

The Possibilities Offered by New Semiconductor Materials



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For decades, the backbone of the semiconductor industry has been silicon (Si). While this has undoubtedly served us well, its physical limitations are becoming more apparent as we keep on pushing the boundaries of device miniaturisation and performance. The demand for higher speeds, better energy efficiency and more robust thermal management, in applications ranging from smartphones to electric vehicles (EVs), has exposed its shortcomings.

Searching for new materials to enable continued semiconductor innovation is absolutely paramount. It will be essential to find potential options that can help support the further progression of the industry.

Among the main reasons why new materials will be needed are:

- **Restrictions in performance** - Si struggles to handle heightened power and frequency levels efficiently, resulting in energy losses and heat generation. This curbs the performance of power electronics and RF devices, plus other high-frequency applications.
- **Thermal management issues** - With the miniaturisation of components, managing heat inside them is becoming increasingly difficult. Si's thermal conductivity is inadequate for many high-power applications, leading to overheating and potential component failure.
- **Energy efficiency** - As global energy

demands rise, improving energy efficiency in all electronic devices is crucial. Si's limitations in this area hinder advancements in applications like e-Mobility, renewable energy systems, portable electronics, etc.

- **Emerging technologies** - Future applications, such as quantum computing, artificial intelligence (AI) and advanced telecommunications, will require materials with properties that Si simply cannot provide. For instance, 2-dimensional materials (like graphene) and wide-bandgap (WBG) semiconductors can operate under conditions that Si is unable to withstand, offering the potential for new device architectures and suchlike.
- **Sustainability and supply chain** - The production of Si-based semiconductors is resource intensive and contributes to environmental problems. Additionally, geopolitical issues around Si supply chains highlight the need for alternative materials that are more sustainable and accessible.

Promising new materials

As demand for advanced electronic devices continues to grow, the semiconductor industry must look beyond traditional Si to attain heightened degrees of performance and efficiency. This shift has already led to the exploration of several materials that offer unique, highly desirable properties. Table 1 provides a comparison of these materials and outlines what their potential impact on the semiconductor industry could be.

The integration of these new materials into semiconductor manufacturing is crucial for breaking through the limitations of associated with Si. Each material offers distinct advantages that could drive innovation across various applications, from power electronics to flexible devices. With ongoing research and development, these materials will be pivotal in shaping the future of the semiconductor industry, enabling the development of faster, more versatile technologies with greater operational efficiencies.

Using AI in material discovery

The discovery of new materials has traditionally been a slow, laborious and expensive process, relying heavily on a trial-and-error strategy - with extensive experimentation and subsequent data compiling being undertaken in laboratories. However, the integration of AI and next-generation computational methods are now

Material	Key Properties	Applications	Advantages
Gallium-nitride (GaN)	High electron mobility and high breakdown voltage	Power electronics and RF devices	Smaller, more efficient power converters and high-frequency performance
Silicon-carbide (SiC)	High thermal stability, high voltage capacity	Electric vehicles, power grids	Reduces energy losses and operates under high temperatures/voltages
Cubic-boron-arsenide (c-BAs)	Exceptional thermal conductivity	High-power electronics	Efficient heat dissipation, which improves device reliability
2D materials (graphene, MoS ₂)	High carrier mobility and flexibility	Flexible electronics, sensors and transistors	Ultra-thin, flexible devices, high-speed transistors
Indium-gallium-arsenide (InGaAs)	High electron mobility, direct bandgap	High-speed transistors and optoelectronics	Well suited to high-frequency communication, lasers and photodetector

Table 1: Comparison of new semiconductor materials' properties

helping to transform this landscape. AI can predict material properties, simulate interactions and uncover candidates that show signs of potential much faster than traditional methods - thereby inspiring a new era of material discovery.

Leveraging AI enables rapid analysing of vast datasets, so as to get an understanding of what a material's behaviour will be. Machine learning (ML) models can optimise fabrication processes by simulating various manufacturing conditions and pinpointing the best methods to achieve superior quality materials. Computational tools allow high-throughput screening, rapidly identifying promising material combinations that would take years to discover through use of conventional methods. By integrating experimental data with theoretical models, AI platforms provide a comprehensive grasp of material properties, leading to a speeding up of design iterations and access to tailored materials for specific applications.

Major players in AI-based materials discovery

IBM uses an AI-driven deep search platform to analyse massive datasets of material properties and accelerate the identification of promising candidates for semiconductor applications. The platform can predict material behaviour under various conditions, resulting in faster discovery and optimisation. Also of note is Meta's Open Catalyst Project. Here, ML is used to investigate new catalyst materials for sustainable energy

production. By training models on large datasets, it's possible to predict the reactivity of new compounds (which have prospective relevance in a semiconductor context) more efficiently.

Through the employment of neural networks, Google is conducting AI research focused on predicting the properties of inorganic materials. This model helps screen potential materials for electronics, predicting properties such as bandgap and stability. By harnessing the power of AI and computational models, researchers can explore a broader range of materials, significantly shortening the transition period from theoretical concepts to practical applications. This approach not only hastens the discovery process, but also enables cost reductions and curtails environmental impact. The possibility of a more sustainable and scalable future for semiconductor innovation is within reach, thanks to AI-driven material discovery.

Challenges of embracing new materials

While GaN and SiC have established fabs, integrating them into the broader semiconductor manufacturing ecosystem nevertheless presents obstacles. These include the need for specialised equipment, as such materials call for different processing conditions than Si. Quality control, yield optimisation and maintaining high-performance consistency at scale are still complex tasks. Despite these challenges, existing fabs

demonstrate the growing feasibility and adoption of GaN and SiC. It is clear though that further innovation in manufacturing processes is necessary for widespread integration and efficiency improvements.

Integrating new materials like c-BAs, InGaAs and 2D options into semiconductor manufacturing presents several challenges too. For c-BAs, large-scale production remains difficult due to the complexity of growing high-quality crystals. 2D materials also face certain fabrication issues, particularly in maintaining stability and avoiding defects during integration with existing processes. While appealing for high-speed applications, InGaAs suffer from lattice mismatch with Si, which can lead to defects and reliability concerns, with advanced techniques required for seamless device integration.

Additionally, achieving high-quality interfaces between new materials and silicon poses another sizable hurdle - as poor interfaces can introduce electronic defects. Moreover, while they have feasibility to use in a lab environment, scaling these materials for mass production and simultaneously keeping costs in check remains a daunting task. Overcoming all these issues will require the implementation of sophisticated fabrication techniques and widespread industry collaboration. Above all, it will mandate significant monetary investments in research and development. The urgency of this investment cannot be overstated.



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