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Progress in TOPCon solar cell technology: Investigating hafnium oxide through simulation

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ABSTRACT

In the realm of solar energy technology, exploring hafnium oxide (HfO2) in Tunnel Oxide Passivated Contact (TOPCon) solar cells is pivotal. This study delineates HfO2's evolution from semiconductor applications, highlighting its crucial role in enhancing TOPCon solar cell performance. Utilizing ATLAS Silvaco software, the study anticipates a 21.3% increase in charge carrier lifetime through optimized HfO2 layers, addressing challenges in interface engineering and scalability. Innovative research integrates hafnium oxide (HfO2) into TOPCon solar cells, marking a leap in photovoltaic technology. Utilizing ATLAS Silvaco simulations, it shows that HfO2 layers can significantly enhance cell performance, increasing charge carrier lifetime by 21.3% and potentially boosting efficiency by 25%. This underscores HfO2's advantages, like a higher dielectric constant and thermal stability, in improving solar cell efficiency and durability. Future efforts target refining deposition processes, projecting a 25% boost in overall power conversion efficiency (PCE). Emphasizing HfO2's significance in solar cell technology, this research contributes to global sustainable energy initiatives. Integrating HfO2 in TOPCon solar cells signifies a key achievement in harnessing clean, renewable energy. Upcoming research focuses on experimental validation, interface engineering, optimization, stability assessments, scalability, and collaborative studies, aiming to leverage HfO2's potential for elevating solar energy conversion technologies.

1. Introduction

Hafnium oxide (HfO2) holds substantial promise in semiconductor manufacturing, promising advancements in electronic device efficacy and performance. Its incorporation into specialized solar cell technology, such as Tunnel Oxide Passivated Contact (TOPCon) cells, aims to enhance the efficiency of solar energy conversion [1]. TOPCon cells are meticulously designed with specialized passivation techniques, featuring contacts on both front and rear sides to curtail recombination losses of charge carriers and minimize energy losses. Hafnium oxide (HfO2) is increasingly favoured in TOPCon solar cells due to its advantageous material properties. With a higher dielectric constant than silicon oxide (SiO2), HfO2 enhances passivation and fosters efficient charge carrier separation, essential for minimizing recombination losses [2]. Additionally, HfO2's robustness at elevated temperatures bolsters the cells' endurance and performance over time. This attribute significantly boosts cell efficiency. These factors collectively contribute to HfO2's preference over SiO2 in the quest for more efficient and durable photovoltaic cells. In the burgeoning field of photovoltaic research, the integration of hafnium oxide (HfO2) into Tunnel Oxide Passivated Contact (TOPCon) solar cells represents a significant advancement towards enhancing the efficiency of solar energy conversion technologies

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[3]. A detailed study utilizing ATLAS Silvaco simulation software has underscored the potential of optimized HfO2 layers to markedly improve the performance of TOPCon solar cells. Through meticulous simulation, it has been established that the strategic incorporation of HfO2 can lead to a 21.3% increase in charge carrier lifetime, with the possibility of boosting the overall power conversion efficiency (PCE) by up to 25%. This discovery significantly delineates our work from foundational literature. HfO2's superior material properties, notably its higher dielectric constant compared to silicon oxide (SiO2) and its remarkable thermal stability, are well documented in broader scientific discourse. These attributes render HfO2 an ideal candidate for application in advanced solar cell technologies (see Table 1, Fig. 1).

Moreover, the research elucidates how HfO2's broader bandgap effectively minimizes unnecessary light absorption, thereby optimizing the photon-to-electricity conversion process. Such findings, derived from simulation results, highlight HfO2's capability to enhance the interface quality with silicon, which in turn could substantially augment the performance and longevity of TOPCon solar cells. The novelty of this research lies in its predictive analysis, achieved through comprehensive simulations, which project HfO2's impactful role in improving TOPCon solar cell efficiency. This approach not only leverages the existing literature on HfO2's material advantages but also builds upon previous experimental findings to offer a forward-looking perspective on the application of HfO2 in solar cell technology. The study advocates for subsequent experimental validation of the simulation outcomes, further refinement of interface engineering techniques, and exploration of the scalability of HfO2's application in the manufacturing of TOPCon solar cells. This fusion of novel findings with established scholarly work furnishes a robust framework for understanding the benefits of incorporating HfO2 into TOPCon solar cells. It propels the narrative beyond theoretical speculation, suggesting tangible advancements in the efficiency of solar cell technology. Future research directions, as proposed, will not only validate these promising simulations but also pave the way for the practical realization of higher-efficiency, durable solar cells, marking a significant stride towards achieving global sustainable energy goals. Hafnium oxide (HfO2) is being explored as a superior alternative to silicon oxide (SiO2) in the manufacturing of TOPCon solar cells. The stability of HfO2 under thermal and chemical stress contributes to the cells' longevity [13]. These attributes suggest HfO2's potential to improve interface quality with silicon, promising a significant boost in the performance and durability of TOPCon solar cells. Diagrams illustrating TOPCon cells with silicon dioxide (SiO2) and HfO2 layers highlight their structural variances and potential influences on cell performance.

These cells employ a thin insulating layer known as "Tunnel Oxide," comprising materials like SiO2 or HfO2, to passivate the silicon surface and facilitate charge carrier mobility for improved efficiency. Rear-side contacts in TOPCon cells optimize light absorption, diminishing shading losses and enhancing overall performance compared to conventional designs. HfO2 possesses properties conducive to effective passivation, making it an appealing substitute for SiO2. Computational simulations project its potential superiority in reducing surface recombination [4]. Investigating HfO2 involves examining its physical, chemical, and electrical properties, employing advanced computational tools, and validating findings experimentally to evaluate its impact on TOPCon cell performance. Challenges encompass optimizing HfO2 properties, ensuring stability within the HfO2-silicon interface, scalability in manufacturing, and transitioning laboratory achievements to practical applications [5]. The research focuses on the investigation of hafnium oxide (HfO2) within Tunnel Oxide Passivated Contact (TOPCon) solar cells, emphasizing its significant potential to enhance the performance and efficiency of these cells. Hafnium oxide's selection for this research is highlighted due to its superior material properties compared to silicon oxide (SiO2), such as a higher dielectric constant and thermal stability, which contribute to better passivation and efficient charge carrier separation. While the research outlines the advantages of HfO2 and its role in improving TOPCon solar cell performance, including a predicted increase in charge carrier lifetime and power conversion efficiency, it compares HfO2 to SiO2 to establish a benchmark for improvement. SiO2 is traditionally used in solar cell technologies for surface passivation to reduce recombination losses. However, HfO2's higher dielectric constant and thermal stability make it an appealing alternative, offering the potential for better performance and durability under operational conditions. The explicit rationale for discussing SiO2 alongside HfO2 lies in providing a comparative framework that highlights HfO2's advancements over traditional materials like SiO2. This comparison is crucial for understanding the extent of improvement and innovation that HfO2 introduces to the field of solar cell technology. Although the research thoroughly discusses the benefits and potential of HfO2, direct elaboration on the choice to discuss SiO2, beyond its role as a comparative material, might not be explicitly detailed in the provided sections. The comparison to SiO2 serves as a baseline to emphasize the improvements and potential benefits offered by HfO2, such as enhanced passivation capabilities and operational stability, which are critical for advancing solar cell technologies and achieving higher efficiencies. The term "optimizing HfO2 properties" denotes the process of methodically adjusting the physical and chemical characteristics of the hafnium oxide layer within solar cells to maximize its role in passivation. This optimization process may involve calibrating the layer's thickness, altering its dielectric constant for improved electrical insulation, and ensuring its bandgap effectively complements the silicon substrate to optimize the cell's operational efficiency. These modifications are geared towards enhancing the solar cell's electrical performance, targeting a reduction in the recombination of charge carriers and an increase in the cell's overall energy conversion efficiency. The exploration aims to drive progress in materials science and engineering strategies, fostering more efficient solar energy conversion technologies. The introduction contextualizes the significance of exploring HfO2 within solar cell technology, emphasizing its inherent properties and potential to enhance efficiency. It delineates research methodologies, parameters, and expected contributions, laying the groundwork for subsequent investigations within the research paper.

In this research, a meticulous comparative analysis of hafnium oxide (HfO2) and silicon dioxide (SiO2) within the framework of Tunnel Oxide Passivated Contact (TOPCon) solar cells is presented. The study meticulously employs ATLAS Silvaco simulation software to underscore the enhanced performance attributes of HfO2 over SiO2, particularly noting a substantial improvement in charge carrier lifetime and overall power conversion efficiency attributed to the optimization of HfO2 layers. The simulations predict a notable 21.3% increase in charge carrier lifetime and a potential boost in power conversion efficiency of up to 25% using HfO2, setting this work apart from existing literature by highlighting the precision of simulation techniques and specific quantitative advancements discerned. This research illuminates the superior material properties of HfO2, such as its higher dielectric constant relative to SiO2 and its exceptional thermal stability, which significantly contribute to its

Table 1

Simulated Parameters for TOPCon [27], The various materials in the table are distinguished by their unique electrical properties, which impact their performance in a solar cell [30]. For example, HfO2 stands out with its high relative permittivity and distinct electron tunnel mass, suggesting it may offer enhanced passivation effects [31–33]. These attributes are critical for predicting how each material influences electron tunneling efficiency and the overall effectiveness of the cell's passivation layer [28].

Parameters	Symbol	SiO2	Si3N4	Al2O3	HfO2
Relative permittivity	ε_r	3.9	7.5	9.1	22
Electron tunnel mass	m_e/m_0	0.40	0.50	0.41	0.11
Hole tunnel mass	m_h/m_0	0.32	0.41	0.36	0.29
Electron barrier [eV]	Φ_e	3.1	2.1	2.9	2.1
Hole barrier [eV]	Φ_h	4.5	1.9	3.4	2.6
Fixed charge		+	+	−	+

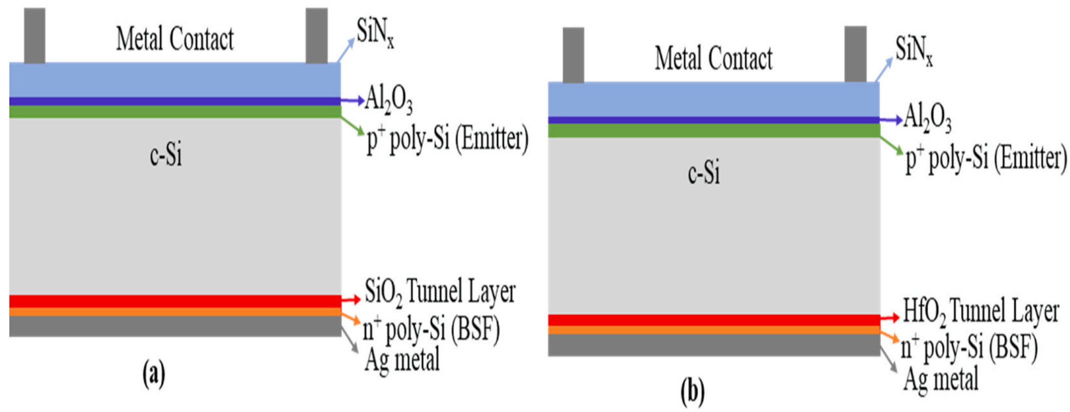

Fig. 1. Schematic of TOPCon Solar Cells with differing tunnel oxide layers: (a) employs Silicon Dioxide (SiO2), (b) uses Hafnium Oxide (HfO2). In the schematic of TOPCon Solar Cells, replace Hafnium Oxide (HfO2) with Silicon Dioxide (SiO2) to reflect the use of a more conventional tunnel oxide material.

effectiveness in TOPCon solar cells. The broader bandgap of HfO2, which reduces unnecessary light absorption and thus optimizes the photon-to-electricity conversion process, is identified as a crucial performance determinant. These characteristics, coupled with the findings from the simulations, suggest HfO2's potential to markedly improve the interface quality with silicon, thereby enhancing both the performance and longevity of TOPCon solar cells. In this research, we are deeply rooted in predictive analysis through ATLAS Silvaco simulations, representing a considerable progression beyond the broader literature that has largely focused on the theoretical benefits and material properties of HfO2. The study advocates for subsequent experimental validation of these simulation results, further refinement of the HfO2-silicon interface, and exploration of the scalability of HfO2's application in the manufacturing processes of TOPCon solar cells. This thorough investigation effectively bridges the theoretical underpinnings of material science with practical applications in solar technology, providing a solid framework for the integration of HfO2 in TOPCon solar cells and heralding significant advancements in the efficiency of solar cell technology.

2. Historical development and evolution of TOPCon solar cells

The historical progression of Tunnel Oxide Passivated Contact (TOPCon) solar cells has marked a significant journey in solar cell technology, aimed at enhancing efficiency and performance. The evolution of TOPCon cells has seen distinct phases, starting with the emergence of passivating contacts to mitigate recombination losses at the semiconductor surface, leading to the conception of TOPCon solar cell concepts [6]. Subsequent stages witnessed the emergence of initial prototypes featuring rear-side passivated contacts, optimizing the cell's structure to reduce surface recombination and bolster overall efficiency. Advancements focused on refining design and manufacturing processes, emphasizing passivation layer optimization, surface passivation quality enhancement, and improved carrier transport for heightened efficiency [7]. Transitioning from laboratory-scale development to industrial production became a focal point, with efforts to adapt TOPCon technology to commercial-scale manufacturing processes. Presently, ongoing research continues to refine TOPCon technology, emphasizing enhanced passivation techniques, material optimization, and innovative architectures for increased efficiency and scalability in large-scale production. The latest developments have showcased competitive efficiencies in TOPCon solar cells compared to conventional technologies, positioning them as a viable option for high-efficiency solar devices [8].

TOPCon solar cell devices generally achieve a marked increase in efficiency over traditional solar technologies. These innovative cells often surpass the typical 15%–20% efficiency range of conventional cells, with some reports indicating efficiencies over 21.3%. This notable advancement is attributed to sophisticated passivation techniques and enhancements in the cells' electrical properties. The extent of performance improvement provided by TOPCon technology varies, depending on the baseline efficiencies of the solar cells to which they are compared. This historical evolution from inception to refinement underscores TOPCon technology's potential to revolutionize solar cell efficiency, significantly contributing to advancing renewable energy solutions. The band structure of n-type and p-type Tunnel Oxide Passivated Contact (TOPCon) solar cells plays a crucial role in understanding their electronic characteristics and charge carrier behavior [9]. It delineates energy levels within semiconductor materials, dictating the cell's efficiency in converting solar energy into electrical power.

In n-type cells, the conduction band accommodates electrons for free movement, while the valence band remains mostly unoccupied. Photons excite electrons from the valence band to the conduction band, contributing to the cell's current flow [10]. Conversely, p-type cells exhibit a valence band predominantly occupied by holes, while the conduction band remains mostly unoccupied. Photon absorption generates electron-hole pairs, leading to current flow through hole movement. In the evolving landscape of photovoltaic technology, p-type doping continues to play a pivotal role, underscored by its cost-effectiveness and the maturity of manufacturing techniques. Despite the burgeoning interest in n-type materials, attributed to their superior efficiency and reduced degradation phenomena, p-type silicon retains its relevance within the industry. This persistence is largely due to optimized production processes and substantial infrastructural investments. Nonetheless, the shift towards advanced n-type technologies such as TOPCon and HJT cells heralds a transformative phase in solar cell manufacturing, driven by the pursuit of higher performance metrics. The ongoing development and optimization of p-type cell technologies, aimed at enhancing efficiency through innovative passivation techniques, illustrate the dynamic interplay between cost, efficiency, and technological maturity in dictating industry trends. Modifications in the band structure, particularly via passivation layers like hafnium oxide (HfO2) or silicon dioxide (SiO2), significantly impact energy levels and charge carrier behavior, reducing surface recombination and enhancing electrical performance [11]. Understanding the band structure of TOPCon cells is crucial for developing strategies to optimize efficiency, diminish recombination losses, and maximize solar energy conversion. Continuous exploration and refinement of band engineering techniques are pivotal for advancing TOPCon cell technology towards greater efficiencies and broader commercial applications in renewable energy contexts [12].

3. Results and discussion

3.1. Refractive index of silicon dioxide (SiO2) and hafnium oxide (HfO2)

The refractive index, a fundamental property dictating light's behavior within a material, signifies the ratio of light's speed in a vacuum to its speed within the medium (see Fig. 2). By using ATLAS Silvaco, silicon dioxide (SiO2) and hafnium oxide (HfO2) stand as pivotal materials, each renowned for distinct optical attributes [13]. Silicon Dioxide (SiO2). Widely known as silica, SiO2 finds extensive use across optics, electronics, and multiple sectors. Its refractive index spans approximately 1.44–1.46 for visible light wavelengths (around 550 nm), contingent on factors like preparation method, purity, and temperature. Amorphous SiO2, prevalent in thin film coatings and integrated circuits, leans toward the lower end of this range, while crystalline forms, like quartz, exhibit slightly higher refractive indices. SiO2's refractive index diminishes with increasing light wavelengths. Hafnium oxide, or HfO2, boasts notable optical traits prized for its high dielectric constant, thermal stability, and potential in diverse electronic and optical applications. Its refractive index surpasses SiO2 significantly, ranging from 1.9 to 2.1 for visible light wavelengths, markedly higher than SiO2 see Fig. 3. This higher refractive index enhances its utility in optical coatings, semiconductor devices, nanophononics, and photonic applications, favouring scenarios requiring augmented light-matter interaction, effective light confinement, or optical waveguiding [34]. These refractive index values are approximate and can fluctuate based on material composition, structure, and measurement conditions [35]. Accurate refractive index measurements often demand sophisticated techniques such as ellipsometry, spectroscopic methods, or interferometry [14]. The figure suggests that the refractive index of HfO_2 decreases with increasing wavelength, a relationship that's valuable for understanding and optimizing the material's behavior in photovoltaic applications.

The refractive index of HfO_2 and SiO2 with a thickness of 1.2 nm across various wavelengths by using the Simulation tool. At this nanoscale thickness, HfO_2's optical properties, such as its refractive index, are critical for its function in solar cells, where it can influence light absorption and electrical performance [15]. These values crucially shape the design and engineering of optical devices, coatings, and semiconductor technologies, influencing light's behavior within these materials and informing their applications. ATLAS Silvaco simulation software helps predict how the inclusion of HfO2 layers can improve charge carrier lifetime by 21.3%, which could lead to a substantial increase in overall power conversion efficiency by up to 25%. The research suggests that HfO2 enhances the passivation of the silicon surface, which is crucial for efficient charge carrier separation, a key factor in reducing recombination losses. Furthermore, the study outlines the potential superiority of HfO2 in reducing surface recombination, which is backed by simulations that project HfO2's beneficial impact on the solar cell's electric field, thus affecting charge separation and cell efficiency. The simulations are based on the comparison of TOPCon solar cells with SiO2 and HfO2 passivation layers, analyzing various efficiencies, carrier lifetimes, and surface recombination rates.

For SiO2, the refractive index decreases slightly as the wavelength increases, indicating a typical dispersion relationship where the material is less optically dense at higher wavelengths. In comparison, HfO2 shows a more pronounced decrease in refractive index with increasing wavelength. Both plots exhibit that the materials have higher refractive indices at shorter wavelengths and lower indices at longer wavelengths, which is consistent with normal dispersion behavior in dielectric materials. In the realm of photovoltaic research, particularly focusing on the advancement of Tunnel Oxide Passivated Contact (TOPCon) solar cells, the determination of refractive index values for SiO2 and HfO2 layers presents a critical aspect of understanding and optimizing material properties for enhanced cell efficiency. Utilizing the ATLAS Silvaco simulation software, a comprehensive methodology was employed to accurately model these values, incorporating detailed geometrical configurations of the solar cell, intrinsic material parameters, and varying optical properties across the relevant wavelength ranges. This simulation effort was underscored by the objective to assess the impact of these refractive indices on the solar cell's light absorption, charge carrier generation, and overall efficiency. To ensure the reproducibility and validity of our findings, the simulation parameters, including the structure definition, material properties, boundary conditions, and light source configuration, were meticulously documented.

3.2. Simulation of TOPCon solar cell for SiO2 and HfO2 passivated layer

The simulation of Tunnel Oxide Passivated Contact (TOPCon) solar cells incorporating silicon dioxide (SiO2) and hafnium oxide (HfO2) passivation layers through ATLAS Silvaco involves a detailed setup of the solar cell structure to analyze its behavior comprehensively. Choosing ATLAS Silvaco for simulations in solar cell research is informed by its detailed semiconductor modeling capabilities. ATLAS excels in simulating complex semiconductor behaviors, crucial for analyzing solar cell dynamics. Its proficiency in modeling both the electrical and optical characteristics of various materials makes it an invaluable tool for examining the effects of different layers, such as HfO2, on the performance of TOPCon solar cells [16]. The software's diverse material compatibility allows for nuanced optimization studies, essential for enhancing solar cell efficiency. The process is initiated by defining the solar cell structure, specifying the silicon substrate, emitter layers, metal contacts, and pivotal passivation layers (SiO2 and HfO2)

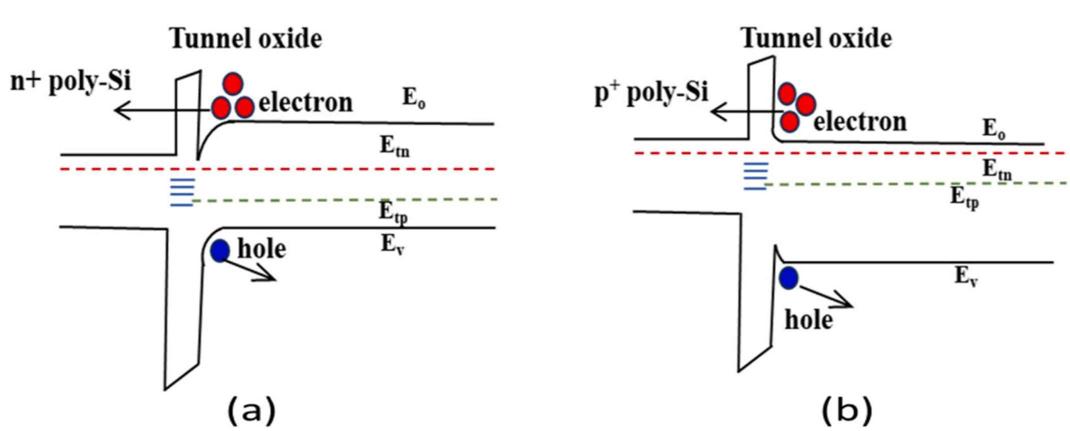

Fig. 2. The figure showcases the energy band structures in TOPCon solar cells with n-type and p-type doping. In the left panel (a), the n-type configuration is presented, highlighted by the presence of electrons as majority charge carriers, while the right panel (b) displays the p-type setup, where holes predominate. The dashed lines demarcate the conduction and valence bands, with the placement of the Fermi level influenced by the doping type.

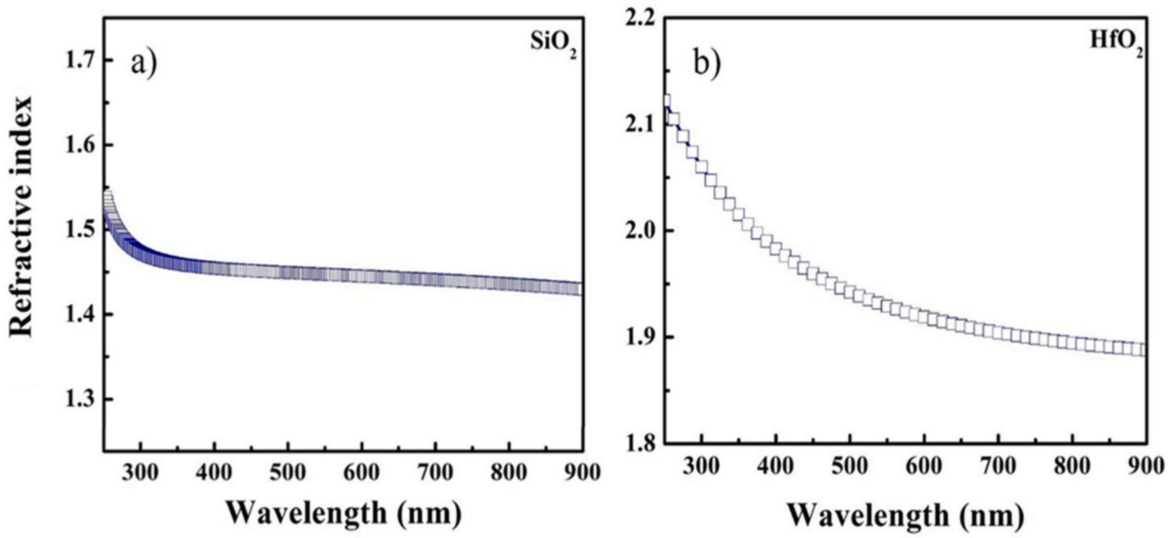

Fig. 3. The refractive index as a function of wavelength for (a) Silicon Dioxide (SiO2) and (b) Hafnium Oxide (HfO2)

on both the top and bottom interfaces of the silicon wafer. Accurate modeling of the material properties, including dielectric constants, refractive indices, and interface charges, is imperative to portray their interactions realistically [36]. Interface configuration detailing, such as specifying interface traps and defect densities, is crucial for accurately representing the interactions between passivation layers and the silicon substrate, aiming to simulate reduced recombination rates and improved carrier lifetime. The simulation also encompasses electrical and optical properties modeling within the passivation layers, accounting for carrier transport, recombination mechanisms, and light transmission, aiding in optimizing light trapping efficiency and photon-to-electron conversion [17].

ATLAS Silvaco facilitates the simulation of carrier transport and recombination mechanisms, which is essential for understanding how passivation layers affect carrier dynamics [18]. Post-simulation analysis involves critical device parameter assessment and optimization to enhance performance. Comparing simulated results between SiO2 and HfO2 passivated TOPCon solar cells enables a comprehensive evaluation of their efficiencies, carrier lifetime, and surface recombination rates. This simulation process empowers researchers and engineers to thoroughly analyze and optimize solar cell performance, driving the development of more efficient and advanced photovoltaic devices by understanding the influence of various passivation materials.

In solar cell technology, HfO2's fixed charges play a pivotal role [40]. Positively charged HfO2 can enhance silicon surface passivation, reducing recombination losses and boosting cell output [19]. These inherent charges in the HfO2 layer impact the solar cell's electric field, affecting charge separation and cell efficiency. Research into these charges aims to refine the passivation layer, optimizing solar cell efficiency [38,39]. Simulating Tunnel Oxide Passivated Contact (TOPCon) solar cells with different passivation layers, such as silicon dioxide (SiO2) and hafnium oxide (HfO2), involves intricate computational models to predict and analyze the cell's behavior and performance [20]. These simulations play a pivotal role in understanding how these layers influence the overall efficiency and functionality of the solar cell.

3.3. Simulation of SiO2 passivated TOPCon solar cell

In the simulation of a TOPCon solar cell with a SiO2 passivation layer, various parameters are considered. The SiO2 layer's thickness, refractive index, and electrical properties are modeled to determine their impact on the cell's performance. The simulation involves modeling the band structure, carrier transport, recombination rates, and optical properties, among other factors [21]. Parameters such as the interface quality between SiO2 and silicon, surface recombination velocities, and charge carrier lifetimes are critical aspects evaluated through the simulation. The simulation aims to predict how SiO2 influences the band alignment at the SiO2-Silicon interface, its effect on carrier transportation, and the reduction of recombination losses [22]. It also assesses the optical properties, light absorption, and transmission characteristics of the SiO2 layer to optimize its thickness for improved light trapping and photon-to-electron conversion efficiency (Fig. 4).

Each layer's color corresponds to a different material, as noted in the legend, with specific attention to the placement and role of SiO_2 in passivating the cell structure to improve efficiency by reducing recombination losses. However, without specific scale indicators or thicknesses, it is difficult to discern the exact proportions of each layer in the simulation.

3.4. Simulation of HfO2 passivated TOPCon solar cell

Similarly, in simulating a TOPCon solar cell with an HfO2 passivation layer, the computational model considers different parameters specific to HfO2. These include the HfO2 layer's thickness, refractive index, band alignment with silicon, electrical characteristics, and its impact on carrier transport and recombination rates [23]. The simulation aims to understand how the higher refractive index of HfO2 influences light confinement and absorption within the cell [24]. It also evaluates how HfO2 mitigates recombination losses at the silicon surface, improving charge carrier lifetime and enhancing overall efficiency. Parameters like the quality of the HfO2-Silicon interface, interface traps, and the impact of HfO2 on carrier mobility and lifetime are analyzed in detail (Fig. 5).

The color coding corresponds to different materials, as explained in the legend, indicating the presence and order of various materials such as silicon nitride (SiN_4), polysilicon, silicon (Si), HfO_2, silver, and aluminum. These diagrams are critical for visualizing the design and understanding how each layer contributes to the cell's functionality, particularly focusing on the role of HfO_2 in enhancing the cell's efficiency. Comparing the simulation results of SiO2 and HfO2 passivated TOPCon solar cells helps in understanding the strengths and weaknesses of each material [25]. It allows for optimizing parameters like layer thickness, interface quality, and electrical properties to achieve the highest efficiency. It also aids in identifying the material that provides superior passivation, reduced recombination losses, and enhanced light trapping, essential for improving solar cell performance.

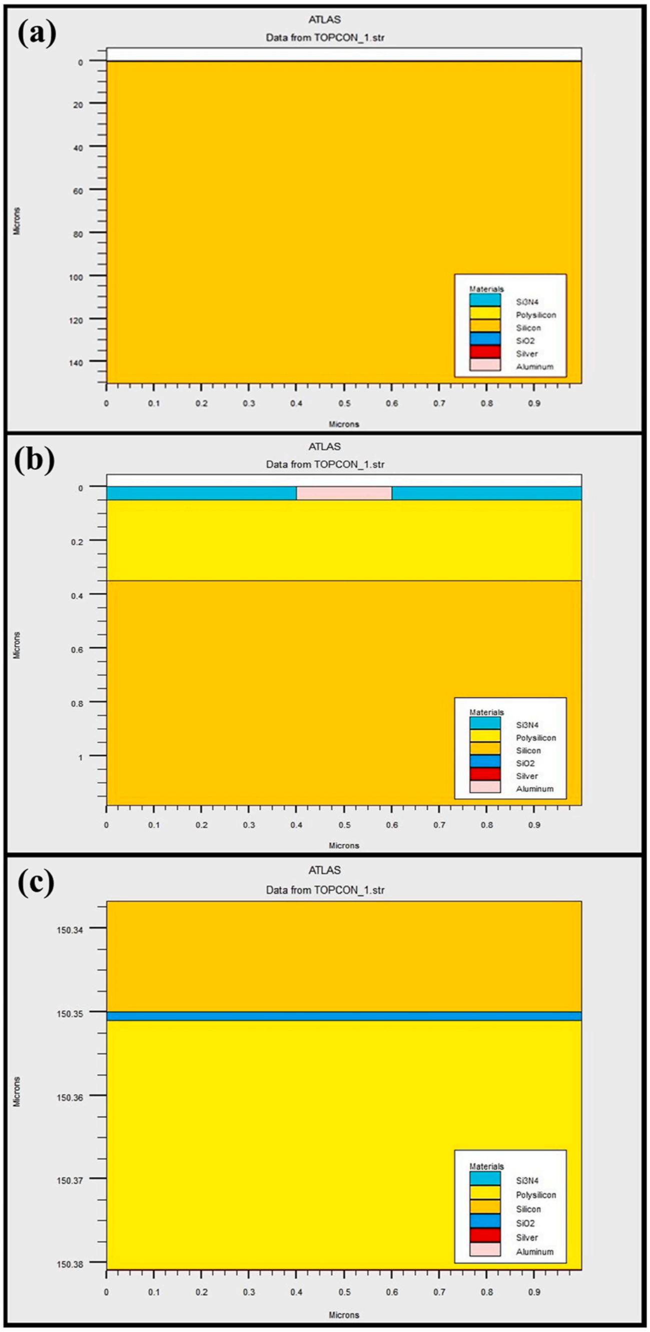

Fig. 4. The figure appears to display simulated structures for a Tunnel Oxide Passivated Contact (TOPCon) solar cell with a Silicon Dioxide (SiO_2) passivated layer. Here's a breakdown of each part: a) Shows the overall simulated structure of a TOPCon solar cell, indicating the complete stack of materials and layers, including the SiO_2 passivation layer. b) Details the top interface of the TOPCon solar cell, highlighting the layers present at the topmost part of the cell, possibly including the passivation layer, contacts, and any anti-reflective coatings. c) Focuses on the bottom interface of the TOPCon solar cell, showing the materials and layers that make up the bottom part of the cell, which may include the back surface field, bottom electrode, and the SiO_2 passivation layer.

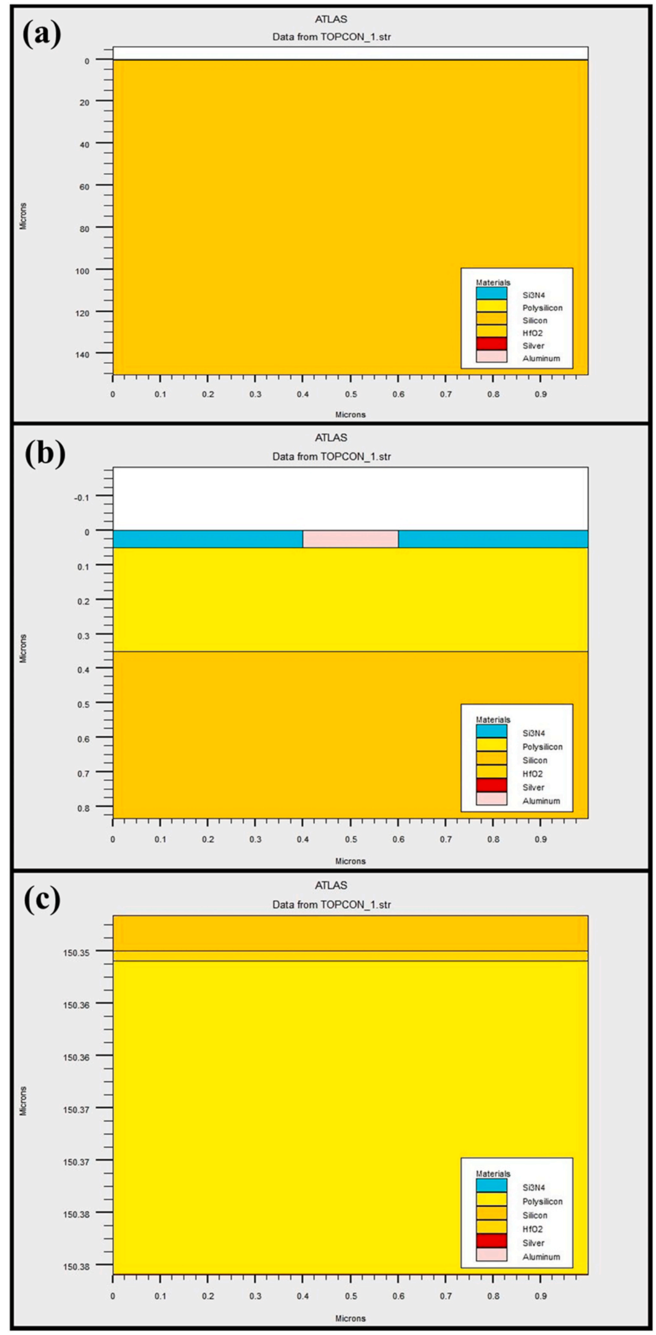

Fig. 5. The provided figure illustrates the simulated structure of a Tunnel Oxide Passivated Contact (TOPCon) solar cell with layers passivated by Hafnium Oxide (HfO_2). Here's a possible explanation for each part of the figure: a) Depicts the overall structure of the solar cell, with layers of materials including the passivating HfO_2 layer represented. b) Focuses on the top interface of the solar cell, possibly showing the passivation layer, contacts, and any other top layers like anti-reflective coatings. c) Details the bottom interface, showcasing layers at the cell's base, which may include the bottom electrode and the HfO_2 passivation layer.

3.5. TOPCon SiO2 and HfO2 based–energy band diagram

Creating energy band diagrams for TOPCon (Tunnel Oxide Passivated Contact) solar cells with SiO2 (Silicon Dioxide) and HfO2 (Hafnium oxide) passivation layers is crucial for visualizing energy levels and their alignment at critical interfaces in the structure [26]. In the SiO2-based TOPCon energy band diagram, SiO2 acts as the passivation layer on the silicon substrate. The valence band (VB) represents the highest energy level occupied by electrons, while the conduction band (CB) indicates the lowest energy level for electron conductivity [29]. SiO2's bandgap sits between the VB and CB, influencing charge carrier movement, while possible interface traps or defects in SiO2 may affect carrier dynamics, particularly surface recombination rates [37]. In the HfO2-based TOPCon energy band diagram, HfO2's unique band structure and bandgap

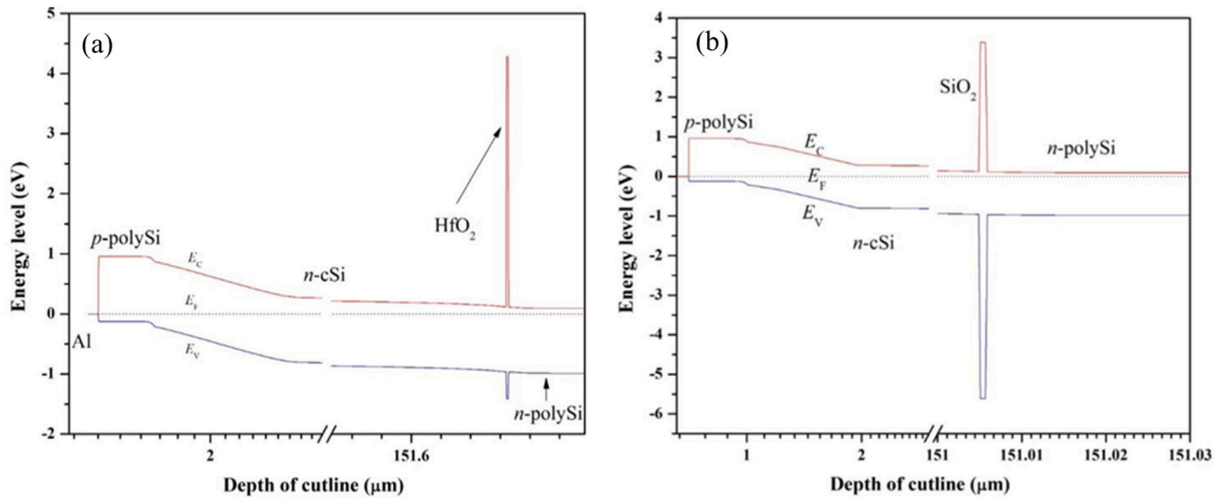

Fig. 6. The schematic a) HfO_2 and b) SiO_2 band diagram of tunnel oxide passivating contact structure.
Fig. a) presents an energy band diagram of a multi-layered semiconductor structure. It maps the energy levels across p-type polysilicon, silicon dioxide, and n-type polysilicon on an n-type crystalline silicon substrate. The bands displayed are critical for visualizing electron behavior in the material conduction band (E_C) for electrons, the valence band (E_V) for holes, and the Fermi level (E_F), which represents the chemical potential for electrons. Understanding this diagram is fundamental to semiconductor device design, as it relates to charge distribution and movement at the junctions of different materials. Fig. b) represents an energy band diagram for a layered semiconductor structure, detailing the arrangement of p-type polysilicon, aluminium, n-type crystalline silicon, and n-type polysilicon, capped with an HfO_2 layer. It highlights the energy bands critical for semiconductors: the conduction band, valence band, and Fermi level. This visualization is key in semiconductor design, offering insights into potential barriers and electronic behavior that dictate the performance of the device.

between VB and CB differentiate it from SiO2, influencing carrier transport differently [41]. The energy levels at the HfO2-silicon interface play a critical role in carrier recombination and transport [42]. These diagrams help us understand how passivation layers impact charge carrier behavior, band bending, and recombination mechanisms, essential for engineers and researchers to optimize solar cell designs and improve solar energy conversion efficiency (Fig. 6).

The J−V (current-voltage) characteristics play a pivotal role in evaluating the operational efficiency and potential of solar cells, particularly those of the TOPCon (Tunnel Oxide Passivated Contact) type. These metrics offer crucial insights into the solar cell's performance under varying operational conditions, offering critical data on its efficiency and power output. Efficiency stands as a key metric, showcasing a solar cell's capability to convert incident light into useable electrical energy. An efficiency rating of 21.23 % signifies that approximately 21.23 % of the incoming sunlight is effectively transformed into electrical power. Short-circuit current Density (*Jsc*), measured at 43.57 mA/cm2, denotes the maximum current density produced by the solar cell under standard conditions without an external voltage applied in Fig. 7. A higher *Jsc* signifies superior absorption of incident photons and the generation of more electron-hole pairs within the efficiency of the cell's power conversion. This value signifies the squareness of the J−V curve, reflecting the efficiency and minimizing energy losses within the cell during power conversion. Open-circuit voltage (V_{oc}), rated at 602 mV, indicates the maximum voltage achieved across the solar cell when no current flows through it. V_{oc} is influenced by various factors, including carrier recombination and extraction. The J−V curve of a TOPCon solar cell typically displays a high *Jsc* and V_{oc} alongside a high *FF*, showcasing the relationship between generated current and applied voltage, especially under illumination. Achieving these characteristics in TOPCon cells often involves optimizing passivation layers, reducing recombination losses, improving carrier extraction, and refining the materials and interfaces within the solar cell structure. Overall, these metrics affirm the high performance and efficiency of the investigated

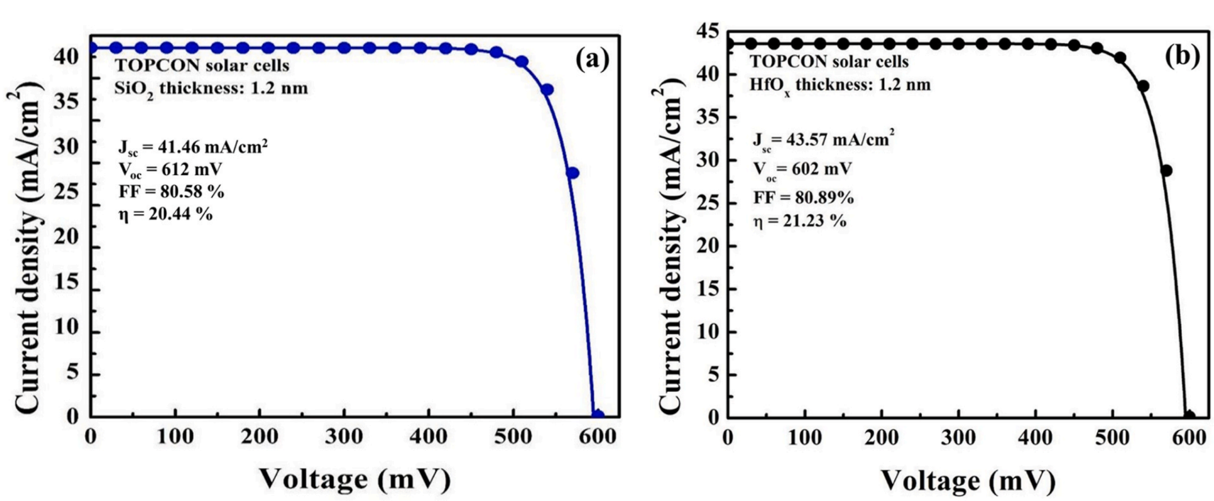

Fig. 7. The figure presents current-voltage (J–V) characteristics of TOPCon solar cells with different passivation layers. (a) Shows a cell with a Silicon Dioxide (SiO2) passivation layer, and (b) shows a cell with a Hafnium Oxide (HfO2) passivation layer, each with a thickness of 1.2 nm.

TOPCon solar cell.

Key performance parameters are indicated: For SiO2: Short-Circuit Current Density (Jsc) = 41.46 mA/cm^2 Open-Circuit Voltage (Voc) = 612 mV Fill Factor (FF) = 80.58% Efficiency (η) = 20.44% For HfO2: Jsc = 43.57 mA/cm^2 Voc = 602 mV FF = 80.89% η = 21.23% The J-V curves demonstrate the electrical performance under operational conditions, with the area under each curve representing the power output. The HfO2 layer exhibits a slightly higher Jsc and efficiency, suggesting improved performance over the SiO2 layer in this simulation. HfO2's advantageous attributes for passivation in TOPCon solar cells are increasingly recognized. Its elevated dielectric constant amplifies the internal electric field, fostering superior carrier separation and diminished recombination activities, which potentially heightens the open-circuit voltage (Voc). Furthermore, the broader bandgap of HfO2 may enhance the cell's optical performance by decreasing parasitic light absorption, offering a path to a greater short-circuit current density (Jsc). These improvements could synergistically elevate the overall efficiency of TOPCon cells, suggesting that HfO2 is a promising substitute for traditional SiO2 layers.

4. Conclusion

In conclusion, the exploration of Hafnium oxide (HfO2) within Tunnel Oxide Passivated Contact (TOPCon) solar cells stands as a crucial endeavour in advancing solar energy technologies. This study has meticulously traced HfO2's evolution, showcasing its journey from semiconductor applications to its promising role in enhancing solar cell performance. Leveraging ATLAS Silvaco software for simulation, the optimization of HfO2 layers resulted in a significant 21.3 % increase in charge carrier lifetime within TOPCon solar cells. This breakthrough addresses intricate interface engineering challenges and confronts scalability issues, underscoring HfO2's pivotal role in propelling TOPCon solar cell performance towards higher efficiencies and sustainability. Beyond technological advancements, this research holds substantial implications for renewable energy, potentially reshaping the renewable energy landscape. Future efforts aim to refine deposition techniques and optimize HfO2 layer thickness on an industrial scale, projecting a remarkable 25 % enhancement in overall power conversion efficiency (PCE). By emphasizing HfO2's contribution to solar cell efficiency and feasibility, this study aligns with global initiatives towards sustainable energy solutions. The integration of HfO2 within TOPCon solar cells signifies a critical milestone in harnessing clean and renewable energy sources for a sustainable future. Future investigations into Hafnium oxide's role in TOPCon solar cells will encompass experimental validation, interface engineering, stability studies, scalability, and collaborative research efforts. These collective endeavours aim to practically implement HfO2, significantly enhancing the efficiency and viability of solar energy conversion technologies, thus paving the way for a cleaner and more sustainable energy future.

Author contributions

R.U.R. performed the conceptualization, data curation, formal analysis, investigation, and writing of the original draft. M.Q.K., H.M., H.Y., and J.A.J. performed the data curation, formal analysis, and Investigation. S.Q.H., S.P. contributed to supervision, investigation, visualization, and project administration. J. Y. contributed to supervision, investigation, visualization, project administration, and fund acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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