



# Novel Materials for AI Chip - Two-Dimensional Materials and the Third-Generation Semiconductors

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**Abstract.** AI chips have a rising demand for high computing power and low power consumption. Traditional silicon-based semiconductors are constrained by inherent properties and process limits, making it difficult to meet the high-performance requirements of AI chips. Therefore the research and exploration of novel materials are particularly significant. This paper focuses on the currently popular two-dimensional (2D) materials and the third-generation semiconductors, deeply analyzing the material properties and comparing four key parameters: bandgap width, electron mobility, thermal conductivity, and breakdown voltage. It is found that graphene has ultra-high electron mobility and thermal conductivity, which can help solve the challenges of high-speed computing and thermal management in AI chips. Molybdenum disulfide with adjustable bandgap width and variable breakdown voltage has excellent switching characteristics, making it suitable for chip memory modules. GaN and SiC can adapt to high-power and high-frequency scenarios by their wide bandgap, high electron mobility and high breakdown voltage characteristics. The four new materials each have their own advantages in physical and electrical properties, demonstrating great application potential in the field of AI chips. If novel materials can overcome the obstacles in manufacturing processes and production costs, they are expected to promote the development of AI chips in the future.

**Keywords:** AI chip, Novel materials, Two-dimensional materials, Third-generation Semiconductors.

## 1 Introduction

In recent years, as information technology has advanced rapidly, the influence of artificial intelligence has continued to strengthen, and its scope of applications has been expanding continuously. This has led to higher and higher performance requirements for related AI chips from artificial intelligence technologies. As the core hardware supporting technologies for tasks such as deep learning and computer vision, achieving

high energy efficiency ratio, high computational density, and excellent thermal management capabilities are the keys to further enhancing the overall performance of AI chips [1]. However, due to the inherent characteristics and process limitations of traditional silicon-based semiconductors, it is difficult to achieve a significant improvement in chip performance in the manufactured devices, and they cannot meet the requirements of AI chips for high parallel computing density and ultra-low power consumption. Therefore, the exploration of new semiconductor materials has become a key path to break through technical barriers.

In this context, this article turns its attention to popular new materials represented by two-dimensional materials (Graphene, MoS<sub>2</sub>) and third-generation semiconductors (GaN, SiC). Two-dimensional materials, with their atomic-level thickness and ultra-high carrier mobility, make ultra-low power edge AI chips possible; while the wide bandgap characteristics and high breakdown field strength of third-generation semiconductors make them show great potential in high power density scenarios [2-3]. This article will discuss these two types of materials from the aspects of their structural characteristics and important parameters, clarify the performance advantages and applicable scenarios of two-dimensional materials and third-generation semiconductors in AI chips, and provide assistance for material selection and manufacturing of AI chips.

## 2 Novel materials

### 2.1 Two-dimensional materials

**Graphene.** Graphene is a thin film carbon material composed of carbon atoms. It features sp<sup>2</sup> hybridized orbitals that form a hexagonal honeycomb lattice. It is also a novel nanomaterial and one of the most popular cutting-edge materials in current research. Compared with general carbon materials, the unique two-dimensional structure of single-atom-layer graphene is remarkable. Graphene possesses extremely high carrier mobility and electron transport velocity. It exhibits exceptional electrical and thermal conductivity at room temperature. Moreover, graphene has extremely high mechanical strength. Compared to other carbon materials like CNT, graphite, and fullerene, graphene is several times stronger. Its carbon atoms are connected flexibly. When external forces are applied, graphene's surface carbon atoms bend to adapt, maintaining structural stability [4]. These unique properties give graphene an advantage over other carbon materials in manufacturing energy storage, conversion devices, and semiconductor devices.

**Molybdenum disulfide (MoS<sub>2</sub>).** MoS<sub>2</sub> is a transition metal dichalcogenide with a layered structure and an adjustable bandgap. As a 2D nanomaterial, it has a high surface-area-to-volume ratio. This gives it good surface conditions for electrical transport and results in higher carrier mobility [5]. A material that integrates photonic and electronic computing in a hybrid architecture enables parallel optical signal processing and low-latency electrical signal transmission, thereby significantly enhancing computational

efficiency [6]. In 2023, the KAUST team developed an optoelectronic synaptic device. It achieved 91% accuracy in image recognition tasks, with an energy consumption as low as 0.1 pJ per pulse [7]. Its excellent performance and mature fabrication technology make it an ideal semiconductor material. Its low static power consumption and good photoresponse characteristics also make it suitable for logic devices and nanoelectronic devices.

## 2.2 The third-generation semiconductors

The third-generation semiconductors, typically represented by GaN and SiC have a bandgap width of over 2.2 eV. They possess advantages such as high electron mobility, high thermal conductivity, and high breakdown electric field, showing stable physical and chemical properties. By virtue of these characteristics, GaN and SiC can adapt well to harsh working environments such as high power, high voltage, and high frequency

**Gallium nitride (GaN).** The crystal structures of GaN material are mainly hexagonal wurtzite and cubic zinc-blende structures, of which the wurtzite structure exhibits higher stability. In practical applications, GaN is usually grown in the form of thin films on substrates such as sapphire and SiC. Technologies like epitaxial growth can be used to control the thickness, crystal quality, and doping concentration of GaN thin films to meet the requirements of different devices [8]. In addition, GaN is often combined with other materials to form heterostructures, or different bandgap materials are introduced into GaN to create GaN quantum well structures, which can also further enhance the performance of the materials [9]. GaN HEMTs display low on-state resistance. When used as the channel material, GaN is capable of withstanding high voltages, which results in the devices being highly dependable and energy-saving for high-power uses. In 2022, Shigeki Yoshida and colleagues used 4-inch wafer processing equipment and metal-organic chemical vapor deposition (MOCVD) to fabricate N-polar GaN high electron mobility transistors (N-polar GaN HEMTs). The non-uniformity of the sheet resistance was as low as 1.2%. The experiment demonstrated a drain current density of 1.74 A/mm and a drain conductance of under 40 mS/mm, attaining the performance standards of high-frequency radio-frequency power amplifiers [10]. At present, GaN, due to its excellent properties, plays an important role in fields such as optoelectronics (LED lighting), power electronics, and microwave radio frequency. It is regarded as a potential material for AI chips.

**Silicon carbide (SiC).** SiC is a non-centrosymmetric compound based on covalent bonds, formed by the accumulation of basic unit structures. Each unit is a tetrahedron consisting of four silicon atoms and one carbon atom arranged in a staggered manner through sp<sup>3</sup> hybridization. Common SiC crystal forms include 3C-SiC, 4H-SiC, and 6H-SiC. The Si-C bond is a strong covalent bond with high bond energy, so SiC has extremely high hardness, excellent wear resistance and chemical stability, enabling it to withstand extreme mechanical stress and harsh environments [11]. Therefore, SiC is considered an ideal material for manufacturing high-power semiconductor devices,

high-temperature semiconductor components, and radio-frequency devices, expected to contribute significantly to future technological advancements.

In practical applications, some silicon carbide-based power conversion devices have demonstrated the capacity to operate stably under high-voltage and large-current conditions while achieving high power conversion efficiency. The DC-DC boost converter, which Zhang Chao and his team developed using SiC MOSFET and SiC SBD, attains a conversion efficiency of 96.1% when operating at a switching frequency of 20 kHz. Studies indicate that under the same voltage, SiC power MOSFETs exhibit lower switching and conduction losses compared to their Si counterparts [12]. These characteristics of SiC devices make them highly suitable for high-frequency systems and will positively impact the field of AI chips.

### 3 Comparison of Important Parameters

In chip manufacturing, selecting appropriate materials is crucial for achieving high-performance devices and ensuring chip quality and stability. These materials need to possess excellent properties. To explore the core characteristics of the materials mentioned above, this paper will investigate key parameters affecting chip speed, energy efficiency, stability, and integration level. A comparative analysis will also be conducted

**Table 1.** Comparison of Important Material Parameters.

Parameter	Graphene	Monolayer MoS <sub>2</sub>	GaN	SiC
Bandgap (eV)	0	1.8	3.4	3.3
Electron Mobility (cm <sup>2</sup> /V·s)	2 × 10 <sup>5</sup>	200	2000	900
Thermal Conductivity (W/m·K)	5300	84	170	490
Break-down Voltage (MV/cm)	/	1	3.3	3.5

Table 1 presents data on bandgap, electron mobility, thermal conductivity, and breakdown voltage for Graphene, monolayer MoS<sub>2</sub>, GaN, and SiC. This article will discuss these important parameters that affect chip performance in detail

### 3.1 Bandgap

The bandgap is the core parameter that determines the carrier excitation efficiency of semiconductors. It reflects the minimum energy required for electrons to jump from the valence band to the conduction band. A smaller bandgap width means that electrons can easily jump from the valence band to the conduction band, so the conductivity is better. On the contrary, a larger bandgap width means that it is more difficult for electrons to jump, thus having better insulation. Generally speaking, materials with a bandgap over 2.3 eV are called wide bandgap semiconductors. Such materials have significant advantages such as high temperature resistance and anti-interference.

Among the third-generation semiconductor materials that are currently being widely studied, GaN and SiC are both typical wide bandgap semiconductors. The bandgap width of GaN is 3.4 eV, and the bandgap width of SiC is 3.3 eV. GaN is suitable for high-frequency and high-power applications due to its high critical electric field and high saturated electron drift velocity, while SiC is widely used in high-power conversion devices and automotive-grade AI platforms due to its high thermal conductivity and good interface compatibility [13]. Wide bandgap materials can reduce thermal effects and improve system heat dissipation efficiency. For example, in GaN-based power converters, experimental data show that compared with traditional silicon materials, gallium nitride can reduce heat accumulation by more than 40% at high frequencies, significantly improving the stability and work efficiency of AI chips during data processing [14].

In addition to traditional wide bandgap materials, two-dimensional materials have also attracted attention in recent years due to their unique structure and adjustable performance. For example, the bandgap width of layered MoS<sub>2</sub> is 1.8 eV when it is a single layer, but the bandgap width drops to 1.2 eV when it is multilayered. Graphene, as a zero-bandgap material, has very special electronic properties: it has extremely high electron mobility, but due to the lack of a bandgap, it is difficult to use in traditional logic devices [15]. Although graphene is not suitable for constructing traditional logic switch devices, its high electron mobility still have great potential in applications that require high-speed electron transmission.

The bandgap width determines their use in AI chips to a certain extent: wide bandgap materials, such as gallium nitride and silicon carbide, are suitable for high-power or high-temperature environments, while two-dimensional materials with adjustable bandgap are more suitable for multifunctional, highly integrated chip designs. These differences in characteristics provide important material foundations and engineering references for AI chips in terms of power density management, heat dissipation path optimization, and device structure innovation.

### 3.2 Electron Mobility

Electron mobility is a key parameter for measuring the conductivity of semiconductor materials. It reflects the speed of electron movement in the material. This parameter directly affects the switching speed of the chip and the efficiency of data transmission. In applications such as AI chips that require high-speed data processing and low power

consumption, the level of electron mobility often becomes an important bottleneck that limits the upper limit of system performance. Generally speaking, the higher the electron mobility of a material, the faster its computing speed and the lower its energy consumption. It is especially suitable for high-frequency data paths such as convolution acceleration and neural network reasoning [16].

Among the third-generation semiconductor materials, the electron mobility of GaN reaches  $2000 \text{ cm}^2/(\text{V}\cdot\text{s})$ , while the electron mobility of SiC is  $900 \text{ cm}^2/(\text{V}\cdot\text{s})$ . Although the mobility of these two materials is lower than the theoretical value of some two-dimensional materials, they have been significantly improved compared with traditional silicon materials. GaN is more suitable for AI accelerators that require high-speed signal transmission and high-frequency switching operations due to its higher electron mobility and high-frequency characteristics [17]. Although SiC has a slightly lower mobility than GaN, it is more stable and reliable in high-temperature and high-voltage working environments, making it more suitable for use in scenarios such as in-vehicle AI systems and industrial edge computing [18].

Among two-dimensional materials, the theoretical value of graphene's electron mobility is as high as  $\text{cm}^2/(\text{V}\cdot\text{s})$ , which is almost one of the materials with the highest electron mobility known so far. This property provides a physical basis for its ultra-high-speed interconnection and cache access in AI chips. However, the material properties of graphene itself as a zero-bandgap material make it difficult to form effective switching characteristics, which limits its direct application in logic devices. To overcome this problem, researchers are exploring doping graphene or combining it with other semiconductor materials in order to find application scenarios in low power consumption, high-speed signal transmission, and high-speed cache of AI accelerators [19]. In contrast, as a typical two-dimensional transition metal sulfide, although its single-layer electron mobility is about  $200 \text{ cm}^2/(\text{V}\cdot\text{s})$ , which is not as excellent as the above materials, its natural band gap is about 1.8 eV and it has excellent switching performance, making it relatively suitable for low-power, high-integration AI chip units.

### 3.3 Thermal conductivity

Today, thermal management issues are also a major challenge constraining the development of AI chips. Materials with high thermal conductivity could be a significant breakthrough. Thermal conductivity is an important physical quantity that measures the heat transfer performance of materials. High thermal conductivity materials enable AI chips to achieve the goals of high computing power and high stability, contributing to the extension of chip service life and the enhancement of integration density. AI chips usually require materials with a thermal conductivity of hundreds of  $\text{W}/(\text{m}\cdot\text{K})$ . Additionally, the materials preferably exhibit isotropic thermal conductivity or can meet heat dissipation design in specific directions, ensuring stable and reliable properties within an operating temperature range of at least  $-40^\circ\text{C}$  to  $125^\circ\text{C}$ .

Graphene has ultra-high thermal conductivity. Theoretical calculations suggest that the thermal conductivity of single-layer graphene could reach  $5,300 \text{ W}/(\text{m}\cdot\text{K})$  at room temperature. In 2024, R. Kunjuveetil Govind and colleagues studied a graphene-based

PCM nanocomposite thermal interface material (TIM). By adding just 3.6 wt.% graphene, the thermal conductivity of the composite was increased from 0.233 W/(m·K) to 0.445 W/(m·K). When applied to heat sink, a combination of graphene-based PCM nanocomposite and heat sink exhibited better thermal performance than an aluminum heat sink, and the heat dissipation effect for integrated circuits was also superior to commercial silver-based TIM [20]. Thus as one of the materials with the best known thermal conductivity, graphene has great potential to help AI chips address thermal management challenges. MoS<sub>2</sub> has a relatively low thermal conductivity, which is 84 W/(m·K) for single-layer MoS<sub>2</sub>. For high-power AI chips, the requirements for molybdenum disulfide are challenging to fulfill [21]. However, MoS<sub>2</sub> has better flexibility and mechanical properties, showing potential applications in some special chip packaging or heat dissipation structures. It can adapt to the design of AI chips with non-planar or bending requirements.

The thermal conductivity of GaN typically ranges between 130 and 180 W/(m·K), which can meet the conventional heat dissipation needs of AI chips. However, compared with graphene and silicon carbide, it is insufficient for heat dissipation in high-power environments. At the same time, GaN is more complex in terms of anisotropic thermal conductivity, which is less straightforward and effective than graphene and SiC. The thermal conductivity of SiC is approximately 342~490 W/(m·K), and polycrystalline SiC materials exhibit good isotropic thermal conductivity, enabling uniform heat conduction in chips. Due to its structure, it has excellent chemical stability and radiation resistance, which can ensure the performance stability of AI chips in harsh environments. Although the thermal conductivity of SiC is slightly inferior to that of graphene, it has good comprehensive performance and is currently a material that more closely meets the heat dissipation requirements of AI chips. The heat dissipation effect can be improved by optimizing the chip packaging structure and combining it with heat dissipation fins.

### 3.4 Breakdown voltage

The breakdown voltage of materials limits the operating frequency of chips, as the operating frequency of chips is generally proportional to the applied voltage. To keep the AI chip operating at a high frequency for a long term, a higher voltage has to be applied inside the chip. If the breakdown voltage of a material is too low, it will be easily broken down after being exposed to high operating voltage for a long time. In severe cases, it may even cause damage to the internal structure of the chip and loss of important functions. Therefore, the breakdown voltage of materials will limit the maximum voltage of chips, thereby restricting the operating frequency. In addition, the integration density of chips is also affected by the breakdown voltage. As the manufacturing process of AI chips evolves towards smaller nanoscale dimensions, the extremely small gap requires materials to have a higher breakdown voltage to prevent electrical breakdown and avoid issues such as signal interference and short circuits. In the future of pursuing high chip integration density, materials with high breakdown voltage will possess significant advantages.

Graphene is a zero-bandgap material. Due to its breakdown characteristics being different from that of traditional semiconductor materials, it is difficult to measure its performance in practical applications using the conventional concept of breakdown voltage. In 2022, Dao Dinh Ha et al. conducted a study on GaN HEMTs with few-layer graphene thermal components and graphite heat sinks. They found that introducing a graphene-based heat dissipation system into GaN HEMTs effectively reduced the maximum temperature of the devices. However, when the graphene layer is close to the gate, it increases the electric field strength near the gate-drain side, leading to an increase in the collision ionization rate and the accelerated generation rate of electron-hole pairs, which will reduce the breakdown voltage of the transistor [22]. Therefore, when applying graphene in the manufacturing of related devices, it is necessary to consider the potential impact on the overall breakdown voltage of the devices.

MoS<sub>2</sub> as a two-dimensional semiconductor material has a non-zero natural bandgap and a layered structure. Its bandgap width can be adjusted by the number of layers. The breakdown voltage characteristics are also affected by multiple factors, such as the number of structural layers, strain conditions, and preparation processes. For instance, MoS<sub>2</sub> has spatial inversion symmetry breaking in odd layers and central symmetry in even layers; tensile strain will decrease the bandgap of MoS<sub>2</sub>, whereas compressive strain may induce the occurrence of a semiconductor-metal phase transition [23]. These differences affect the electron distribution and energy band structure of MoS<sub>2</sub>, altering its breakdown voltage characteristics. Therefore, one of the valuable research directions for MoS<sub>2</sub> is developing multi-layer MoS<sub>2</sub> structures suitable for AI chips.

Both GaN and SiC, as wide-bandgap semiconductors, have remarkably high breakdown voltages, reaching  $3.3 \times 10^6$  V/cm and  $3.5 \times 10^6$  V/cm respectively, which are an order of magnitude higher than those of Si and GaAs. A wide bandgap means that electrons need to acquire higher energy to transition from the valence band to the conduction band. In such materials, charge carriers are difficult to excite under low electric fields, which effectively restricts the generation and migration of charge carriers. In the crystal structure of GaN, the strong covalent bond energy between nitrogen atoms and gallium atoms is as high as 8.9 eV. The crystal has high symmetry and stability, making it less prone to lattice distortion or ion migration due to electric field effects. For many crystal types of SiC (such as 4H-SiC and 6H-SiC), the bond energy of Si-C (approximately 7.3 eV) is generally higher than that of Si-Si (approximately 4.6 eV). The strongly bonded structure suppresses atomic displacement and defect generation under high electric fields, reduces leakage current paths, and thus enhances the breakdown voltage. The high breakdown voltage characteristics of GaN and SiC make them ideal alternatives to traditional silicon, helping improve the power conversion efficiency, reliability, and system integration.

### 3.5 Application fields and development

Graphene has an electron mobility far exceeding that of traditional semiconductor materials and can achieve faster transmission speeds. Utilizing this feature, graphene can play a huge role in sensor modules, helping AI chips to perceive environmental information faster and achieve faster computing and data processing. At the same time, its

excellent thermal conductivity can help solve the thermal management problems of AI chips and can be added to the chip cooling system to promote the development of packaging technology, ensure the stability of the chip under high computing power operation, and extend its service life. MoS<sub>2</sub> has an adjustable bandgap width and variable breakdown voltage. Its special layered structure enables it to exhibit excellent switching performance when constructing field-effect transistors. This feature has obvious advantages in chip storage modules, and can help chips flexibly adjust performance according to different storage requirements, achieving efficient storage and reading of data. It is an ideal logic switching device material.

The third-generation semiconductors, GaN and SiC, have the advantages of wide bandgap, high thermal conductivity, and high electron mobility, which can help AI chips effectively improve computing power, reduce power consumption, and enhance stability. Devices such as GaN HEMT and SiC MOSFET based on third-generation semiconductors have shown performance characteristics that can better adapt to the high-power working scenarios of AI chips. They can be used in high-frequency power amplifier modules and RF modules for high-speed signal transmission to help chips control output power consumption and achieve the performance requirements of efficient processing and transmission of data under high temperature and high load conditions. In addition, the high breakdown voltage characteristics of third-generation semiconductors also allow related devices to withstand higher operating voltages, which can help chips increase switching frequency while enhancing reliability, and can play an important role in power management modules where AI chips require high-frequency conversion and stable power supply.

## 4 Application Challenges of Novel Materials

Today in practical applications, two-dimensional materials and third-generation semiconductors still face significant challenges in material production and device fabrication. Novel materials need to overcome the difficulties in material growth, fabrication process and application cost in order to achieve widespread application in the field of AI chips.

In terms of material growth, when growing high-quality large-area thin films of two-dimensional materials, the current preparation methods (such as CVD) have problems in film uniformity, defect density control, and adhesion to the substrate. The quality of thin films is difficult to meet the high requirements of device manufacturing during large-scale production. The production of third-generation semiconductor materials requires harsh conditions such as high temperature and high pressure. Throughout the material growth phase, defects like dislocations and stacking faults tend to emerge readily, thereby impacting the electrical attributes of the materials and the dependability of the devices. Moreover, attaining precise doping control demands an extended time frame, which in turn heightens the complexity of production. In terms of manufacturing processes, two-dimensional materials have process compatibility issues with traditional semiconductors. There are differences in lattice constants, thermal expansion coeffi-

cients, and processing conditions. Traditional semiconductor processes such as photolithography, etching and other technologies are not directly applicable to two-dimensional materials either. Third-generation semiconductor materials are relatively hard, posing challenges to traditional etching processes. Meanwhile, nano-sized devices have extremely high requirements for photolithography precision and resolution, necessitating more advanced photolithography technology to fabricate smaller-sized devices. In terms of Ohmic contact, the issue of contact resistance (the hindrance to carrier transport at the interface with metal electrodes) is a core challenge restricting device performance. MoS<sub>2</sub> has a high intrinsic resistivity, which tends to generate high Schottky barriers and impede carrier transport when the interconnecting metal is deposited directly on the source and drain during device fabrication. Forming good Ohmic contacts on third-generation semiconductors is also quite challenging, requiring processes such as optimizing electrode materials, surface treatment, and annealing to reduce contact resistance.

In addition, novel materials represented by two-dimensional materials and third-generation semiconductors still need to overcome dual challenges in cost and technological maturity before industrial production and commercial application in the AI chip field. At present, the circuit and architecture design of AI chips for two-dimensional material devices is still in the exploratory stage, lacking a mature application system and having adaptability issues with existing device manufacturing processes. Compared with traditional silicon semiconductors, third-generation semiconductors suffer from low product yield and high production costs due to complex manufacturing processes and immature device applications, making them unsuitable for mass production. Currently, the development costs of AI chips are high, thus there is still a long way to go before two-dimensional materials and third-generation semiconductors can be commercially applied in the field of AI chips.

## 5 Conclusion

The four popular new materials have their own advantages in material properties, and have exciting application potential under different scenarios and performance requirements of AI chip design, bringing new development opportunities for AI chips. However, the industrial production and commercial application of new materials still face challenges in material preparation, device manufacturing and production costs. In today's technology cycle, the semiconductor industry and AI technology have formed a mutually reinforcing relationship. The application of AI technology within the semiconductor industry is also expected to help new materials break through existing research and application bottlenecks. New materials with excellent properties can promote AI chip design to move towards higher computing power, lower power consumption and greater stability, and accelerate the development of artificial intelligence technology.

**Authors Contribution.** All the authors contributed equally and their names were listed in alphabetical order.

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