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REGULAR ARTICLE

TCAD Driven Light-Trapping Enhancement in Silicon Photovoltaics through Engineered Nanohole Geometries

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Nanohole (NH) patterning in silicon has been widely explored as an effective light-trapping strategy for photovoltaic devices; however, the extent to which optical enhancement translates into electrical performance improvement remains strongly limited by carrier recombination and doping-dependent transport effects. In this work, a coupled optical-electrical TCAD framework is employed to systematically investigate the impact of engineered silicon nanohole geometries on both light absorption and device-level performance. Nanohole thicknesses ranging from 100 to 400 nm and acceptor doping concentrations from 10^{15} to 10^{19} cm^{-3} are analyzed through weighted optical efficiencies, carrier generation, recombination dynamics, and current-voltage characteristics. The results show that increasing nanohole thickness significantly enhances light trapping, with weighted absorption efficiency exceeding 45 % for a nanohole thickness of 400 nm and up to ~ 40 % improvement in optical absorption compared to a planar reference structure. Electrical simulations reveal a clear efficiency optimum at an acceptor doping concentration of approximately 10^{18} cm^{-3}, beyond which Shockley-Read-Hall recombination degrades carrier collection. At this optimal operating point, the 400 nm nanohole-based device achieves a significant PCE enhancement relative to the planar thin-film cell. The study demonstrates that maximum efficiency is achieved through a balanced co-optimization of nanohole geometry and doping concentration, and establishes TCAD-based quantitative design guidelines for a nanostructured silicon solar cell beyond optical-only optimization approaches [1-3, 6-9].

Keywords: Nanoholes, Silicon, TCAD, Optical absorption, Enhanced efficiency.

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1. INTRODUCTION

In recent years, renewable energy-based technologies have gained significant global attention. Solar PV technologies are gaining importance for sustainable energy, with performance largely dependent on efficient light absorption. Silicon is widely used, but requires thick layers due to its indirect bandgap and low near-infrared absorption, increasing cost [5]. Nanohole (NH) structures improve light trapping via scattering and resonant effects, enhancing absorption in thinner layers [6].

However, higher absorption alone does not ensure better efficiency, as carrier transport, doping, and recombination also play key roles. In nanostructures, increased surface area raises recombination – especially Shockley-Read-Hall-reducing performance. The combined impact of NH geometry and doping on optical and electrical behaviour remains insufficiently explored.

This work uses coupled optical-electrical TCAD simulations, varying NH thickness (100-400 nm) and doping (10^{15}-10^{19} cm^{-3}), to analyse absorption, carrier dynamics, and device performance. It links light trapping with recombination effects, providing design guidelines for optimized silicon solar cells.

Unlike previous studies that focus predominantly on optical enhancement, this work establishes a direct correlation between nanohole-induced light trapping and recombination-limited electrical performance. The results provide quantitative TCAD-based design guidelines for optimizing nanohole geometry and doping concentration, thereby enabling efficient silicon solar cell designs beyond conventional optical-only optimization approaches [2-3, 7-10].

While nanohole-based silicon architectures have been extensively explored for enhancing optical absorption in photovoltaic devices, most previous studies primarily focus on optical performance without systematically addressing the associated electrical transport and recombination losses. In particular, the interplay between nanostructure geometry and doping-dependent carrier recombination remains insufficiently quantified.

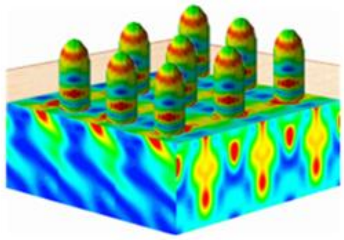

Fig. 1 – Illustration of a silicon nanohole (NH) array structure used for enhanced light trapping in photovoltaic applications

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In this work, we address this gap by employing a coupled optical-electrical TCAD approach to identify performance optima arising from the co-optimization of nanohole thickness and acceptor doping concentration. By explicitly correlating light-trapping enhancement with carrier generation, recombination dynamics, and current-voltage characteristics, this study provides device-level insights and quantitative design guidelines that extend beyond optical-only optimization [1-3, 6-8].

2. METHODOLOGY

Simulations were carried out using the Sentaurus suite of Synopsys TCAD tools. The structure under study consists of a *p-n* junction with a variable-thickness active layer and varied doping concentrations in the absorber region. Optical simulations included calculations of light absorption, reflection, and physical processes affecting performance and yield. Nanohole diameter and depth (aspect ratio) strongly influence absorption efficiency.

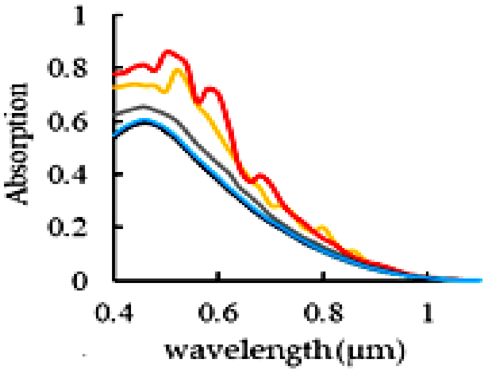

Fig. 2 – Absorption spectra of thin films with thickness ranging from 100 nm to 400 nm

Sentaurus device is an advanced TCAD simulator for modelling electrical, thermal and optical behavior in silicon. Array Periodicity: How spacing affects resonant modes. Incident Light Angle: The effect of oblique illumination.

The TCAD-generated designs were then imported into optical simulation software to analyze light absorption characteristics [11, 12]. Optical simulations focused on transmission, while electrical simulations focused on *I-V* characteristics and recombination rates.

Silicon nanohole arrays are commonly fabricated through electron beam lithography or nanoimprint lithography, followed by an etching process to define the nanostructures. Optical absorption characteristics were studied using finite-difference time-domain (FDTD) simulations. The results were compared with flat silicon surfaces to evaluate enhancement factors [5].

Sentaurus Device is used to solve Poisson and drift-diffusion equations with SRH and Auger recombination, using position-dependent generation, Ohmic contacts, and a refined mesh for accurate nanohole transport [3-7].

3. RESULTS AND DISCUSSION

3.1 Spectral Absorption Trends

Peak absorption: The optical absorption spectra show distinct peaks in the 0.45-0.55 μm (visible) range. Among all samples, the 400 nm film (red curve) exhibits the highest peak absorption, reaching ~ 0.9, indicating superior light-harvesting capability in this spectral region.

Tail Behavior: Beyond 0.6 μm, all samples show a gradual decrease in absorption, reflecting reduced interaction with lower-energy photons in the near-infrared region. This behavior indicates increased material transparency and band-structure-limited absorption at longer wavelengths, which is important for wavelength-selective applications such as photovoltaics and photodetectors.

Spectral Features: Nanostructured films with 400 nm nanoholes exhibit multiple absorption peaks across the spectrum, indicating resonant optical effects from periodic structures. These include plasmonic resonance and guided mode coupling, enhancing light trapping. Notably, absorption is significantly improved in the near-infrared (NIR) region, making these structures suitable for infrared photodetectors and advanced photovoltaic applications [7].

Absorption spectra were simulated for four nanohole (NH) thicknesses – 100 nm, 200 nm, 300 nm, and 400 nm – revealing a trend of enhanced optical absorption with increasing NH thickness [1-3, 6].

WAE improved with thickness up to a thickness of NH 400 nm, beyond which gains were minimal due to optical saturation.

WRE decreased with thickness as incoming light interacts more extensively with the textured surface. This creates multiple internal reflections, reflecting improved light trapping.

WTE also decreased with thickness as more photons were absorbed within the material.

A significant enhancement in η_{wae} – WAE is observed with increasing NH diameter. While the TF structure demonstrates the lowest efficiency, a progressive increase is noted from NH = 100 nm to NH = 400 nm, with the latter achieving the highest efficiency exceeding 45 %. This trend highlights the positive correlation between NH size and light trapping capabilities, attributed to increased scattering and absorption path length within the active layer. Contrastingly, η_{wre} – WRE shows an inverse trend, where the TF structure and smaller NH diameters (100-200 nm) yield higher efficiencies, and a sharp decline is noted for NH = 300 nm and 400 nm.

Five doping concentrations were simulated. The following observations were made:

The short-circuit current density (*J*sc) represents the maximum current a solar cell can deliver when the terminals are shorted (i.e., under zero external load). In the context of silicon nanohole-based [4-6] absorption or optical losses in the larger NH configurations under specific conditions, such as wavelength sensitivity or angular light incidence. Again η_{wte} – WTE confirms the superior performance of NH = 400 nm, which surpasses all other configurations, including TF. The slight differences in among NH sizes indicate a more moderate sensitivity in this operational condition but still emphasize the advantage of nano-structuring for performance enhancement.

Photovoltaic cells: *J*sc exhibits a non-linear dependence on doping concentration. At low to moderate doping levels, increased carrier concentration supports efficient current generation. However, at high doping, the minority carrier diffusion length (electrons in *p*-type or holes in *n*-type) decreases significantly due to enhanced impurity scattering and increased recombination. Consequently, although optical absorption remains high, reduced diffusion length limits effective carrier collection, leading to a decline in *J*sc. This effect is further aggravated by increased defect-assisted (SRH) recombination at higher doping levels. Additionally, the shortened carrier lifetime restricts charge transport, making carrier extraction less efficient and ultimately degrading device performance. Furthermore, bandgap narrowing and Auger recombination at very high doping concentrations can further suppress carrier collection efficiency. Therefore, an optimal doping range is essential to balance carrier generation and recombination losses for maximizing *J*sc. In nanostructured devices, this effect becomes more pronounced due to the increased surface-to-volume ratio, which enhances surface recombination. As a result, surface passivation becomes critical for maintaining high carrier collection efficiency. Overall, achieving high *J*sc requires careful control of both bulk doping and surface recombination mechanisms.

Open-circuit voltage (*V*oc) is the maximum voltage a solar cell can produce when no current is drawn (i.e., the circuit is open). Voc generally increases with moderate doping levels because doping enhances the built-in electric field and reduces the recombination of minority carriers, particularly in the depletion region. With fewer recombination events, the separation between electron and hole quasi-Fermi levels increases, leading to a higher *V*oc.

PCE is the ratio of electrical power output to the incident solar power input. In this study, PCE reaches its peak at an optimal doping level. At this point, the doping is sufficient to establish strong built-in fields and limit recombination without introducing excessive defects or reducing carrier mobility. Beyond this optimal doping point, both *J*sc and Voc begin to suffer due to increased recombination and shorter carrier lifetimes, leading to a decline in overall efficiency.

SRH recombination is a non-radiative process that occurs via defect states in the bandgap, typically introduced by impurities or lattice defects. This recombination mechanism becomes significantly more active at higher doping concentrations. The increase in doping leads to more defect-related trap states that act as recombination centers. As a result, SRH recombination rates increase, reducing the carrier lifetime and contributing to both lower *J*sc and *V*oc.

Optical generation refers to the creation of electron-hole pairs due to light absorption. In nanohole arrays, the optical generation remains relatively stable across different doping concentrations because the physical nanostructure governs how light is trapped and absorbed. These structures effectively enhance light absorption via mechanisms like multiple scattering and resonance effects, especially in the visible and near-infrared regions. However, while generation remains high, the ability to collect the generated carriers (collection efficiency) is heavily influenced by the doping level. Higher doping may result in shorter diffusion lengths and increased recombination, reducing the fraction of generated carriers that contribute to the electrical output.

3.2 Performance Comparison

Graphical data and spectral studies demonstrate that silicon nanohole arrays have superior absorption efficiency compared to flat silicon surfaces. The best-performing nanostructure design shows an improvement of up to 40 % in absorption, leading to enhanced photocurrent output [10]. TCAD-enabled modelling provided precise control over nanohole geometries, facilitating systematic design variations. The ability to visualize and adjust parameters in TCAD before simulation helped refine the structures for optimal light absorption performance [1-4, 6-8]. The integration of AutoCAD into the design process proved invaluable in achieving precise and efficient nanostructures. Continued advancements in nano structuring techniques and design tools like TCAD will pave the way for more efficient and cost-effective solar technologies [12].

4. APPLICATIONS AND FUTURE PROSPECTS

Silicon nanohole arrays enhance light absorption and PCE by optimizing doping and NH thickness without added cost, and can be applied to perovskite, organic, and CIGS solar cells. Thicker NH layers improve carrier generation and reduce recombination, making them suitable for low-light use. They also enable applications in flexible electronics, sensors, and tandem cells, with further gains possible using advanced materials and improved AutoCAD-based design.

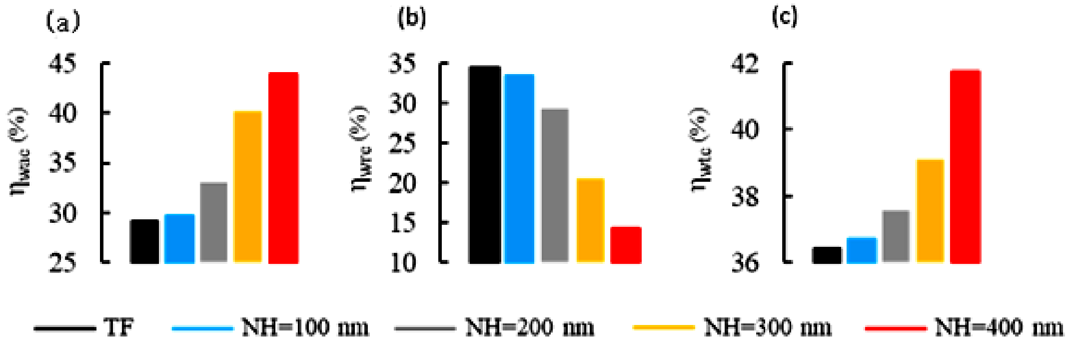

Fig. 3 – Comparison of nanostructures (NHs) of varying sizes in terms of (a) weighted absorption efficiency (η_{wae} – WAE) (b) weighted reflection efficiency (η_{wre} – WRE), and (c) weighted transmission efficiency (η_{wte} – WTE) (cm^{-3} s^{-1}) 10^{15}

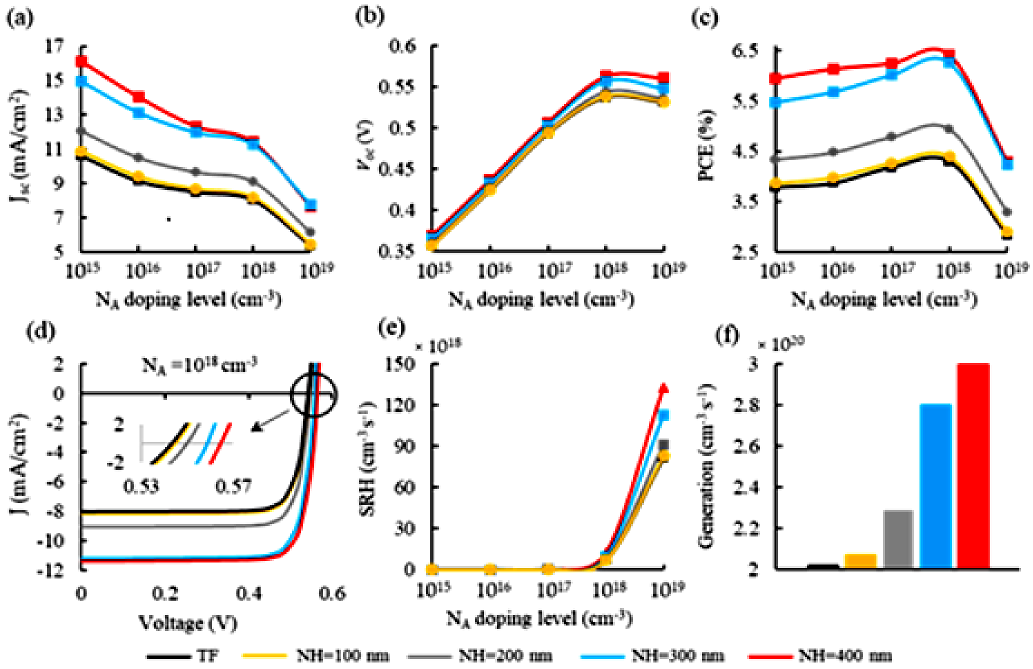

Fig. 4 – (a) Short-circuit current as a function of acceptor doping levels; (b) Open-circuit voltage depending on acceptor doping levels; (c) Power conversion efficiency (PCE) as a function of doping levels; (d) *I-V* characteristics for all five considered geometries; (e) SRH recombination rates as a function of doping levels; (f) Optical generation rates based on doping levels

5. CONCLUSION

In this work, a comprehensive TCAD-based optical-electrical investigation of silicon nanohole (NH)-engineered photovoltaic devices has been presented, with a particular emphasis on correlating nanohole geometry and acceptor doping concentration with recombination-limited device performance. By systematically varying the nanohole thickness from 100 nm to 400 nm and the acceptor doping concentration from 10^{15} to 10^{19} cm^{-3}, distinct performance regimes governing optical absorption, carrier transport, and power conversion efficiency were identified [6-8]. Optical simulations demonstrate that nanohole patterning significantly enhances light trapping compared to planar thin-film silicon. The weighted absorption efficiency (WAE) increases monotonically with nanohole thickness, exceeding 45 % for a nanohole thickness of 400 nm. Compared to the planar reference structure, the optimized nanohole configuration exhibits up to ~ 40 % enhancement in optical absorption, particularly within the visible and near-infrared spectral regions. Electrical analysis reveals that device performance is strongly influenced by the interplay between optical generation and recombination dynamics. The short-circuit current density decreases with increasing acceptor doping due to reduced minority-carrier diffusion lengths; however, thicker nanohole layers (300-400 nm) consistently maintain higher current densities owing to enhanced optical generation. The open-circuit voltage increases with doping and reaches a maximum near 10^{18} cm^{-3}, beyond which Shockley-Read-Hall recombination increases sharply, leading to degradation in carrier collection. As a result, the power conversion efficiency exhibits a clear optimum at an acceptor doping concentration of approximately 10^{18} cm^{-3}, with the 400 nm nanohole structure delivering the highest efficiency among all investigated configurations. The key contribution of this study lies in demonstrating that nanohole-induced optical enhancement alone is insufficient to maximize photovoltaic efficiency unless accompanied by proper electrical optimization. This work establishes quantitative design guidelines for nanohole-engineered silicon solar cells. These results confirm that optimal device performance is achieved through the co-optimization of nanohole thickness and doping concentration, providing a predictive pathway for improving silicon photovoltaic efficiency beyond conventional optical-only optimization strategies.

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Покращення захоплення світла, кероване TCAD, у кремнієвих фотоелектричних елементах за допомогою спроектованих геометрій наноотворів

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Формування наноотворів у кремнії широко досліджується як ефективна стратегія захоплення світла для фотоелектричних пристроїв; однак ступінь, до якої оптичне покращення призводить до покращення електричних характеристик, залишається сильно обмеженою рекомбінацією носіїв заряду та залежними від легування транспортними ефектами. У цій роботі використовується пов'язана оптико-електрична структура TCAD для систематичного дослідження впливу спроектованих геометрій кремнієвих наноотворів як на поглинання світла, так і на продуктивність пристрою. Товщина наноотворів від 100 до 400 нм та концентрація легування акцепторами від 10^{15} до 10^{19} см$^{-3}$ аналізуються за допомогою зваженої оптичної ефективності, генерації носіїв, динаміки рекомбінації та вольт-амперних характеристик. Результати показують, що збільшення товщини наноотворів значно покращує захоплення світла, причому зважена ефективність поглинання перевищує 45 % для товщини наноотвору 400 нм та покращує оптичне поглинання до ~ 40 % порівняно з планарною опорною структурою. Електричне моделювання виявляє чіткий оптимум ефективності при концентрації легування акцептора приблизно 10^{18} см$^{-3}$, за межами якої рекомбінація Шоклі-Ріда-Холла погіршує збирання носіїв заряду. У цій оптимальній робочій точці пристрій на основі наноотворів розміром 400 нм досягає значного покращення PCE порівняно з планарною тонкоплівковою коміркою. Дослідження демонструє, що максимальна ефективність досягається завдяки збалансованій кооптимізації геометрії наноотворів та концентрації легування, а також встановлює кількісні рекомендації щодо проектування наноструктурованого кремнієвого сонячного елемента на основі TCAD, що виходять за рамки лише оптичних підходів оптимізації [1-3, 6-9].

Ключові слова: Наноотвори, Кремній, TCAD, Оптичне поглинання, Підвищена ефективність.