Diffusion Process Strategies for Semiconductor Devices

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Abstract. The semiconductor industry is rapidly advancing toward high precision and miniaturization. As a core process in semiconductor device fabrication, diffusion technology plays a crucial role, with its selection directly impacting device performance. This paper delves into the fundamental principles of diffusion processes in semiconductor devices, presents relevant case studies, and explores future development trends. First, the conventional diffusion process flow is introduced. Subsequently, the focus shifts to three classic diffusion techniques employed in the core diffusion step: constant-source diffusion, limited-source diffusion, and two-step diffusion. Based on their typical boundary conditions, the characteristics of these diffusion techniques are analyzed through formula-based mechanism studies. Through a comprehensive analysis of existing research findings and industrial practices, this paper not only systematically reviews the core aspects of semiconductor device diffusion processes but also provides valuable theoretical support and practical guidance for the industry to optimize process solutions and drive technological innovation in diffusion processes.

Keywords: Diffusion Processes, Constant-Source Diffusion, Limited-Source Diffusion, Two-Step Diffusion, Scene Selection.

1. Introduction

In semiconductor manufacturing, the diffusion process serves as a critical step, which is most commonly applied in the production of integrated circuits and discrete devices [1]. It plays a vital role in forming the core structures of semiconductors, thereby influencing the operational efficiency and quality of the final products [2]. With the ongoing miniaturization of semiconductor devices, characterized by integrated chips, and the increasing demands for enhanced performance, higher requirements are now placed on the precision and application of the diffusion process.

In diffusion processes, there exist not only traditional constant-source diffusion and limited-source diffusion methods, but also multi-step diffusion techniques represented by the two-step diffusion method [2,3]. These three classical and mature technologies are indispensable in microprocessor manufacturing and are also widely applied across various semiconductor fields, including photovoltaic cells, power devices, and sensors. In 1978, Fair and Tsai proposed a diffusion model for phosphorus in silicon and explained the emitter dip phenomenon, establishing diffusion processes as fundamental to emitter/source-drain region design and simulation. By 2014, Fraunhofer ISE validated APCVD-BSG and $POCl_3$ co-diffusion on mass production lines, enabling one-step formation of emitter/BSF. This demonstrated that combined optimization of diffusion processes is critical for photovoltaic scaling and consistency. Then in 2023, Xu and others proposed a “low-high-low” stepwise temperature $POCl_3$ diffusion scheme. This approach maintains a low surface concentration while enhancing open-circuit voltage and fill factor in mass-produced batteries, further demonstrating the universal value of refined diffusion process control in improving industrial-grade performance [4-6]. Different diffusion processes exhibit distinct characteristics in terms of diffusion source supply mechanisms, impurity concentration gradient control, and process compatibility, while also presenting unique technical challenges.

Investigating the precision value differences among various diffusion processes and selecting the optimal diffusion strategy for diverse manufacturing scenarios has become a critical challenge in enhancing semiconductor device performance and production efficiency. This paper first introduces the fundamental principles and operational procedures of impurity diffusion, analyzes three typical diffusion methods, and presents relevant case studies highlighting their characteristics. Finally, it summarizes and compares the three approaches, discussing their applicable scenarios and future prospects.

2. Diffusion Process and Fundamental Principles

The general process flow for diffusion is shown in Figure 1 below.

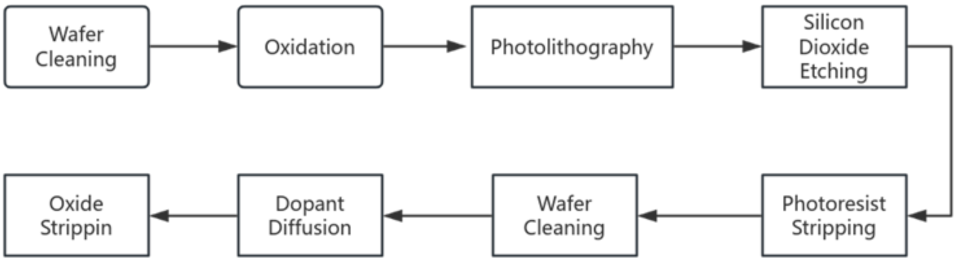

Figure 1. General Process Steps for Diffusion

The first step in the doping process is cleaning the silicon wafers to remove particles, organic matter, and other metallic impurities from their surfaces, creating a clean substrate. This is followed by thermal oxidation to form a uniform silicon dioxide film on the wafer surface, which serves as a masking layer for subsequent etching. The process then proceeds to photoresist coating. After completing photolithography through steps such as exposure and development, the mask pattern is transferred onto the photoresist layer. Using dry or wet etching techniques, the silicon dioxide not protected by photoresist is selectively removed, exposing the silicon substrate areas requiring doping. After etching, the residual photoresist is stripped away, revealing the patterned silicon dioxide structure. Then, wafer cleaning is performed to remove chemical residues and particles generated during etching and stripping. After completing the preparatory steps, the core doping process is carried out using diffusion phenomena and appropriate diffusion techniques. Finally, the oxide layer is stripped away, achieving precise doping in localized areas. Diffusion primarily utilizes concentration gradients to drive impurity diffusion, with the process adhering to Fick's first and second laws within the diffusion law system [7]. Diffusion technology employs thermal activation to enable directed migration of impurity atoms within silicon crystals from high to low concentration regions, achieving precise control over specific impurity concentration gradients and junction depths. Based on differences in impurity source supply methods within integrated circuit manufacturing processes and distinct diffusion process control strategies, diffusion techniques can be systematically categorized into three typical types: constant-source diffusion, limited-source diffusion, and multi-step diffusion represented by two-step diffusion.

2.1. Constant-Source Diffusion Method

2.1.1. Basic Principles of the Constant-Source Diffusion Method

Constant-source diffusion is continuously replenished by an external impurity source during processing, maintaining the wafer surface concentration at the solubility limit [8]. The one-dimensional model typically assumes boundary/initial conditions of surface $C(0,t) = Cs$ and an initial bulk concentration is approximately equal to 0. Under these conditions, applying Fick's second law reveals that the concentration profile in devices with constant-source diffusion follows an erfc distribution. Total dose and junction depth increase linearly with time, while the diffusion coefficient exhibits Arrhenius dependence on temperature. Consequently, the profile exhibits high surface concentration and steep gradients. While process control is straightforward, this approach is unfavorable for achieving low surface concentrations and gentle gradients.

2.1.2. Constant-Source Diffusion Case Analysis

From the formula, it can be seen that the surface concentration in this diffusion method remains constant at the solubility limit Cs. To maintain a constant surface concentration, impurities must be continuously replenished. As diffusion time increases, the junction depth gradually deepens. In industrial research on tubular diffusion, Li Hongzhao et al. employed a constant-source diffusion operation with continuous impurity supply, clamping the wafer surface concentration at the solubility limit while achieving a proportional increase in total doping dose over time [9]. At EU PVSEC 2020, the Fraunhofer ISE team optimized the emitter of photovoltaic cells in an industrial-scale $POCl_3$ tube diffusion process by lowering the phosphorus-silicon glass deposition temperature and independently extending the diffusion time. This demonstrated that under constant-source diffusion, the surface concentration is continuously supplied by an external source ($POCl_3$ vapor source) and can be controlled by temperature, while the junction depth progresses over time. the combined adjustment of these two parameters further yielded a more uniform sheet resistance of approximately 105 Ω/sq [10]. Cao Chuhui conducted experiments using a diffusion apparatus with phosphorus oxychloride as the source, setting and validating the process parameters of temperature and time. The sheet resistance was measured as the control variable using the four-probe method. Numerical simulation results indicated that increasing the temperature at the same diffusion time, or extending the diffusion time at a constant temperature, both deepened the junction depth [11].

In conclusion, constant-source diffusion exhibits distinct characteristics: it stabilizes surface concentration at the solubility limit, causing total dose and junction depth to increase proportionally over time. Cross-section analysis reveals high surface concentration and steep gradient profiles. However, while this diffusion method is easy to control, it is unsuitable for achieving low surface concentration and gentle gradient doping effects.

2.2. Limited-Source Diffusion

2.2.1. Basic Principles of the Limited-Source Diffusion Method

Unlike constant-source diffusion, limited-source diffusion pre-deposits a finite amount of impurities on the wafer surface before diffusion begins and does not replenish new sources during the process, meaning the total impurity amount remains constant [8]. Subsequently, only redistribution occurs during thermal diffusion. At this stage, the surface concentration continuously decreases over time as impurities diffuse into the bulk. The profile gradually flattens from a peak, exhibiting a smoother gradient and a Gaussian distribution. Due to the conservation of total dose and the gradual increase in junction depth over time and temperature, limited-source diffusion is suitable for scenarios requiring low surface concentration, gentle gradients, and precise control of dose/resistance per wafer. However, it is less efficient than constant-source diffusion when high surface concentration and extremely steep gradients are needed. The following case studies analyze the characteristics and applicable scenarios of limited-source diffusion.

2.2.2. Limited-Source Diffusion

Compared to constant-source diffusion, the deepening of PN junctions in limited-source diffusion also scales proportionally with diffusion time. However, limited-source diffusion exhibits lower surface concentrations and gentler gradients. Guo Qin et al. simulated limited-source diffusion using Mathematica to model impurity distribution after pre-dosing, yielding images showing decreased surface concentrations and profiles that flattened into Gaussian distributions [12]. In arsenic (As) metered injection studies, a pre-set dose was injected at 950°C using 80 keV ions. The relationship between drive-in time and sheet resistance/junction depth was investigated, demonstrating the characteristics of constant total dose, reduced surface concentration, and deepening junction depth over time in limited-source diffusion. This confirms the applicability of limited-source diffusion for manufacturing power semiconductor doping regions [8]. Heilig and colleagues prepared BSG/PSG multilayer pre-doped layers via APCVD. Following laser diffusion and thermal processing, they achieved reduced surface concentration, profile smoothing, and mask-free selective doping. This approach eliminated lithography, lowered costs, and reduced surface recombination, addressing the challenges of complex photolithography and high carrier loss in photovoltaic devices [13]. What's more, Keding et al. employed PECVD-deposited thin layers as a defined source, achieving low surface concentration and a gentle gradient profile through diffusion at 950 °C for 30 minutes. This approach enabled precise quantity control and process stability within thermal budget constraints, facilitating stable and consistent emitter sheet formation without altering the furnace program [14].

According to these cases, limited-source diffusion has the outstanding advantages of slowing down the profile, controlling the amount accurately, and reducing the cost and improving the efficiency; however, due to the limitation of its own characteristics, this kind of diffusion is not applicable to the scenarios that require high surface concentration.

Based on these characteristics, source-limited diffusion is well suited for the fabrication of photovoltaic devices, as well as industrial semiconductor devices, which share the common characteristics of slow gradient and low complexity.

2.3. Two-step diffusion

2.3.1. Basic Principles of the Two-Step Diffusion Method

The two-step diffusion method combines the advantages of constant-source diffusion and limited-source diffusion, which is usually divided into a pre-precipitation phase and an advancement phase in applications [15].The two-step diffusion method employs constant-source diffusion in the preprecipitation stage to introduce impurities at lower temperatures to form a shallow distribution of high surface concentrations, and switches to finite-source diffusion without an external source in the advancement stage to advance the impurities deeper at higher temperatures while lowering the surface concentration.

It should be pointed out that there is a significant difference between two-step diffusion and source-limited diffusion. Source-limited diffusion is where the total amount of impurities is limited before diffusion begins and no new sources are added throughout the process, so its surface concentration decays with time, making it suitable for scenarios with low surface concentrations and gentle gradients. However, the two step diffusion, although in the second stage it is also a limited source diffusion without external new sources, the dopant layer with high surface concentration has been pre-formed in the first stage after pre-precipitation from a constant source. In this way, the two-step diffusion separates the “dose control” from the “junction depth regulation”, where the pre-deposition phase ensures a sufficient total amount of doping, while the advancement phase utilizes a source-limiting mechanism to distribute the impurities deeper and reduce the surface concentration. Compared with pure source-limited diffusion, two-step diffusion can achieve lower surface concentrations while maintaining independent regulation of junction depth and sheet resistance, which is more suitable for the combined uniformity and performance needs of modern devices.

2.3.2. Two-Step Diffusion Case Analysis

As one of the more commonly used diffusion strategies in modern integrated circuit manufacturing, the two-step diffusion method can independently control the total doping amount and the junction depth, and through the optimization of the temperature and time parameters, it solves the problem that the solid solubility does not change much within the range of 900-1200 °C, and it is difficult to obtain a low surface concentration by purely constant source diffusion. This technique stands as one of the most commonly employed diffusion strategies in modern integrated circuit manufacturing. R.M. Ali et al. employed the two-step diffusion method with $POCl_3$ as the source to fabricate n-type emitters in monocrystalline silicon solar cells. During the pre-deposition stage at 775–850°C, continuous source supply formed phosphorus-silicon glass enabling shallow impurity deposition. The drive-in stage at 825–900°C ceased additional source supply to promote deep phosphorus diffusion. By adjusting temperatures, the junction depth increased from 1.44 μm to 2.79 μm while significantly reducing sheet resistance, highlighting its segmented control characteristics: pre-deposition controls dosage and post-deposition controls junction depth [16]. Mourad and others addressed charge recombination issues caused by high impurity concentrations at the emitter surface. They employed a two-step diffusion process in a low-pressure tube furnace at 200 mbar: pre-deposition followed by a 2-hour push-up phase. The constant-source pre-deposition ensured total impurity content, while the limited-source diffusion during the push-up phase reduced surface concentration. This approach effectively suppressed charge recombination and improved doping uniformity [17]. Facing the problem of poor uniformity in the conventional process of P-type emitter for N-type crystalline silicon cell, Ma Xiaobo et al. used the two-step diffusion method to pre-precipitate N_2 carrying BBr_3 with a constant source at 900-1000℃ under low pressure to lay the foundation for the total amount of impurities, and then promoted the distribution of impurities through the limited source diffusion to ultimately realize the stable square resistance (uniformity ≤4%) of 40-60 Ω and the conversion efficiency of 19.33% [18]. This demonstrates the ability of the two-step diffusion method to precisely control the resistance and improve the performance.

These cases demonstrate that the two-step diffusion method, through its segmented operation of "pre-depositing a fixed total amount and advancing to adjust distribution," can independently regulate junction depth, sheet resistance, and surface concentration. It simultaneously addresses the challenge of achieving low surface concentrations within the 900–1200°C range, where solubility varies little and constant-source diffusion alone proves inadequate.

Given these characteristics, limited-source diffusion aligns well with photovoltaic device manufacturing requirements and is also suitable for industrial semiconductor device production. It is particularly applicable to semiconductor devices demanding high doping uniformity and performance stability, such as the emitter in monocrystalline silicon solar cells and the p-type emitter in n-type crystalline silicon cells.

3. Summary of Diffusion Process Comparison Analysis

Based on the above theoretical analysis and case studies, we can compare the characteristics, advantages, and applicable fields of the three diffusion processes, forming a horizontal comparison table (Characteristics-Advantages-Applicable Fields) as shown in Table 1:

Table 1. Comparison of Characteristics, Advantages, and Applicable Fields for Three Diffusion Processes

	Constant-Source Diffusion	Limited-Source Diffusion	Two-Step Diffusion
Characteristics	Surface concentration held constant; The longer the time, the more impurities enter the wafer and the greater the increase in junction depth.	No replenishment; As time progresses, the surface concentration gradually decreases, but the total dose Q remains constant.	Constant-source predep fixes dose; limited-source drive-in deepens junction. Used for lower C_s profile with limited solubility.
Advantages	High surface conc., steep profile; simple and repeatable	Precise total dose; drive-in lowers surface conc.; smoother profile	Decouples dose-setting from depth tuning; low surface concentration at target depth
Applicable Fields	Scenarios requiring high target surface concentration and steep curves	Device processes requiring precise dose control or low surface concentration/gentle gradient	scenarios requiring both low surface concentration and sufficient junction depth

Three diffusion processes serve as key methods for controlling doping concentration and junction depth distribution in integrated circuit manufacturing. The selection of these processes and the control of their parameters directly impact device performance.

Constant-source diffusion maintains a constant surface concentration through continuous source supply. Over time, the total impurity content increases synchronously with the deposition depth, facilitating the attainment of high surface concentrations and steep concentration gradients. This method features a simple process with good reproducibility, making it suitable for scenarios requiring high surface concentrations and steep deposits. However, it carries the risk of surface over-doping leading to increased composite formation. The limited source diffusion process has no additional new sources, the total dose remains unchanged, and the surface concentration gradually decreases with time. The limited source diffusion can precisely control the total doping amount, and can reduce the surface concentration and form a gentle gradient while deepening the junction depth, which is suitable for device processes that require precise dose control or low surface concentration and gentle gradient, but need to pay attention to the contact difficulties caused by insufficient dose. Two-step diffusion combines the advantages of the first two, first pre-precipitation with a constant source to set the dose, and then through a limited source to promote the deepening of the knot, to realize the decoupling of the dose control and the knot depth, the surface concentration adjustment, to be able to obtain a low surface concentration and the target depth of the knot when the solid solubility is limited. Although the two-step diffusion method is more complex, it can achieve a good compromise in the solid solubility-limited zone, and is suitable for scenarios where low surface concentration and sufficient junction depth need to be balanced to meet the combined needs of device uniformity and performance.

4. Conclusion

This paper systematically compares three diffusion processes, constant source diffusion, limited source diffusion and two-step diffusion, and reveals the significant differences between different diffusion modes in terms of surface concentration, junction depth control and other aspects. Among them, constant-source diffusion exhibits high surface concentration and steep gradient, limited-source diffusion has the advantages of controllable total doping amount and smooth gradient, and two-step diffusion strikes a balance between optimized junction depth and surface concentration. In the future, with the continuous improvement of the requirements for device microstructure and electrical properties, the diffusion process is expected to further evolve towards the development of high precision, adjustability and wide adaptability, providing better process support for advanced semiconductor manufacturing.

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