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Molecular Engineering in the Semiconductor Industry: Progress and Prospects

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Abstract. Along with population growth and economic development, human demand for energy and information will be more than ever, and humans need to rely on semiconductor devices to achieve energy storage, signal and other conversions. So how to design and prepare semiconductor materials with better performance, and industrialise and commercialise the materials has become a new hot topic. Typically, semiconductor materials are nanomaterials, and the current mainstream industrial processing is a top-down process, which raises the cost of production and leads to a waste of resources. Because of this, scientists are starting to believe that molecular engineering—a bottom-up strategy based on molecule self-assembly can save resources, energy, and production costs by constructing semiconductor material structures. This paper examines the bottom-up conceptual approach of molecular engineering and discusses the potential challenges in applying molecular self-assembly technology, which is a crucial method in molecular engineering, to the semiconductor industry. It ultimately concludes that molecular engineering plays a significant role in the semiconductor production process due to its advantages and vast potential for development.

Keywords: Semiconductor materials, Nanomaterials, Molecular engineering, Molecular self-assembly.

1. Introduction

Semiconductor materials have come to dominate the energy sector and the electronic communications sector. Both fields need semiconductor materials with better performance. In addition, to meet the needs of human life and the production of electronic communication, the semiconductor materials used in the field should also have the characteristics of integration, miniaturisation and flexibilization. Such as intelligent terminal mobile phone chips, both want to follow Moore's law but also want to build more transistors in the original size or even smaller size range to improve computing performance and reduce energy consumption. In order to achieve many of the characteristics of a particular semiconductor material, it is necessary to change the size and structure of the semiconductor material, not only to be processed into materials with nanometer dimensions but also to ensure that there is a special structure. As a result, materials engineers no longer employ the popular top-down mechanical processing (cutting, lithography, etc.) and preparation methods that are currently available. Instead, they employ a bottom-up approach that relies on the molecular self-assembly of semiconductor materials to achieve the

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synthesis of molecular engineering preparation at the molecular level under the assembly process. This method is also referred to as molecular engineering.

2. Literature review

In the last few decades or so, molecular self-assembly has received a great deal of attention due to its ability to form larger colloids or nano-aggregates and technological applications and products based on the principle of self-assembly, e.g., in the pharmaceutical field to prepare shells of drugs for the treatment of specific cancerous tissues have a targeted binding effect [1, 2]. In addition, supercapacitors with helically structured V2O5 electrodes have been designed using molecular self-assembly to have high specific capacitance and strong electrochromic colours to indicate the charging status of the capacitor [3]. In the field of environmental engineering, such as catalytic degradation of organic matter and wastewater treatment, people rely on molecular self-assembly or molecular engineering to prepare semiconductor catalysts or catalyst carriers, so that they have a certain forbidden bandwidth or skeleton structure to increase the catalytic material's specific surface and so on, to improve the catalytic ability [4, 5]. The above cases of using molecular self-assembly to successfully achieve material preparation and performance enhancement also provide ideas for semiconductor manufacturing. However, in recent years, the rapid development of smart devices and wearable devices has benefited from the advancement of semiconductor chips in the hardware part. However, there are still some challenges if we want to realise flexible wearable devices. Therefore, there is a great need to understand the technical principles of molecular self-assembly in molecular engineering in light of recent advances. This review provides a general overview of the subject. Firstly, the concept of molecular engineering and the techniques of molecular self-assembly are introduced, as well as the shortcomings. Then, practical examples of material preparation by some research groups are described. Finally, the challenges and outlook for the future application of molecular engineering in the semiconductor industry are predicted. It is hoped that the review of this paper will clarify the significance and application prospects of molecular engineering in semiconductor material preparation and provide insights into the development of the semiconductor industry.

3. Concepts of molecular engineering and molecular self-assembly

Molecular engineering is a new way of thinking about engineering problems. Instead of using pre-fabricated materials and trying to design engineering applications that are consistent with their macroscopic properties, it involves building materials from molecules as needed. Among them, molecular self-assembly can be regarded as one of the important strategies or means of molecular engineering. Molecular self-assembly refers to the process of spontaneous assembly of molecules to form ordered structural or functional units through intermolecular forces (e.g. hydrogen bonding, van der Waals forces, etc.).

3.1. Key drivers of molecular engineering

Called driving forces when they are applied, and which include intermolecular hydrogen bonding, van der Waals' forces, Coulombic forces, ionic dipole interactions, inter-dipole interactions, hydrophobic effects, site-barrier interactions, depletion interactions, and so on. The motivating factors include Molecular self-assembly, which is reversible due to a multitude of driving forces. This is significant since it provides molecular engineering with the functional benefits of error correction and "self-repair" because of the presence of specific driving forces.

3.2. Molecular self-assembly techniques

Molecular self-assembly is a technique based on intermolecular interactions, whereby molecules are spontaneously assembled into specific structures or functional materials by controlling their interactions. Molecular self-assembly has also been classified as static self-assembly and dynamic self-assembly according to kinetics. In addition to this, George and Bartosz also defined two additional types of self-assembly: templated self-assembly and crystallization of colloids in three-dimensional optical fields [6].

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3.2.1. Static self-assembly & Dynamic self-assembly

Static self-assembly involves systems that are in global or local equilibrium and do not dissipate energy. For example, molecular crystals [2, 3] are formed by static self-assembly; as are most folded globular proteins. In static self-assembly, the formation of an ordered structure may require energy (e.g., in the form of agitation), but once formed, it is stable. Most self-assembly studies have focused on this static type. Dynamic self-assembly refers to the interactions between components that lead to the formation of structures or patterns only when the system consumes energy. Patterns formed through competition between reaction and diffusion in oscillatory chemical reactions are simple examples of dynamic self-assembly; biological cells are more complex examples. The study of dynamic self-assembly is still in its infancy.

3.2.2. Templated self-assembly

Template self-assembly is where the interaction between components and regular features of their environment determines the structure that is formed. An example is crystal growth on surfaces with defined morphology. Template self-assembly has important applications in nanotechnology. It is often the case that templates are prepared using block copolymers, and products are subsequently processed based on the templates, as theoretically modeled in Figure. 1 (thanks to Synthesis and Applications of Double-Gyroid-Structured Functional Materials). For example, Di Wei et al. prepared V2O5 supercapacitor electrodes with a helical structure using templated self-assembly, and the electrodes exhibited high specific capacitance[7].

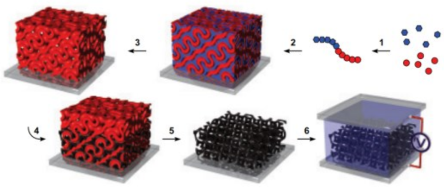

Figure 1. BCP templates - from generic templates to functional material architectures [7]

In addition, there are some shortcomings of block copolymers, such as the fact that the theoretical phase diagram and the actual preparation cannot be matched, as shown in Figure 2. There are also some regional errors. This is also a deficiency of the current block copolymer, or molecular self-assembly technology, and perhaps a more suitable theoretical model of thermodynamics and kinetics is needed.

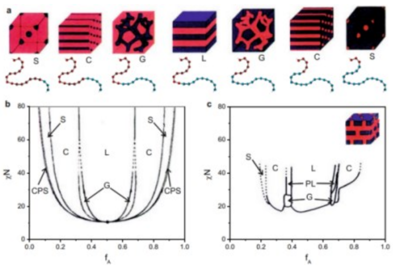

Figure 2. Phase separation of diblock copolymers.

(a) Schematic representation of diblock copolymer chain asymmetry and the corresponding morphological arrangements after phase separation. Self-consistent mean-field theory predicts five arrangements at thermodynamic equilibrium with decreasing asymmetry: densely packed spheres (CPS, not shown), body-centred cubic sphere arrangement (S), hexagonally arranged cylinders (C), gyroscopes (G)), and layered phases (L). b) The phase diagram can be parameterised by the volume fraction (fA) of=block A and the combined parameter χN. c) Experimental data for BCP model systems such as poly(isoprene-b-styrene) are in good agreement with the calculations [8]. a) - c) Adapted with permission from [9]. Copyright 1999 American Institute of Physics. [INORGANIC NANOARCHITECTURES BY ORGANIC SELFASSEMBLY page 7 of the book].

4. Molecular Engineering in Materials Preparation

This section focuses on molecular engineering, using molecular self-assembly techniques for applications in the field of materials.

20 nm diameter silica columns. Figure 3 shows the transfer of square-packed PFS microdomain arrays to prepare silica columns with heights of 30 nm and aspect ratios (height/diameter) ∼1.6, which are larger than those of the pristine PFS columns (aspect ratios ∼1). The use of triple block terpolymers in self-assembly can create nanostructures with unique geometries that are not achievable with diblock copolymers. This advancement greatly improves the effectiveness of block copolymer lithography [10]. What's more, the use of templated self-assembly of triblock terpolymers can create nanostructures with unique geometries that are not achievable with diblock copolymers. This technique greatly improves block copolymer lithography [10].

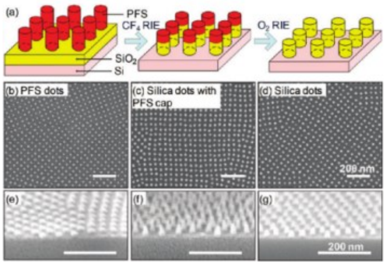

Figure 3. BCP etching process for silicon dioxide dots [10]

A. Baruth et al. report the successful execution of a nanolithography process based on a solvent-annealed, cylindrically molded, readily degradable polystyrene-polypropylene cross polymer block copolymer film, which completely avoids the stripping of the most challenging aspects of the etch. And demonstrated by the formation of large area arrays of 25 nm diameter ferromagnetic Ni80Fe20 nanodots with a hexagonal dense stacking sequence, which A. Baruth et al. believe can be scaled to smaller feature sizes achieved to minimise etch damage, thus preserving the essential functionality of the patterned material [11].

Yidong Zou et al. demonstrated the spontaneous orthogonal stacking of poly(ethylene oxide)-block polystyrene and silicotungstic acid composite nanorods using tungsten oxide semiconductor nanowires as an example to obtain a controllable construction of 3D multilayered cross-metal oxide nanowire arrays, which were prepared using the principle of molecular self-assembly, which solves the problem of manual assembly or transfer printing and therefore the lack of synthesis flexibility and controllability [12].

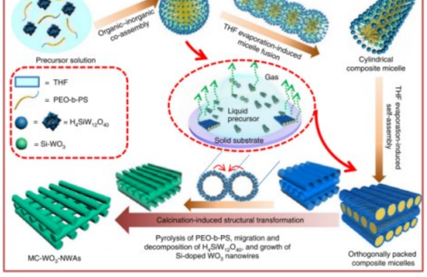

Figure 4. Schematic diagram of the formation process of MC-WO3-NWA [12]

Edward J. W. Crossland et al. reported the first successful application of ordered bicontinuous gyrosemiconductor networks in hybrid heterojunction solar cells [13]. Their freestanding helical networks were made by electrochemical deposition into 10 nm wide void channels of a self-assembled, selectively degradable block copolymer film, and solid-state dye-sensitised solar cells only 400 nm thick exhibited power conversion efficiencies of up to 1.7%.

5. Challenges for molecular engineering in the industrialisation of semiconductors

5.1. Challenges

Even though molecular engineering can create or prepare unique structural functional materials from the bottom up, the process also has drawbacks, such as difficult-to-control molecules or unsatisfactory self-assembly, which leads to uneven material structure in large-scale industrial production. This means that a batch of materials will perform differently even if they are polished into a granular powder and then processed to produce a uniform effect. Additionally, the powder's surface free energy prevents material agglomerates from achieving a uniform arrangement of nanometer size, so the material performance is not ideal. Even if the powder is polished into particles and processed to achieve uniformity, the free energy on the surface of the powder will cause the material to agglomerate and fail to achieve a uniform distribution of nano-size, resulting in less than ideal material properties. Because commercialisation places great importance on product stability, this is an important reason why industrialisation has not made extensive use of molecular engineering, a bottom-up design approach to materials production. In particular, the semiconductor industry requires strong and stable properties. Certainly, in the second part, this paper introduced some applications of molecular engineering, it can be seen in the semiconductor industry in some of the production steps also use molecular engineering concept or molecular self-assembly technology to produce intermediates, so molecular engineering in the semiconductor industry is facing certain challenges, this section mainly describes the use of molecular self-assembly technology for the production of semiconductor materials need to face the challenges. This section focuses on the challenges of producing semiconductor materials using molecular self-assembly techniques, which are summarised below.

5.2. Limitations

Molecular self-assembly is usually limited by interactions between components and environmental conditions. This means that only specific types of molecules can be self-assembled and specific conditions are required for this to occur. This limits the applicability and flexibility of self-assembly. b) Lack of controllability: although it is possible to influence the self-assembly process by designing the molecular structure and environmental conditions, it is actually difficult to fully control the outcome of self-assembly. This is because self-assembly is a complex process involving many interactions and kinetic parameters. Therefore, achieving precise self-assembled structures remains a challenge. c) Instability: Since self-assembly is a dynamic process, the stability of the structure may be affected by external conditions. For example, changes in temperature, solvent, pH, etc. may lead to dissociation or reorganisation of the self-assembled structure. This limits the long-term stability and reliability of self-assembled structures. d) Lack of complexity: Although molecular self-assembly can produce several ordered structures and functions, its complexity is still relatively low compared to that of complex self-assembly in living organisms. Currently, people have not fully understood and mimicked the mechanism and function of complex self-assembly in organisms.

6. Conclusion

With the rapid development of modern society, human production and living needs are oriented towards miniaturiation, wearability, and other directions, which have higher requirements on the production and preparation of materials, requiring the production of materials not only at the nano level but also need to have a special structure, to achieve materials with special functions. This paper found that in the idea of material preparation, molecular engineering is different from the previous top-down approach, but similar to Lego blocks like bottom-up construction. It is conceivable that the self-assembly of molecules ranges from the microscopic nano-size to the macroscopic, and researchers need to figure out why

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molecules self-assemble, which is built based on studies of self-assembly kinetics, thermodynamics, and so on, coupled with artificial intelligence such as mathematical modeling. Due to the limitations of this article, there is a lack of data to support it. For the application of molecular engineering in the semiconductor industry as a whole, although it is still at the stage of local application, one day molecular engineering can be more widely used in industry, especially in the semiconductor industry, as well as in biomedicine, aerospace and other fields, to solve the energy crisis, environmental crisis and climate problems that mankind is facing. The use of materials by human beings has contributed to the progress of human civilisation, in order of the Stone Age, the Iron Age, etc. Nowadays, the bottom-up design concept of molecular engineering provides unlimited prospects for the development of civilisation in human society, and it is believed that one day, the great era of molecular engineering will eventually come and become another milestone in the history of human industrial civilisation.

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