

Performance evaluation of nanostructured ZnO on silicon based solar cells

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Zinc oxide (ZnO) has garnered significant attention in photovoltaic research due to its exceptional optical and electronic properties, which complement traditional silicon (Si) solar cells. This work investigates the characteristics of integrating nanostructured ZnO layers over silicon substrates to enhance the performance of silicon solar cells. It also discusses the fabrication techniques for depositing ZnO on silicon, such as sol-gel method and highlights the performance of ZnO with various analysis. Additionally, the potential of ZnO/Si hetero junctions in reducing recombination losses and enhancing the open-circuit voltage and short-circuit current in solar cells have been discussed. The findings suggest that the integration of ZnO into silicon solar cells paves the way for more cost-effective and scalable photovoltaic solutions.

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1. Introduction

Electricity production is a significant concern in today's world. Over the past two to three decades, researchers and scientists have concentrated their efforts on finding solutions to this global crisis. As a result, various methods for converting natural, renewable resources into electricity have been developed. Among these, solar radiation stands out as a well-known renewable energy source (RES). Through the use of solar cells, photon energy can be efficiently transformed into electrical energy [1].

Following the advent of semiconductor technology, materials such as silicon, cadmium became prominent in fabricating conversion mediums for electricity generation [2-4]. The pursuit of higher efficiency in silicon solar cells is critical for making photovoltaic technology more competitive with conventional energy sources. Traditional silicon cells face limitations in light absorption, especially at longer wavelengths and suffer from reflection losses at the cell surface. Nanotechnology, particularly the use of ZnO nanomaterials, offers innovative solutions to these challenges.

ZnO nanostructures can significantly reduce surface reflection when applied as anti-reflective coatings (ARCs). By minimizing the reflection of incident sunlight, ZnO allows more light to enter the silicon substrate, thereby increasing the number of photons available for conversion into electricity. Studies have shown that ZnO-based ARCs can reduce surface reflection to less than 5%, leading to a noticeable improvement in cell efficiency [5-7].

In addition to reducing reflection, ZnO nanomaterials can enhance light trapping within the solar cell. The nanostructured ZnO scatters incoming light, increasing its optical path length inside the silicon layer. This enhanced scattering effect is particularly beneficial for trapping longer-wavelength light, which silicon absorbs less effectively. As a result, more photons are absorbed, boosting the overall power conversion efficiency [8-11].

Hence, this study explores the integration of nanostructured zinc oxide (ZnO) into silicon-based photovoltaic (PV) cells to enhance their performance. ZnO, a transparent conductive oxide (TCO) with unique optical and electrical properties, plays a vital role in improving light absorption

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and charge carrier dynamics within the solar cells. Using a simple and cost-effective co-precipitation method, ZnO nanoparticles (NPs) were synthesized and incorporated into silicon PV cells [12-15]. The study focuses on how ZnO nanostructures, acting as an anti-reflective coating (ARC) and transparent electrode, increase photon absorption, reduce recombination losses, and enhance charge collection. The results demonstrate a significant improvement in the overall efficiency of silicon solar cells, offering a sustainable, scalable, and economically feasible solution for energy conversion. This research provides valuable insights into the development of advanced PV technologies aimed at maximizing energy harvesting from solar resources.

2. Methodology

2.1. Materials

The materials used for synthesis includes $[\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}]$ were sourced from Merck. Deionized and double distilled water was used in the preparation of these solutions.

2.2. Synthesis

A water-based solution of zinc salts was made by using zinc acetate dihydrate and zinc chloride as the starting materials. Sodium hydroxide was added as a precipitating agent, with each ingredient having a concentration of 1M in 100 ml of water. The zinc salt solution was then added slowly, drop by drop, into the sodium hydroxide solution. The two solutions were mixed thoroughly at room temperature using a magnetic stirrer for 2 hours. As the sodium hydroxide solution was added to the zinc chloride or zinc acetate dihydrate ZnO began to form immediate, causing the solution's color to change from transparent to white. The mixture was stirred for 2 hours and then sealed and left to sit overnight. By the next day, zinc hydroxide and its impurities had deposited at the bottom, while the excess liquid, known as the mother liquor, remained at the top and it was then removed. Then, the same solution was set apart for 5 minutes. The precipitate formed was then eroded with methanol and deionized water to remove any byproducts. Afterward, the precipitate was dried in air at about 200°C, during which the zinc hydroxide was converted into pure ZnO nanoparticles.

3. Results and discussion

The structure of the ZnO nanocomposites was analyzed through X-ray diffraction (XRD) patterns. Optical properties were assessed using a UV-VIS spectrophotometer, while the chemical structure was analysed using X-ray photoelectron spectroscopy (XPS).

3.1. XRD examination

The XRD patterns of prepared ZnO nanoparticles is depicted in figure 1. This XRD examination of ZnO coated silicon cell provides a critical insight into the crystalline structure, orientation, and quality of the ZnO layer.

The analysis reveals that the lattice parameters of ZnO, including the unit cell parameter (\AA), volume (\AA^3), and density (g/cm^3), remain consistent regardless of the precursor used in their synthesis. This suggests that the type of precursor does not influence the lattice structure of the oxide. The XRD data confirms that ZnO has a hexagonal structure, matching the crystallographic data of JCPDS Card No: 80-0075. It shows good crystallinity, with minimal dislocations, stacking faults and elastic strains.

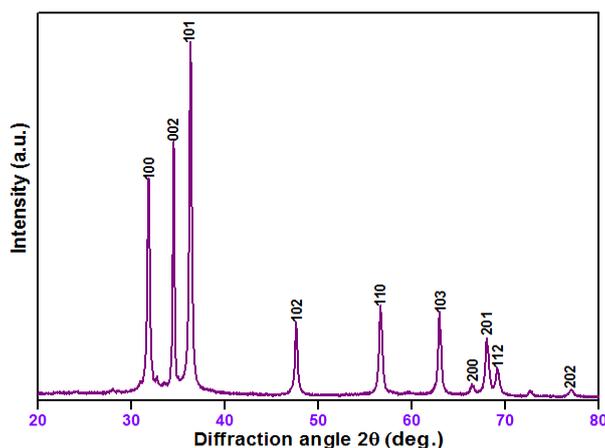


Fig. 1. XRD patterns – ZnO.

The presence of sharp and well-defined diffraction peaks at specific angles confirms the hexagonal wurtzite crystal structure of ZnO. This indicates a high degree of crystallinity, which is essential for efficient charge carrier mobility in the ZnO layer. The dominant diffraction peak at the (002) plane suggests a strong c-axis orientation and ZnO is vertically aligned on the silicon surface. This orientation enhances the light-trapping capabilities and charge transport properties of the PV cell.

Table 1. Structural parameters of prepared ZnO.

ZnO precursor	Planes	Peak position 2θ ($^{\circ}$)	Crystallite Size D (nm)	Stacking faults probability (\AA)	Elastic strains ϵ
$\text{Zn}(\text{CH}_3\text{COO})_2$	100	31.80	24.87	0.0029	0.0053
	002	34.41	37.31	0.0018	0.0033
	101	36.31	30.40	0.0022	0.0038

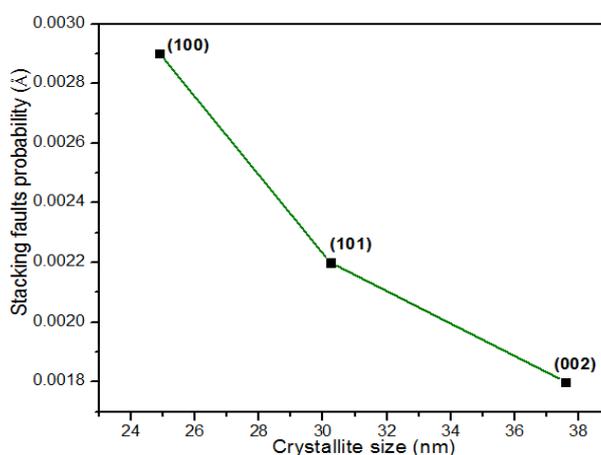


Fig. 2. Variation of stacking faults probability.

Stacking fault probability is an important parameter in assessing the quality of ZnO used in PV applications. A low stacking fault probability is generally desired to minimize defects and

optimize the efficiency of PV cells. A high stacking fault probability can lead to an increase in defect density, which in turn may create localized energy states within the bandgap. This could enhance non-radiative recombination rates, reducing the efficiency of charge transport in ZnO-based PV cells. From the Figure 2 and table 1, it has been noted that the values of the stacking faults and elastic strains gets decreased with increase in crystallite size for and hence, it is concluded that the ZnO nanoparticles prepared with Zn (CH₃COO)₂ precursor has less dislocation, stacking faults and elastic strains.

3.2. Optical characteristics

Figures 3 and 4 depicts the optical absorption and transmission spectra of the ZnO nanoparticles, respectively.

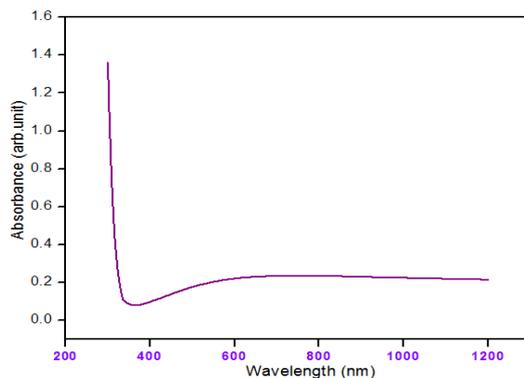


Fig. 3. Absorbance spectra (optical)- ZnO.

This material shows strong absorbance in the ultraviolet (UV) region, particularly between 200 and 400 nm. This is typical for ZnO, which has a wide bandgap (~3.37 eV) and therefore strongly absorbs UV light. The peak absorbance around 300-350 nm suggests this material is absorbing most UV light, a property useful for UV protection or applications where UV blocking is needed. After UV Region, there is a sharp drop in absorbance. This indicates that the material becomes transparent to visible light. Beyond 400 nm, absorbance levels off to a low, nearly constant value, indicating that the material is highly transparent to visible and near-infrared light (400-1200 nm). This is beneficial in applications like photovoltaic cells, where ZnO needs to allow visible light to pass through to the silicon layer while blocking harmful UV radiation.

Figure 4 indicates that the material has a relatively high transmittance (around 70% or more) from approximately 400 nm and beyond. This suggests that the material, is highly transparent to visible light, making it an effective transparent conductive oxide (TCO) for PV applications.

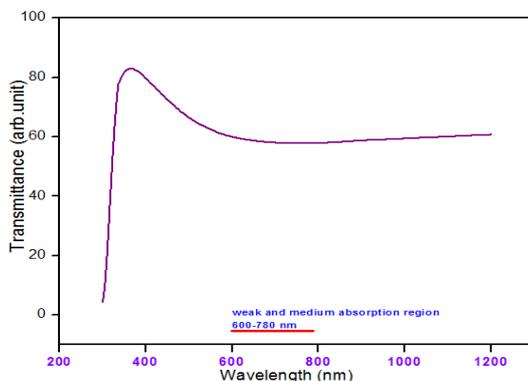


Fig. 4. Transmittance spectra (optical) – ZnO.

Figure 5 shows the Tauc-Plot, which graphs $(\alpha h\nu)^2$ against energy.

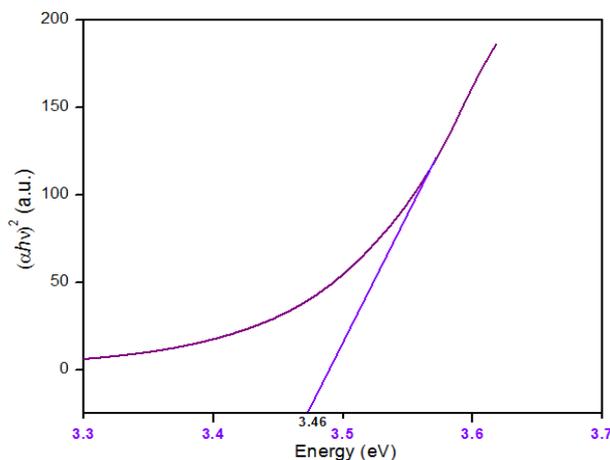


Fig. 5. Optical bandgap.

Thus, with a bandgap of 3.46 eV, ZnO can effectively capture high energy ultraviolet (UV) and blue light, which is beneficial for converting sunlight into electrical energy. By capturing more of the higher energy from a solar spectrum, ZnO with a 3.46 eV bandgap has the potential to improve the overall power conversion efficiency of solar cells. Additionally, it is generally higher than that of silicon (1.1 eV), which means ZnO can be used to complement silicon-based PV cells by enhancing their performance in specific wavelength ranges. This characteristic, makes it a promising candidate for improving solar cell performance.

3.3.4. SEM / EDS analysis

The morphology of the ZnO nanoparticles synthesized through the sol-gel method is revealed on the surface of the sample, as captured by high-energy electrons in the scanning electron microscope (SEM). This depiction is illustrated in Figure 6. From the SEM images, it is found that the ZnO coating has a porous structure that could enhance light absorption in PV applications.

From the figure 6, it is found that the majority of the pores seem to be in the range of 1-3 nm, with a few larger pores up to 7 nm. Smaller pores (around 1-2 nm) might help in enhancing the surface area for light interaction, but larger pores (3-5 nm) might allow better electron mobility. An optimal pore size distribution can thus balances both the optical and electrical properties of the ZnO coating in solar cells.

Form the figure 6b, it is found that the surface roughness of ZnO nanoparticles is found high as compared with others. This in turn, enhances the light scattering, increases the optical path length in the solar cell. This leads to improved light absorption. It can also reduce reflection losses, functioning as an anti-reflective coating. At the same time, a rough ZnO surface provides a larger area for dye adsorption, leading to higher photocurrent.

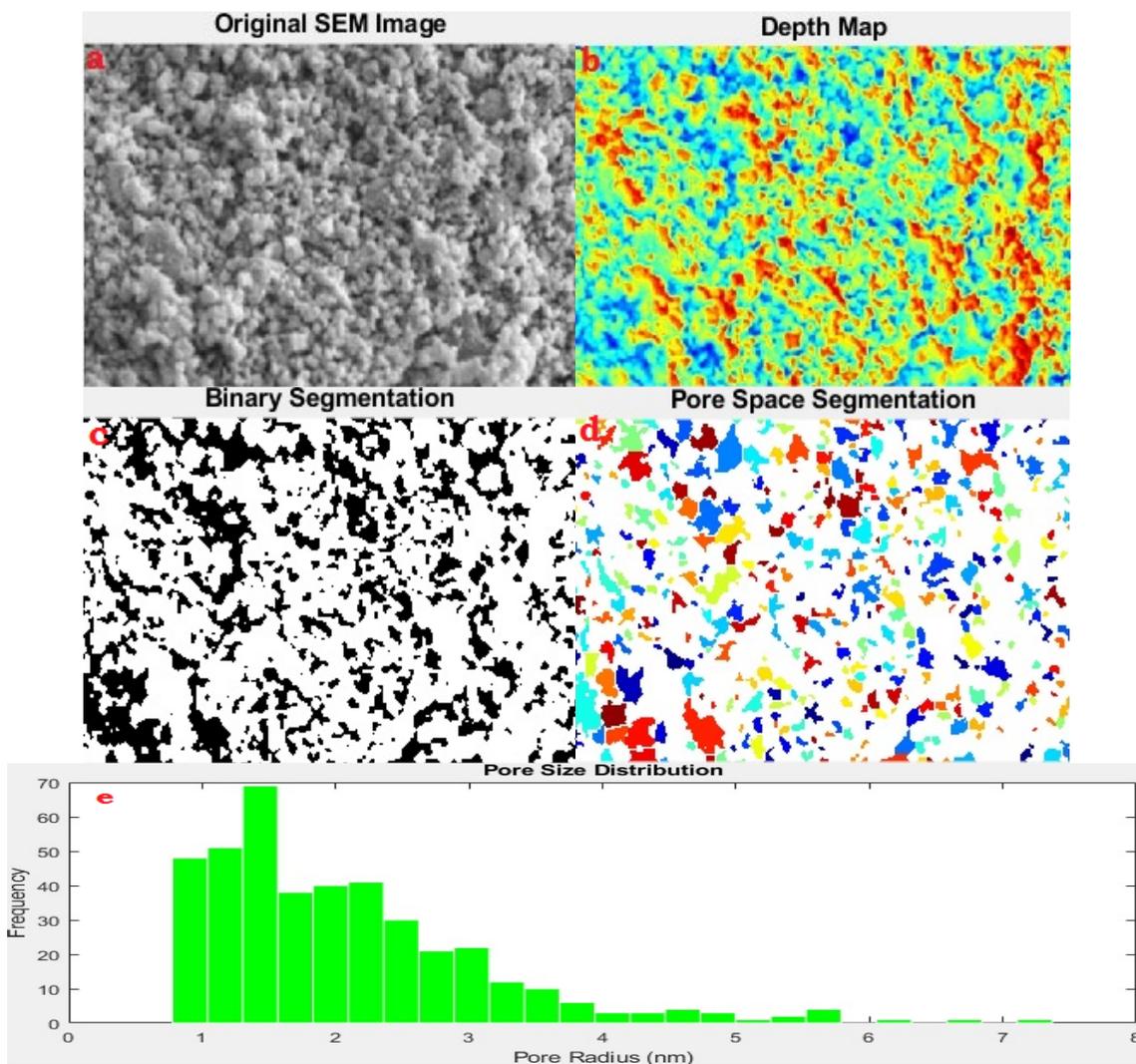


Fig. 6 (a). SEM micrographs – ZnO.

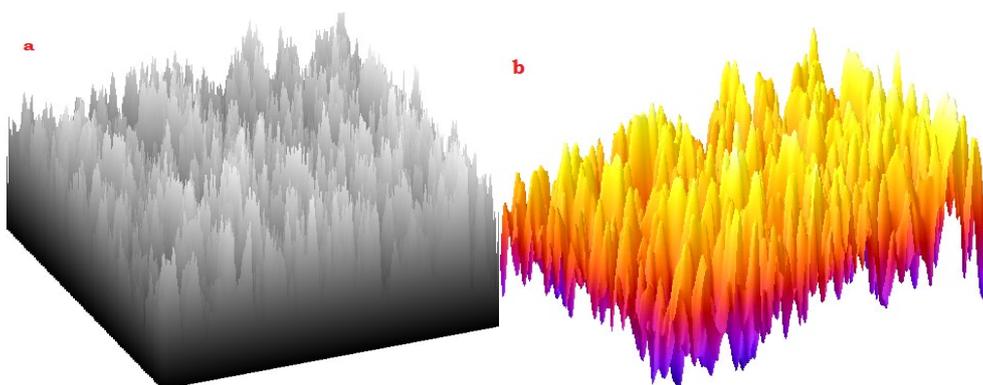


Fig. 6 (b). Surface roughness – ZnO.

EDS spectra also have been recorded during the SEM imaging technique as depicted in figure 7. The EDS results confirm the high purity of the synthesized ZnO nanoparticles, demonstrating that they consist exclusively of zinc and oxygen in the ZnO wurtzite structure. As a result, the wurtzite structure's high transparency in the visible spectrum allows more light to pass

through to the underlying silicon, potentially increasing the amount of light that contributes to electricity generation and reduced energy losses.

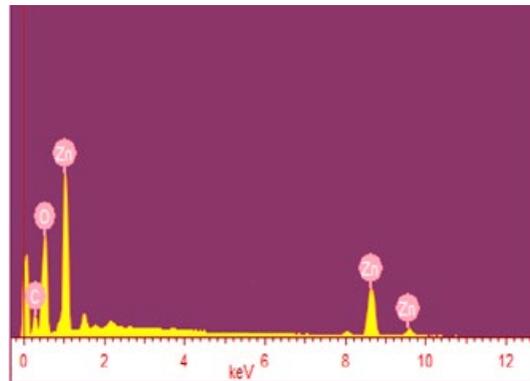


Fig. 7. EDS analysis (Exposed by EDX analysis).

3.3.5. HRTEM analysis

HRTEM reveals the details of the crystalline, elemental and structural composition of ZnO nanoparticles and it is revealed in Figure 8.

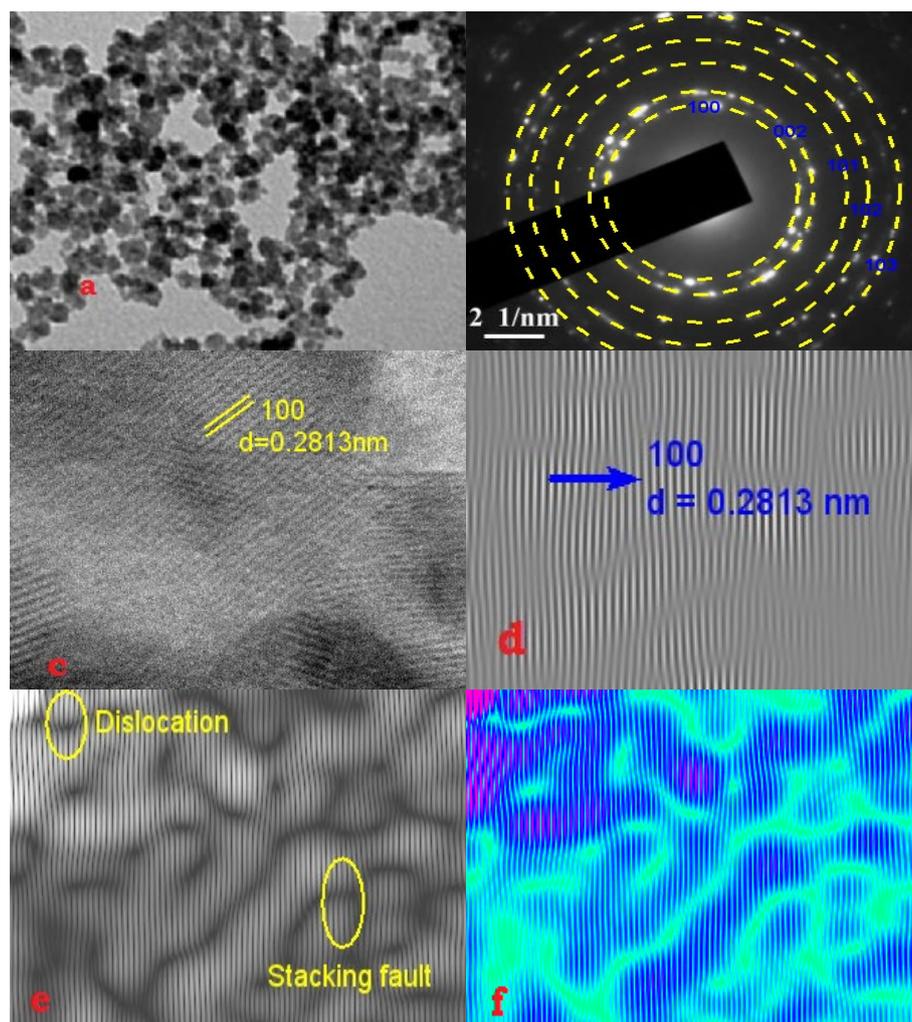


Fig. 8. HRTEM analysis.

The hexagonal wurtzite structure of the ZnO samples is confirmed by the hexagonal facet and spherical structure having dimensions of approximately 24-37 nm and over the hexagonal facet and spherical like morphology the small particles were decorated. In the Figure 8, the SAED patterns shows the existence of ZnO in (100) (002) and (101) and it also confirms the polycrystalline nature of ZnO and this fact is found to be in good accordance with the XRD analysis. The d spacing (Figure 8) of (100) planes of ZnO exhibit in 0.2817 nm, 0.2813 nm and 0.2813 nm which is in close match with the corresponding standard values, respectively.

These types of analyses are crucial for understanding the structural and defect characteristics of ZnO, which can significantly influence their electronic, optical, and mechanical properties. From all those above structural analyses, it is observed that ZnO exhibits good transparency, electrical conductivity, and ability to transport electrons and thus, maximizes the efficiency of solar cells where ZnO is used as a key material.

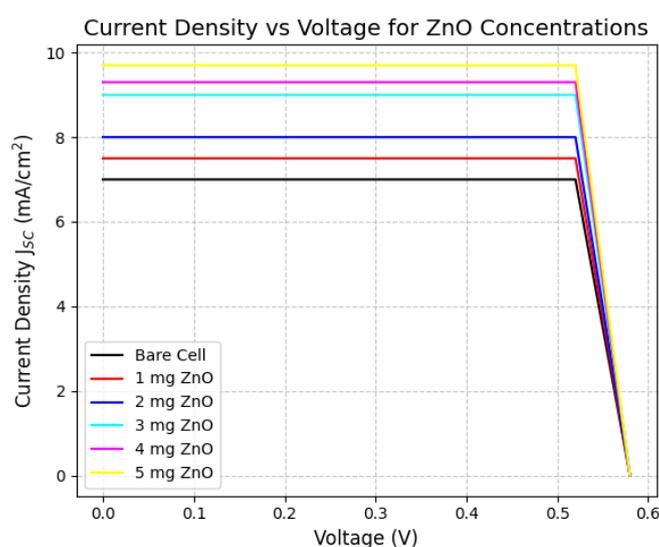


Fig. 9. *J-V* curves - ZnO NPs - solar cell.

Figure 9 shows the *J-V* curve for a single crystalline silicon solar cell coated with ZnO nNPs at different concentrations (1-4 mg/ml). The "Bare Cell" (black curve) represents a PV cell without ZnO. It shows the lowest current density when compared cell with ZnO. As ZnO is added (1 mg to 3 mg), the current density increases, indicating better charge carrier collection and possibly enhanced electron transport due to the ZnO layer. Beyond 3 mg of ZnO, the performance begins to decline (as seen with the 4 mg and 5 mg curves), which could indicate that excess ZnO is causing charge recombination or hindering charge transport. Thus, the highest efficiency, 7.30%, was achieved with a ZnO concentration of 3 mg/ml. However, increasing the concentration beyond this point led to a decrease in performance. The best results included an open-circuit voltage (V_{oc}) of 0.56 V, a short-circuit current density (J_{sc}) of 9.67 mA/cm², and a fill factor (FF) of 75.4%, leads to a maximum efficiency. Coating the silicon solar cells with ZnO nanoparticles improved their efficiency by at least 1.1% compared to uncoated silicon cells.

4. Conclusion

Nanostructured ZnO significantly enhances silicon solar cell performance by improving electron transport and light absorption. Its high electron mobility and wide bandgap reduce recombination losses, while the nanostructures provide effective light trapping and anti-reflective properties, increasing photon absorption. Optimal ZnO thickness or concentration improves current density and efficiency, with a balance between charge transport and minimal resistive losses. ZnO

also acts as a surface passivation layer, reducing surface recombination and enhancing open-circuit voltage.

However, excessive ZnO can increase series resistance, lowering efficiency. Overall, nanostructured ZnO enhances power conversion efficiency (PCE) and holds great promise for boosting silicon solar cell performance.

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