

Impact of Doping and Surface Modification on Solar Cell

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ABSTRACT

Such massive research in material engineering technique like doping and surface modification has been brought about by the need to make sure that solar cells are efficient and durable. The methods play an essential role in maximizing electronic, optical and structural properties of photovoltaic materials to eliminate the limitation to the charge transport, recombination and long-term stability. Doping allows controlled amount of carrier, carrier band construction and carrier defect passivation on the absorber layers that would directly influence the performance factors, open-circuit voltage, short-circuit current and fill factor that are very important. In the meantime, surface alteration methods, including chemical passivation, plasma treatment and self-assembled monolayers are convenient in eliminating surface flaws, supplementing the light capture in addition to the increase in interfacial contact. Synergistic optimization of power conversion efficiencies of over 25 percent in silicon, perovskite, CdTe and CIGS technologies, has been carried out using controlled doping in addition to engineered interfaces. The current review is a systematic review of the underlying mechanisms of such processes on the basis of the experimental and theoretical advances in the subject. It is emphasized using novel-fangled approaches such as nanostructured dopants, gradient doping, and surface treatment by atomic layer and interface design with the aid of machine learning. Persistent challenges are critically appraised including the dopant stability, scalability of the processes and environmental sustainability. Finally, the paper also talks of the future projections of the generation of next-generation, defect-tolerant

and environmentally-friendly solar cells by clever material architecture and architectural designs of hybrid devices.

Keywords: Doping, Surface modification, Photovoltaics, Perovskite solar cells, Silicon solar cells, Charge carrier dynamics, Interface engineering, Bandgap tuning, Passivation, Power conversion efficiency.

1. INTRODUCTION

Sustainable energy systems making solar energy a central solution to solving the increasing crisis of climate change, environmental degradation and fossil fuel depletion. Photovoltaic (PV) devices, also known as solar cells, work on the physical basis of photovoltaic effect which transforms incident solar radiation directly to electrical energy [1]. Results aimed at improving the efficiency of these devices in conversion and this is an important factor that defines their commercial feasibility and environmental performance [2]. New developments of materials, especially the development of perovskite, quantum dot, and tandem cell technologies, have transformed the workings of photovoltaics to reach conversion efficiencies of more than 30 percent in the laboratory [3]. The incorporation of nanostructured materials and the ability to manage light has helped to reduce optical and thermal losses [4]. With these developments, carrier recombination, thermal instability, large cost of production, among other issues remain as persistent challenges limiting large scale implementation [5]. The importance of renewable energy in the modern global development has become even stronger over the last ten years mainly as a result of the growing problems of climate change and the exhaustion of traditional fossil fuel supplies [6]. Solar energy has become one of the key elements of sustainable energy systems due to its scale, environmental friendliness, and scaled ability to be introduced into the world of technologies [7].

The performance of solar cells that defines the capacity to transform sunlight into a useful electrical power is a determining factor of its financial as well as environmental sustainability [8]. The recent studies are dedicated to the increase of conversion efficiency, utilizing new material engineering, such as perovskite and tandem cell architectures, and surface modification and doping approaches, enhancing the movement of charge carriers and light absorption [9]. There is many researches done on nanostructured surfaces and passivation layers to help minimize

recombination loss and stability in the real life scenario [10]. The conversion of the countries to cleaner energy mixes, the optimization of solar cell efficiency is still to be at the core of achieving the global sustainability goal, reducing the carbon footprint, and contributing to the achievement of energy security of the future generation [11]. The surface modification material engineering and doping plays a significant role in enhancing the performance and stability of solar cells [12]. The effectiveness of photovoltaic devices depends basically upon the effectiveness of materials to take in luster, to create charge carriers and to minimize the loss of energy [13]. Fabrication of impurities in semiconductor materials purposely is referred to as doping with the aim of controlling electrical conductivity, carrier density and transportation of charges of the solar cell assembly [14]. It is viewed in silicon, perovskite and thin-film substances where precise doping may decline recombination loss by numerous factors and consequently raise open-circuit voltage [15]. Visual appearance techniques such as texturing, coating and passivation are required to increase absorption of light as well as minimizing the surface defects which locally clump the charge carriers [16]. These Nanostructured and plasmonic surfaces designs as well have improved the manipulation of light by facilitating increased photon capture and angular response [17]. These combined strategies not only increase conversion efficiency, but also increase thermal stability, durability and environmental degradation resistance [18]. Controlled doping and surface modification of materials will still continue to play an indispensable role in the further development of high efficiency, low cost and sustainable solar cell technologies [19].

1.1 Types of Solar Cells

Solar cells have progressed in numerous generations of material development giving rise to several different types, each with its own benefits and difficulties [20]. The first generation of photovoltaic technology, silicon-based solar cells, is the most commercial dominant, as they have reached their mature fabrication processes and stability, as well as stable functioning [21]. Monocrystalline and polycrystalline silicon cells are usually able to reach 20-27 percent wastes, and ongoing research has sought to eliminate the price of production and increase the power output [22]. The new type of hybrid material perovskite solar cells has received a lot of attention in

the last five years due to their high absorption capacity of light, tunable bandgap, and low prices that can be solved through solution processing [23]. Their laboratory efficiencies have already significantly exceeded 25 making them an excellent choice as the next-generation photovoltaics [24]. Cadmium Telluride (CdTe) solar cells are of the thin-film type and are appreciated by being comparatively cheap to manufacture with great performance in low light environments [25]. The Copper Indium Gallium Selenide (CIGS) solar cells offer flexibility and high absorption efficiency as well as high temperature tolerance, hence, can be used in the terrestrial as well as in portable powering devices [26]. All these technologies are representative of the various material approaches currently used to improve the efficiency of conversion of solar energy, its scale, and its sustainability..

1.2 Doping Concept

The concept of doping is one of the fundamental concepts in semiconductor physics that has been instrumental in the determination of the electrical and optical properties of solar cell materials [27]. When a n-type doping is used, donor atoms (which are usually more electronegative than the base material) are added to supply additional electrons and therefore the number of negative charge carriers [28]. P-type doping provides atoms with fewer valence electrons and provides holes or positive charge carriers in the crystal lattice [29]. This balance of n-type and p-type regions is controlled to create the key p-n junction in control of charge separation and charge transportation of solar cells [30]. Relationship between acceptor and donor doping in semiconductors is depicted in Figure 1.2 where the development of n-type and p-type regions that control charge separation and transport in solar cells is revealed.

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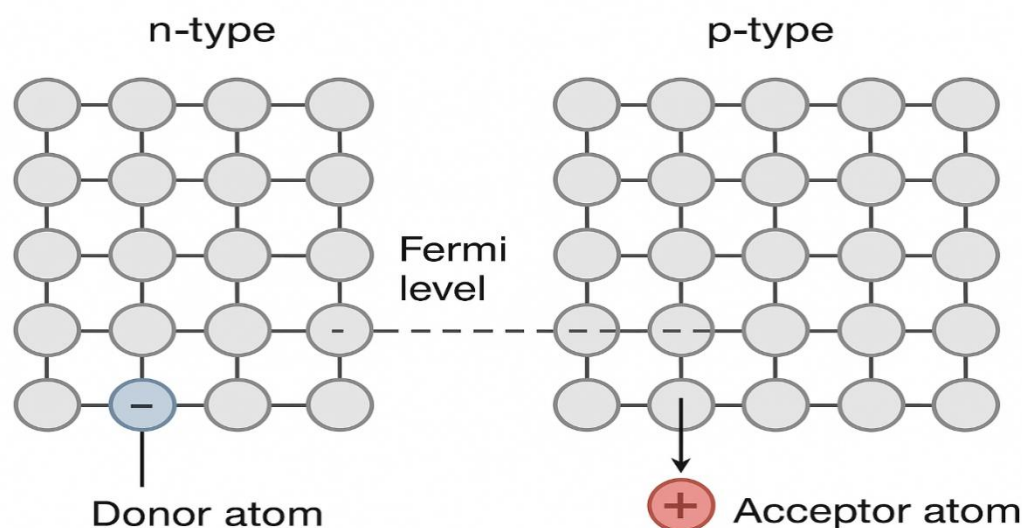
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Figure 1.1 n-Type and p-type Semiconductor Doping Schematic

Intentional doping, intrinsic defects, including vacancies, interstitials and antisite defects, may determine the behavior of the semiconductor by being sources of recombination, or shallow traps, and hence influence device behavior [31]. The direct and significant effect of doping on carrier concentration, Fermi level position and electrical conductivity of semiconductor materials in solar cells is notable [32]. Doping changes the natural equilibrium in the number of electrons and holes in the crystal lattice by adding known quantities of donor or acceptor atoms into the crystal lattice. The donor atoms of n-type semiconductors inject some extra electrons in the conduction band which increases the concentration of electrons and moves the Fermi level nearer to the conduction band edge. P-type doping puts acceptor impurities that open holes in the valence band, in effect, reducing the Fermi level to the valence band. This change in the Fermi level determines the distribution of the energy levels of charge carriers and it determines the conductivity of the material to electricity [33]. Electrical conductivity of a doped semiconductor is therefore dictated by the carrier concentration as well as mobility- parameters that can be adjusted by the type of dopant used, its concentration and distribution [34]. Studies shows increased doping control, which has made it possible to modify the band structure to a high degree and reduce recombination loss especially in perovskite, silicon, and thin-film technologies. This control has the added advantage

of not only improving the level of photovoltaic efficiency, but also increases stability, and engineering doping is one of the tools that cannot be ignored in optimizing the performance of solar cells in the next generation [35].

1.3 Impact on the open-circuit voltage (Voc), short-circuit current (Jsc) and fill factor (FF).

Doping and surface modification have a significant effect on the main performance parameters of solar cells open-circuit voltage (Voc), short-circuit current density (Jsc), and fill factor (FF), which subsequently have an impact on the total conversion efficiency [36, 37]. The difference between the quasi-Fermi levels of holes and electrons mainly determines the open-circuit voltage (Voc); effective doping increases this distance by increasing the concentration of charge carriers as well as decreasing junction recombination [38]. Oxidized n-type and p-type doping designs generate high strength built-in electric fields and thus raise Voc. The current density at the short-circuit (Jsc), the rate of charge carrier collected by photogeneration at illumination, takes advantage of doping and surface modification in both improvement of charge mobility, light absorption, and reduction of the losses during reflection [39]. Nanostructured dopants and textured surfaces enhance photon harvesting whereas carrier trapping is inhibited by defect passivation resulting in increased Jsc values. The fill factor (FF) of the current flow in the device is dependent on the series and the shunt resistances that are affected by the homogeneity of doping and the quality of the interfaces [40]. Accurate doping density and surface engineering is essential to achieve optimal Voc, Jsc, and FF at the same time and the optimal compromise between the electronic and the optical performance of solar cells in the next generation [41]. The comparative effect of varying levels of doping on the fundamental photovoltaic parameters Voc, Jsc, and FF is shown in Figure1.3 indicating the improvement in efficiency through optimized doping.

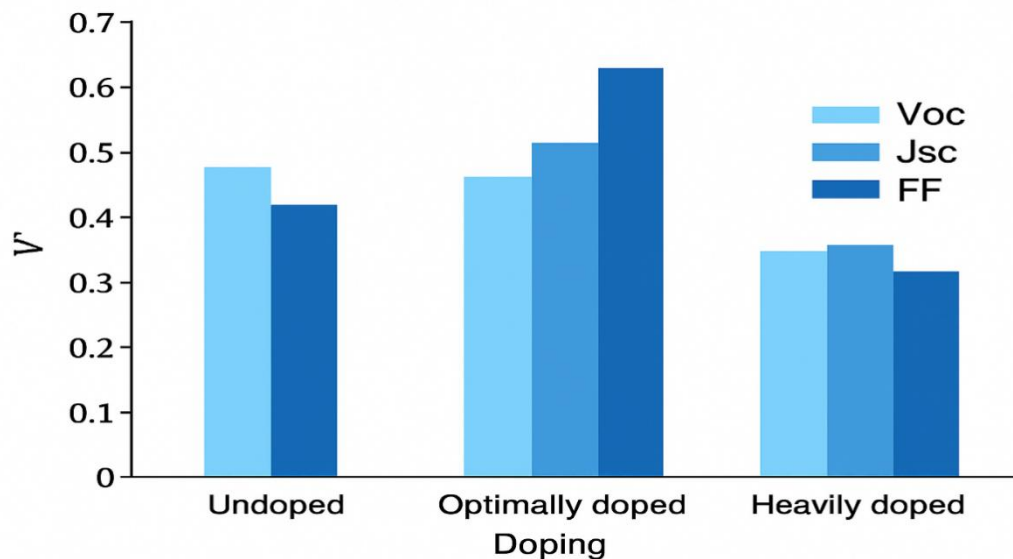


Figure 1.2 *Effect of doping level on photovoltaic performance parameters.*

2. TECHNIQUES OF SURFACE MODIFICATION

Surface modification has become an essential practice in the contemporary solar cell engineering as it has been instrumental in decreasing carrier recombination, as well as interface contact among various layers [42]. The major techniques are:

- Passivation of chemical (HF, SiO₂, Al₂O₃ layers).
- Plasma or UV-Ozone treatment.
- Self-Assembled Monolayers (SAMs) of interface engineering.
- Ultra-thin control by Atomic Layer Deposition (ALD).

A number of sophisticated surface modification methods have been invented to improve the performance of solar cells in terms of their efficiency, stability and charge conductivity by reducing surface recombination and maximizing the quality of interfaces [43]. One of the most developed ones is the chemical passivation, during which the surface defects and dangling bonds are neutralized by using hydrofluoric acid (HF) or by the deposition of thin dielectric layers like silicon dioxide (SiO₂) and aluminum oxide (Al₂O₃). SiO₂ layers are also very good conductors of electricity and Al₂O₃ is a good conductor of electricity and also a good passivation layer because of its high density of fixed negative charges hence it is especially good in p type silicon surfaces [44]. Plasma or UV-ozone treatments are extensively used to treat surfaces to make them functional and clean, increase

adhesion and eliminate organic contaminants that prevent the transfer of charges [45]. Surface modification has a strong influence on three aspects of solar cell performance, which are interrelated; light absorption, surface stability, and contact resistance, that determine energy conversion efficiency and long-term performance. Light absorption is enhanced by ensuring better photon trapping and lower surface reflectance by designing the surface morphology, optical properties, using nano-texturing, anti-reflective coating, and plasmonic layers and integration [46].

2.1 Interaction of Doping and Surface Modification

The overall performance, efficiency, and durability of the modern solar cells are greatly improved because of the synergistic effect of the doping and the surface modification [47]. Controlled doping creates high internal electric fields that enable the carrier transport and surface passivation and texturing reduces losses of carriers at the interfaces [48]. Recent technology in material engineering, especially through accurate doping and surface treatment has propelled Power Conversion Efficiency (PCE) in solar cells over the 25% mark- a mark that was previously deemed as being close to the theoretical limit of single-junction devices [49]. Both bulk and interface optimization innovations have been developed to record efficiencies in silicon, perovskite and tandem solar cells [50]. In perovskite-silicon tandem cells, this synergy has been extended to efficiencies over 29 per cent, as has been shown in a number of studies over the past five years [51]. The interplay between interface engineering and defect control has helped to improve the efficiency, stability and long term reliability of the modern solar cells by targeting two of the most serious performance-defining phenomena, namely interfacial recombination and defect-related charge trapping [52]. In photovoltaic devices, photovoltaic interfaces between the absorber and charge transport layers are frequently associated with structural discontinuities, lattice mismatches, and chemical imperfections, which are recombination centers [52]. Using interface engineering, scientists fabricate optimized interfacial coatings (e.g. self-assembled monolayers (SAMs), ultrathin dielectric coating (e.g. Al₂O₃, TiO₂), or 2D materials) in order to obtain the optimal energy band alignment and smooth charge transfer pathways [53]. Figure demonstrates the layer architecture of a generic solar cell, showing where interface engineering and defect control schemes operate to suppress recombination and

facilitate charge transport at junctions and

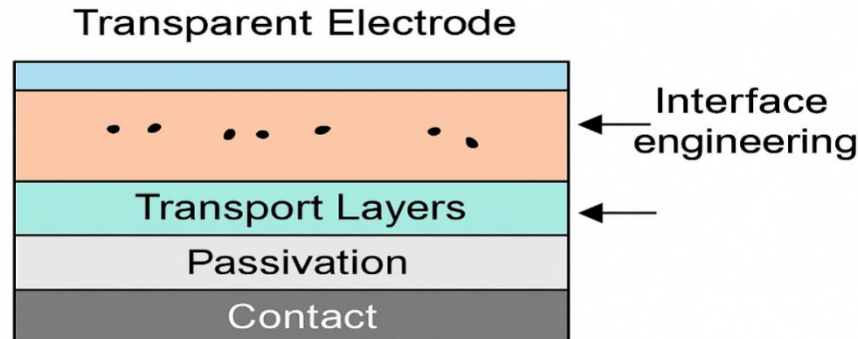


Figure 2.1 *Interface engineering and defect control in layered solar cell architecture, showing defect-prone regions and optimized interfaces for improved charge transfer.*

Defect control strategies are focused on intrinsic and extrinsic defects in the bulk or in the interfaces with the help of chemical passivation, doping control and post-deposition methods such as plasma exposure or UV-ozone exposure [54].

2.2 Nanostructure Layers, Perovskite-Silicon Tandem Designs

Nanostructured films and perovskite-silicon hybrid tandem cell designs have emerged as one of the most influential solutions in the area of escalating effectiveness and scalability of solar cells [50]. To achieve more efficient photon harvesting in thinner absorber layers, the use of nanostructured layers, as quantum dots, nanowires, and plasmonic nanoparticles may facilitate light absorption based on a high level of scattering and localized surface Plasmon resonance [46]. Perovskite-silicon tandem solar cells are hybrid to achieve the combination of a high degree of optical tunability and high absorption coefficient of perovskites and the established stability of crystalline silicon and carrier mobility [51]. This tandem architecture allows it to be sensitive over a broader region of the solar spectrum- perovskites are able to absorb high-energy photons better, and silicon absorbs the low-energy photons- and has no longer the single-junction Shockley-Queasier efficiency limit [55]. Efforts towards interface passivation, bandgap engineering and defect control now have perovskite-silicon tandem efficiencies up to over 29 percent with 33 percent potential theoretically and in ideal laboratory settings [56]. Nanostructured interlayers and graded doping are also included with the purpose of increasing optical coupling and low lattice mismatch. The combination of

nanostructured and hybrid tandem architecture makes a great breakthrough to high-performance, low-cost and long-term solar energy technologies that could be applied on a large scale [4].

3. CHALLENGES AND LIMITATIONS

Despite the enormous progress in the field of materials science and photovoltaic design, several issues still hinder large-scale application and extended exploitation of high-efficiency solar cells. The inhomogeneous carrier distribution and interface degradation are common in the process of dopant diffusion and instability during the process of high-temperature or solution-based processing [57]. There is also a problem of scalability, because techniques like atomic layer deposition, gradient doping, and Nano structuring are only effective in laboratories, at a cost, throughput, and uniformity, limiting them to commercial-scale manufacturing [58]. The use of noxious solvents and precursors in perovskite and CdTe systems are ecological problems, whereas humidity, light and temperature exposure accelerates the degradation of the devices [59]. The performance has to be aligned with price and sustainability by setting up of friendly to environment, low-priced, and scalable fabrication techniques that will assure durability of the system and truly sustainable solar energy system [60].

4. FUTURE DIRECTIONS

Future solar cell technology focuses on improved efficiency, extended lifetime, and complete environment friendliness by applying smarter materials and technologies. Creating defect-tolerant, self-healing materials can greatly improve longevity through dynamic bonding and passivating defects. Data-assisted and artificial intelligence -optimized design and material discovery enhance speed and precision in material fabrication. Hybrid and tandem perovskite–silicon cells approaching 30% efficiency continue to improve through interface and composition control. Shifts to green manufacturing, recyclable materials, and future architectures like multi-junction, quantum dot, and all-perovskite tandems will make photovoltaic systems scalable, carbon-neutral, and cost-efficient to achieve sustainable energy conversion.

5. CONCLUSION

The development of the solar cell technologies, especially the material engineering, doping, and surface alteration, has become central in improving the efficiency, stability, and sustainability of the photovoltaic systems. Controlled doping controls the concentration of carrier and electrical conductivity whereas surface modification reduces recombination and maximizes interfacial contact. A combination of these strategies can be used to achieve increased power conversion efficiencies and long term performance. Although there are problems of dopant instability, environmental issues, and scalability to manufacturing, new developments, such as nanostructured interfaces, tandem architectures, and AI-assisted design, can eliminate these constraints. The state of persistence in the defect control and interface engineering will be crucial to the achievement of sustainable and high-efficiency solar energy solutions in the future.

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