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A New Method of Industrial Passivation for Characterization of Surface Defects in Silicon-Based Materials or Solar Cell Precursors

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Accurate defect passivation is critical for characterizing intrinsic carrier lifetimes in semiconductor materials, as surface defects induce recombination centers that distort lifetime measurements. While conventional passivation coatings (e.g., SiO_2, SiN_x, Al_2O_3, a-Si:H(i)) require complex high-temperature/vacuum processes, this work proposes an innovative low-temperature solution-based approach utilizing organic passivation materials. The Nafion/Polystyrene sulfonic acid-based system achieves electrochemical interaction between sulfonic groups (SO_3^-) and silicon dangling bonds, forming interfacial silicon oxides that effectively neutralize trap states. This versatile technique accommodates multiple deposition methods—including spin coating, blade coating, spraying, and brush coating—without vacuum requirements. Demonstrated for silicon, CuInxGa(1-x) Se2, and perovskite thin films, the solution-processed passivation enables rapid, large-area characterization while maintaining exceptional stability. The combined advantages of ambient processing conditions, material compatibility, and scalability position this methodology as a cost-effective industrial solution for high-throughput semiconductor evaluation.

1. Introduction

Semiconductor surface defect management remains a critical challenge in advancing silicon photovoltaics manufacturing. Crystalline silicon substrates, along with emerging materials like CuInxGa(1-x)Se2[1] and perovskites,[2] require precise defect characterization to optimize their optoelectronic properties. In industrial silicon solar cell production spanning from wafering to metallization,[3] surface recombination control directly determines final device efficiency and production yield. Although dielectric passivation layers (e.g., SiO_2,[4–6] SiN_x,[7–9] Al_2O_3,[10–12] and a-Si:H,[13]) effectively reduce interface states, their dependence on high-temperature (>400 °C) or vacuum-assisted deposition significantly increases manufacturing complexity and energy consumption.

The semiconductor industry has long sought alternative passivation strategies combining process scalability with environmental sustainability. Since Semilab's pioneering work on iodine-based solutions in 1992,[14] liquid-phase passivation has gained attention for its low-temperature compatibility and cost-effectiveness.[15–19] However, practical limitations persist: 1) transient passivation stability (<24 h) impedes inline characterization workflows; 2) operator-dependent immersion techniques hinder process standardization; and 3) incompatible with subsequent high-throughput coating processes. These constraints underscore the need for novel liquid-phase methodologies that bridge the gap between laboratory-scale innovation and industrial-scale production demands.

Recent developments in functional polymers present new opportunities for solution-processed passivation. Materials such as Nafion[20–22] exhibit unique advantages including tunable rheology for various deposition techniques (spray, spin, or blade coating) and intrinsic chemical stability under photovoltaic processing conditions. Crucially, their molecular design flexibility allows simultaneous passivation and surface functionalization—a feature unattainable with conventional inorganic or small-molecule approaches.

In this study, we develop an industrially adaptive passivation protocol using sulfonated tetrafluoroethylene-based polymers. The proposed method addresses three key industry requirements: 1) room-temperature processing compatible with inline quality control; 2) long-term stability for passivation; and 3) seamless integration with existing photovoltaic manufacturing sequences. By combining defect termination mechanisms with scalable coating technologies, this approach establishes a unified framework for surface engineering across silicon wafers, textured substrates, and cell precursors.

2. Results and Discussion

Figure 1 illustrates the current mainstream iodine solution passivation used in production lines and the commonly used spin-coating organic solution passivation in laboratories, along with

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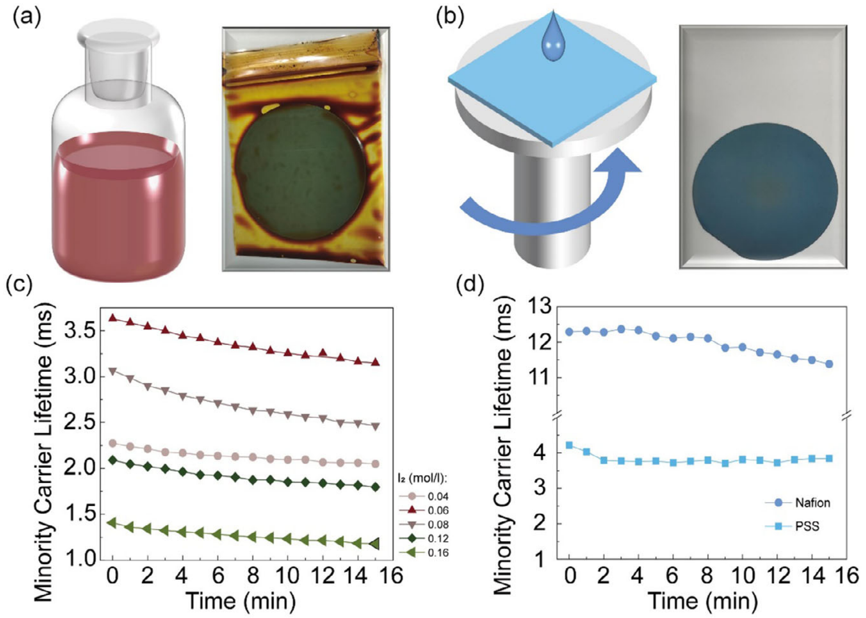

Figure 1. a,b) Schematic diagram and physical image of the immersion and spin-coating passivation process for silicon wafers; c) variation trend of τ_{eff} of silicon wafers passivated with iodine solution at different concentrations over time; and d) variation trend of effective minority carrier lifetime of silicon wafers passivated with different organic passivation materials over time.

their corresponding effective minority carrier lifetime (τ_{eff}) data.[23–25] In Figure 1a, the schematic of iodine solution passivation involves pretreating the sample, sealing it in acid-resistant plastic bags, and immersing it at room temperature. Excess solution and bubbles are expelled to ensure a thin layer of iodine solution covers both sides of the sample. However, this method is inconvenient and relies heavily on the operator's skills. Additionally, as observed in Figure 1a, iodine solution passivation fails to form a film and can only be used for lifetime measurement through the immersion method. Figure 1b depicts the schematic of spin coating with organic solution, which is the most commonly used solution-gel method in laboratories.

Figure 1c presents the variation in τ_{eff} of n-type silicon wafers with different molar concentrations of iodine solution. The highest τ_{eff} is measured at a concentration of 0.06 mol L^{-1}. Figure 1d displays τ_{eff} of various organic high-molecular-weight materials, including Nafion solution and Polystyrene sulfonic acid (PSS) solutions. From τ_{eff} in Figure 1c,d, it is visually evident that organic solution passivation outperforms iodine solution passivation, exhibiting better and more stable lifetimes in a short duration. On the other hand, iodine solution passivation shows a rapid decay in τ_{eff} over time, indicating that the Si—I bonds formed are not sufficiently stable and are prone to decomposition.[18,26–28] Therefore, this method of capturing high lifetime values in a short period poses significant challenges.

The organic solution not only possesses highly efficient and stable passivation performance but can also be implemented through various techniques, including spin, spray, pull, and passivation brush coating. Through these methods, it is possible to successfully prepare films with high durability, uniform, and dense characteristics. Schematic diagrams of these different methods and their corresponding τ_{eff} are presented in **Figure 2**. Spray coating and pull coating are common industrial techniques that can achieve rapid and uniform passivation effects. In Figure 2c, the passivation brush is a self-developed tool for optimizing photovoltaic products, employing precise and convenient localized fine coating technology to provide targeted and efficient passivation effects. Examining the data in Figure 2d reveals that films prepared using spray coating and passivation brush techniques exhibit excellent τ_{eff}, while the drawdown technique is noticeably inferior to these two. However, all three methods demonstrate good stability.

In the preparation process of crystalline silicon solar cells, the stability of the production line process is a critical factor in determining product yield. Typically, the quality of silicon materials is assessed using τ_{eff} and the PL mapping luminous intensity, with real-time monitoring of the stability of the production process to analyze any anomalies on the production line. Currently, the production lines commonly employ the iodine solution passivation method for defect detection. However, this method is inconvenient to operate and can cause irreversible damage to the samples being tested.

Figure 3 illustrates a liquid-based passivation method suitable for large-scale industrial applications, where a high-performance organic passivating solution is coated onto silicon wafers after various processes. This demonstrates the universality of the organic passivation solution process and its effective application in both solar cell preparation and silicon solar cell manufacturing processes. By measuring the PL intensity on silicon wafers (182 × 182 mm) under different solar cell manufacturing processes, we can conduct defect detection to assess surface contamination, diffusion uniformity, and the removal of phosphorous-silicon/boron-silicon glass. This method allows for the timely identification of anomalies in the production process, enabling adjustments to be

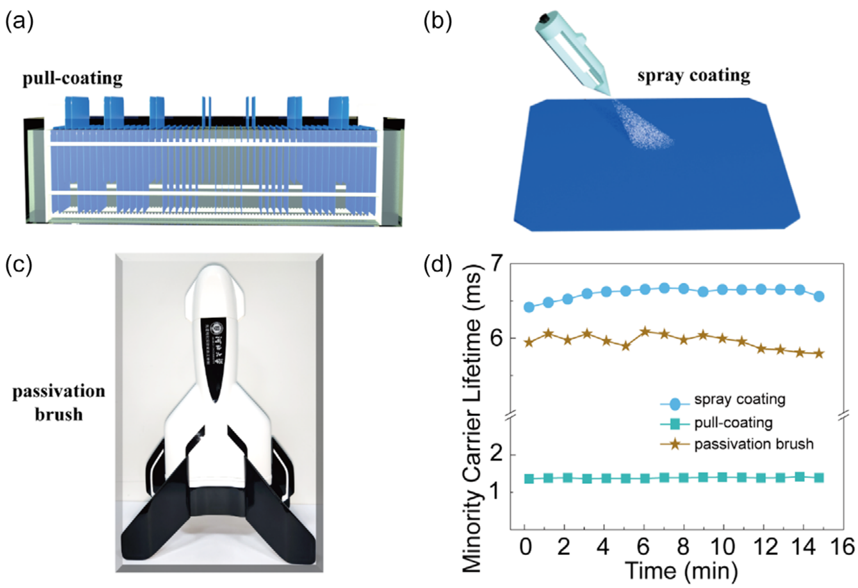

Figure 2. a–c) Schematic diagrams of the pulling, spraying, and brushing processes and d) trends of minority carrier lifetime with time under different processes.

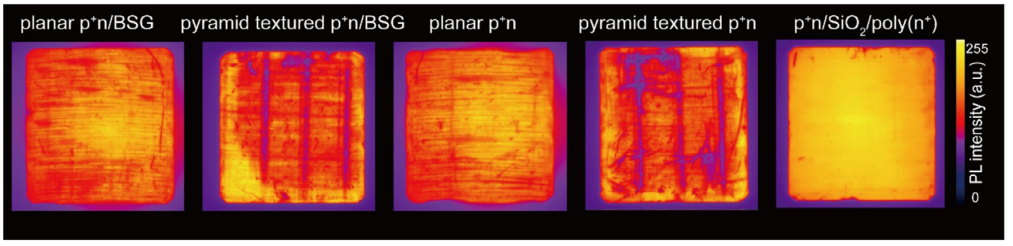

Figure 3. PL intensity mages of silicon under different process flows.

made to ensure the stability of production and the yield of high-quality silicon wafers and silicon solar cells.

3. Conclusion

After comparing with the current mainstream defect detection methods on the production line, the liquid-based passivation method demonstrates advantages that are more real time, efficient, stable, and suitable for large-scale industrialization. Compared to traditional iodine alcohol passivation, the use of organic high-molecular-weight materials for passivating double-polished silicon wafers can extend τ_{eff} to 12 ms. Through a 15 minute tracking, it was found that various existing organic passivation materials can obtain stable data.

This novel passivation method can also employ various coating techniques, applicable to different process stages, including silicon wafers, and the entire production process. Under multiple coating techniques, it is only necessary to uniformly coat the surface of silicon wafers with passivation solution to form a passivation film, enabling the testing of τ_{eff} on silicon wafers. Moreover, the τ_{eff} can still be maintained at a stable and efficient level. It can offer visual inspection methods for the commercialization process of silicon solar cells.

4. Experimental Section

Solution and Thin Film Preparation: Nafion (Sigma–Aldrich, 5 wt% in water), PSS solution (Sigma–Aldrich, 18 wt% in H_2O), PSS_2 solution (Sigma–Aldrich, 5 wt% in H_2O). Prior to film preparation, silicon wafers were immersed in a 10% hydrogen fluoride solution for 3 min to remove the oxide layer from the silicon surface. The iodine solution was applied using an immersion method, with double-polished silicon wafers sealed in acid-resistant plastic bags and immersed at room temperature. There were four methods for preparing organic films: spin coating at a speed of 3500 rpm; spray coating; pull coating; and passivation brushing.

Solar Cells: N-type (100) FZ wafer (Tianjin Institute of Semiconductor Technology), resistivity 3–5 kΩ cm, thickness 400 μm surface polished on both sides. Silicon (Das Solar Co., Ltd. 182 × 182 mm) under different process flows: planar p^+n/BSG, Pyramid textured p^+n/BSG, planar p^+n, Pyramid textured p^+n, p^+n/SiO_2/poly(n^+).

Characterization: PL imaging measurements of the thin films were performed with a BT imaging LIS-R1 system. The minority carrier lifetime test was conducted using Sinton WCT-120 instrument.

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Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

Xiao Wang: conceptualization (lead). **Rui Yang**: methodology (supporting). **Wenheng Li**: data curation (lead). **Jingwei Chen**: formal analysis (lead). **Ziqi Zhao**: investigation (supporting). **Yuhua Bai**: software (supporting). **Bingbing Chen**: supervision (lead); writing—original draft (lead). **Xuning Zhang**: writing—original draft (lead). **Jianhui Chen**: writing—review and editing (lead). **Xiao Wang**, **Rui Yang**, and **Wenheng Li** contributed equally to this work.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

large-scale industrial, organic passivation, silicon, stability

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