layer is about 0.65 nm, generally defined as, at most, five layers.

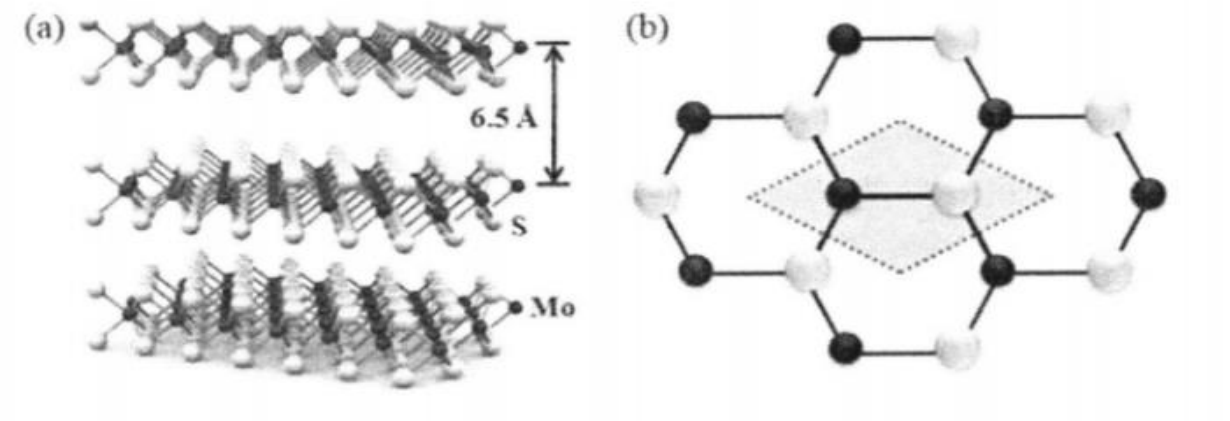

Figure 2. Structure of 2D layered molybdenum disulfide.

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The energy band structure of two-dimensional layered molybdenum disulfide is shown in Figure 3. The connecting line between the center of the Brillouin region and every point on the plane constitutes a K vector, and each K vector has its energy level E_k.

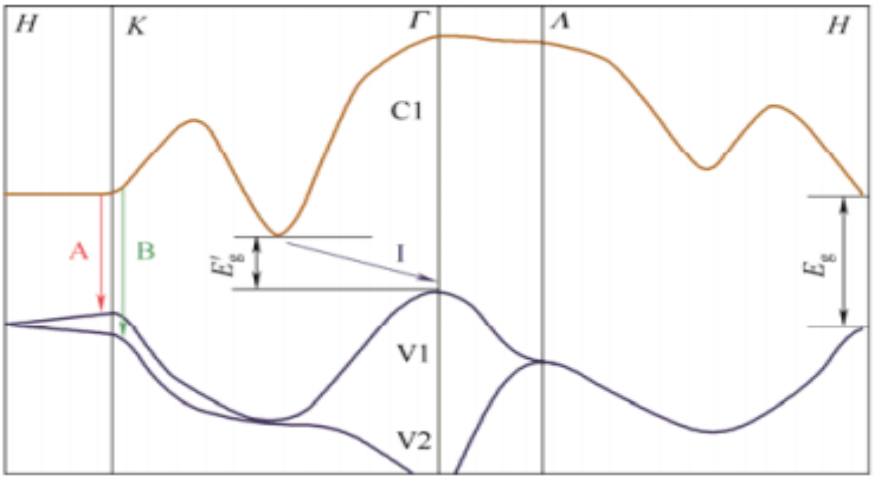

Figure 3. Simplified band structure of 2D layered MoS_2 [1].

K, H, and Λ represent high symmetry points of the Brillouin zone; *Γ* represents the center of the Brillouin zone; V1 and V2 represent two separate valence bands; C1 represents the conduction band; A and b represent two vertical transition modes from the conduction band to the valence band; I mean the non-vertical transition mode from the conduction band to valence band; Eg stands for the energy gap of abrupt transition, and Eg stands for the energy gap of non-vertical transition. The band gap of molybdenum disulfide crystal is Eg=1.29 eV, and its electronic transition is a non-vertical transition. When the thickness of molybdenum disulfide is reduced, the band gap will be widened. In the case of a single layer, the transition mode of electrons becomes vertical transition, and its band gap reaches Eg=1.9 eV, and its band gap changes from indirect band gap to direct band gap. Molybdenum disulfide has unique properties in light absorption due to its band gap change and particular geometric structure, so it has excellent potential in photoelectric applications. Because of its unique microstructure and physical and chemical properties, it has many advantages over graphene. It overcomes the disadvantages of zero band gap graphene, such as large specific surface area, good electron mobility, and high electron density of states. Therefore, molybdenum disulfide also shows excellent photoelectric properties and has broad prospects in applying optoelectronic integrated circuit devices. [2]

3. Industrial production and application

Two-dimensional materials have such high performance that they have entered people's field of vision instead of silicon materials. This section focuses on manufacturing and applying graphene and hydrogen sulfide.

For example, in 2022, researchers at Tsinghua University made a transistor with a completely new structure using graphene and two-dimensional single-layer molybdenum disulfide. Before they made

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this transistor, the gate length of the transistor could not break through the limit due to the limitation of silicon material, which reduced the gate length to less than 1nm and made a device with better performance. In this device, graphene is used as the gate, and molybdenum disulfide is used as the channel material. The graphene edge gate controls this two-dimensional sidewall transistor, and the molybdenum disulfide channel that holds atoms has a gate length of only 0.34 nm.

3.1. Graphene

Graphic research has also aroused interest in material analysis. The preparation methods of graphite materials, such as mechanical stripping, chemical oxidation, crystal growth, chemical vapor deposition, organic synthesis, and carbon nanotube stripping, are reported.

The mechanical stripping method uses labels and relative movement between objects and graphics to create thin materials that are easy to use. Therefore, in 2004, two British scientists usually stripped natural graphite one layer at a time, which is an effective mechanical method and cannot be manufactured at the industrial level.

Chemical vapor deposition (CVD) is a method of preparing graphene thin films by vapor deposition using carbon-containing organic gases as raw materials. CVD is the use of heating, plasma Methods of excitation, or light radiation, through chemistry Reactions among gas-phase atoms and molecular, the technical means of generating a thin film on a specific substrate surface—currently, Many applications in the semiconductor process of insulating layer and semiconductor layer preparation. Theoretically speaking, it is easy to introduce two or more gas components into the reaction chamber and then interact with each other to decompose a new material on the surface of the substrate. This is the most effective method to manufacture graphene thin films, which have a large surface area and high quality, but they must be fixed by micro-gap equipment such as a touch screen and heater.

Some scientists used low-level deposition gas to form monochrome on the infrared surface. Further research shows that this graphene structure goes through metal steps and gradually starts a continuous single-layer carbon crystal graphene structure on the infrared surface. This polyester is formed by condensing graphene and graphene on a polycrystalline film in centimeters. When the surface of the laminated plate is heated at 300nm℃ and exposed to CH4, a large area of the graphene film surface is formed after a specific reaction.

Graphene is also widely used today. In 2005, some research groups found that graphene was ten times faster than commercial silicon wafers at room temperature. 10 am/V·S) is transported, and there is less temperature and noise, which shows sub-micron ballistic transmission characteristics (up to 0.3 m at 300 K). This is another significant advantage of electronic devices based on graphene. Even if they are reduced in nano-computing, they can maintain good stability and electrical properties, thus making it possible to study simple electronic devices.

Some scientists have also found that graphene is the most widely known conductive material. This property of graphene is beneficial for high-frequency circuits. High-frequency circuit is the leading part of the modern electronic industry. Some electronic devices, such as mobile phones, need higher and higher frequencies, and engineers try to fill in more and more information. The higher the mobile phone frequency, the more heat it generates, so the promotion of high frequency is minimal. Due to the appearance of graphene, the improvement and development prospect of high frequency seems endless. Therefore, it has great application potential in the microelectronics field. Researchers even regard graphene as a silicon substitute for future supercomputers.

Some scientists have also found that graphene is the best conductive material. This characteristic of graphene is especially suitable for high-frequency circuits. The high-voltage course is the leader of the modern electronic industry. Some electronic devices, such as mobile phones, are forced to use higher and higher frequencies because engineers try to fill signals with more and more information. The higher the frequency of mobile phones, the greater the heat, so the promotion of high frequency is minimal. Thanks to the chart, the rising prospect of graphene seems infinite. Therefore, it has great

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potential in the field of electronics. Researchers even regard graphene as a silicon substitute for future supercomputers.

3.2. Molybdenum disulfide

Some researchers use the micro-mechanical cutting method to make single-layer sulfur compounds and transfer them to a silicon dioxide substrate. Using gold as an electrode, the single-stage binary instrument of trisulfide and three-component carbon dioxide are assembled into an upper intermediate insulating layer. The experimental results show that the ripple voltage is -4V, the switching current ratio reaches 10^8, and the electron mobility is 217 cm^2 $V^{-1}S^{-1}$. Then, the researchers synthesize the single-layer disulfide bond into the logic integrated circuit, and the experiment proves that it can perform basic logic operations well. This provides greater confidence for the practical application of monosulfide transistors.

There are many applications of molybdenum disulfide, such as the single-layer MoS2 nonvolatile switch developed by the French research team, which can work in the 6G communication band. (Fig.4) [3]. The field effect transistor with a channel length close to 0.34 nm developed by Ren Tianling's research team at Tsinghua University further develops Moore's Law(Fig.5) [1]. Wang Xinran of Nanjing University proposed the technical scheme of driving a display chip with MoS2 transistor and realized a high-performance microdisplay(Fig.6) [4].

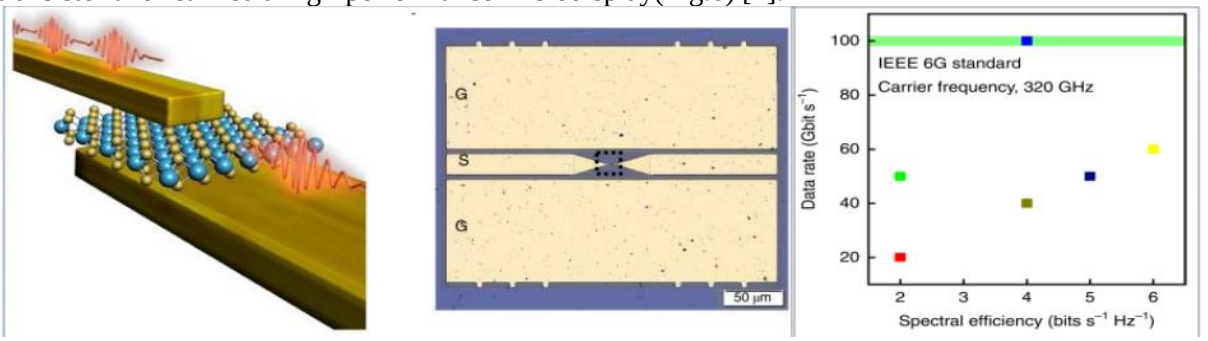

Figure 4. Single-layer MoS2 non-volatile switch, which can work in the 6G communication frequency band [3].

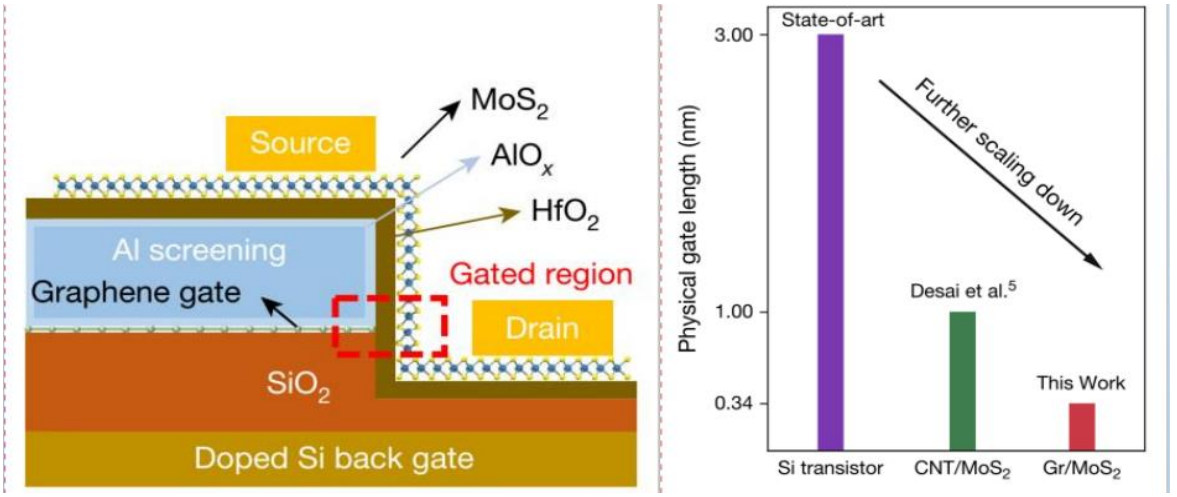

Figure 5. The channel length is close to 0.34 nm field effects transistors [2].

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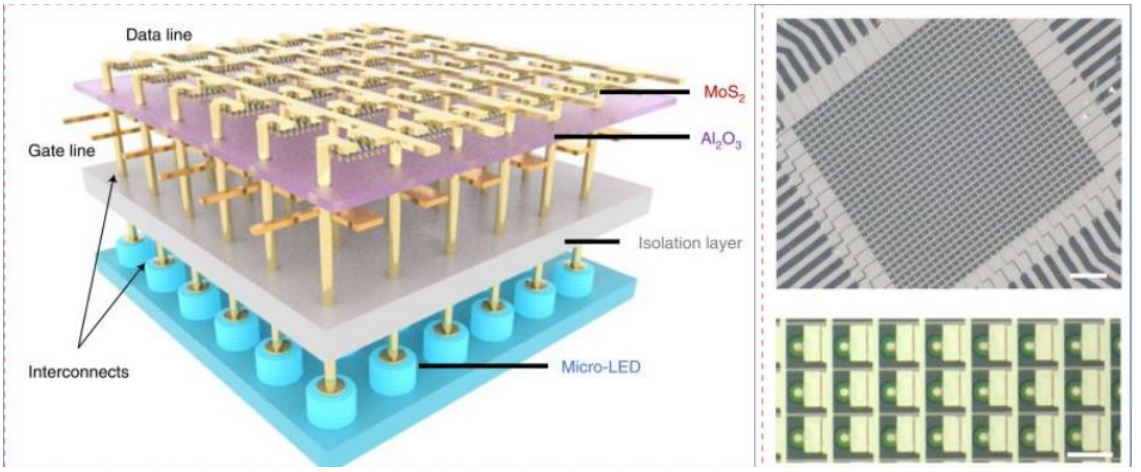

Figure 6. MoS2 Transistor drive display chip technology solution to achieve high-performance microdisplay [4].

Up to now, many methods have been developed to prepare wafer-level MoS2 thin films, such as chemical vapor deposition (CVD), film vulcanization, atomic layer deposition (ALD), metal-organic chemical vapor deposition (MOCVD), pyrolysis and so on.

At present, there are two central schemes for preparing MoS2 by CVD. The current scheme 1 is sapphire substrate epitaxy. The advantages are high mobility, relatively mature process, and large-area continuous film growth, but the disadvantages are high cost and low growth rate (Fig.7) [5]. Scheme 2 is epitaxial on a soda-lime glass substrate. Its advantages are low production cost and fast growth rate. Still, its disadvantages are low mobility, small crystal domain size, and immature large-area preparation process (Fig.8) [6], so the low-cost preparation of large-area high-performance MoS2 is a critical problem that restricts its industrial application!

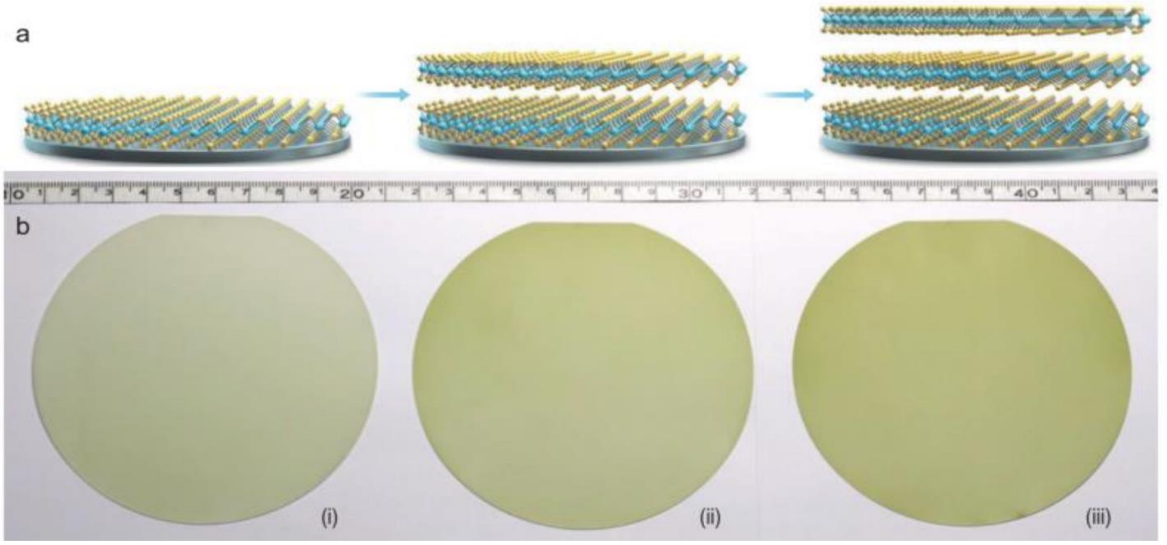

Figure 7. Sapphire substrate epitaxy [5].

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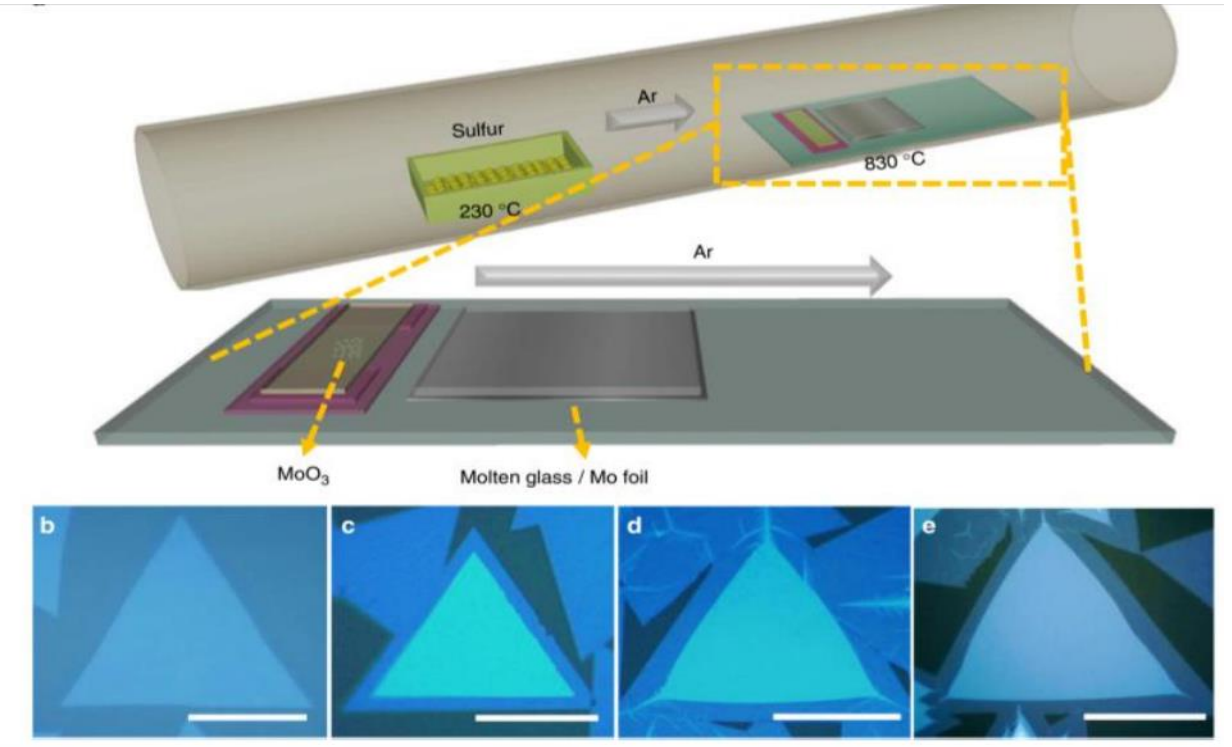

Figure 8. Nanocalcic glass substrate epitaxy [6].

4. Conclusion

Although molybdenum disulfide (MoS_2) or other two-dimensional materials, such as graphene, have better physical and chemical properties, many problems still exist in replacing silicon with them.

Even if graphene may have better mobility, it has many defects and may look unremarkable in a transistor, but there are hundreds of millions of transistors in integrated circuits. The chip may not work correctly when even a few transistors have problems.

Although molybdenum disulfide may have many better characteristics than silicon, such as thinner thickness and excellent electrical characteristics, it also has characteristics that are not suitable or worse than silicon. Its industrial production also has problems, such as higher production costs. So it seems complicated, even impossible, for these materials to replace silicon completely.

However, does this mean that our research and understanding of new materials is meaningless? Admittedly these new materials can only partially replace silicon. We can still use these materials, give full play to their advantages, and use them as parts of transistors, such as making gates or channels, to improve the performance, such as those I mentioned earlier. These are also significant scientific and technological progress, which are very meaningful. I want to say that in scientific research, the results may be different from our original goal, but when we look back, we have done a lot and gone a long way.

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