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Impact of Thickness and Doping Concentration on Heterojunction InP/Si-Based Solar Cell Performance: Insights from PC1D and Wafer Ray Tracer Simulations

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ABSTRACT

The study aimed to investigate how different doping concentrations and n-region layer thicknesses affected the efficiency of InP/p-Si solar cells. The n- and p-regions were represented by indium phosphide (InP) and silicon (Si), respectively, with band gaps of 1.35 eV and 1.124 eV. To optimize the efficiency and performance of InP/p-Si solar cells, the study systematically varied the doping concentrations over six orders of magnitude, ranging from 1×10^{14} cm^{-3} to 1×10^{17} cm^{-3}, and adjusted the thickness of the n-region layer from 5µm to 30 µm. Reflection, absorption, and transmission characteristics of heterojunction InP/Si layers in the wavelength region of 300-1200 nm were also modelled by wafer ray tracer software. At 450-700 nm wavelength, 50 nm InP sample exhibited minimum reflection compared to all other samples. Trends showed that the absorption decreased with increasing thickness of InP layer between 300 and 920 nm. The data obtained from the absorption measurement at different thicknesses was in agreement with the data obtained from the result of impact of different n-region thickness of InP/p-Si solar cells, where the reduction in InP layer thickness resulted in the increase of absorption, which in turn increased the current due to the higher absorption of photons and the generation of excess electron carriers.

1. Introduction

A binary semiconductor made up of indium (In) and phosphorus (P) is known as indium phosphide (InP). InP falls into the same category as gallium arsenide (GaAs) semiconductors, which have a zincblende crystal structure [1]. These materials are categorized as III-V semiconductors. High-frequency and high-power electronics use InP semiconductors because of their high electron velocity [2]. The performance of InP solar cells is primarily evaluated by their efficiency, a critical metric in assessing the ability of a solar cell to convert sunlight into electricity. With a direct bandgap of approximately 1.35 eV, InP is well-suited for efficiently absorbing photons from the solar spectrum [3]. This characteristic contributes to the creation of electron-hole pairs, initiating the generation of electrical current. InP is often integrated into tandem solar cells, where multiple semiconductor materials with different band gaps are combined [4-7]. This approach enhances the absorption of a broader spectrum of sunlight, pushing the boundaries of efficiency and paving the way for advanced solar technologies. Silicon substrate is normally used for the solar cell's fabrication due to its cheap substrate and can be integrated with well-

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established technology. However, research on the simple heterojunction InP/Si based-solar cells is limited in the literature review. For the tandem solar cells, the fabrication of InP/InGaAs tandem system solar cell to incorporate InP on a Si template resulted in an efficiency of 18.4%, following the Metal-Organic Vapor Epitaxy (MOVPE) method [8]. Besides that, fabricating wafer bonded GaInP/GaInAsP/Si triple-junction solar cell generates a conversion efficiency of 36.1%, combining a rear-heterojunction for the middle together with light trapping layer, improving the current cell [9]. InP nanowire arrays grown on Si substrates have indicated significant results in solar cells, showing high onset potential and photocurrent [10].

Most researchers used advanced heterostructures of InP-based solar cells to reach the maximum efficiency of solar cells [11-15]. In another improvement application, InP shell layer was formed vertically on SiNWs core based solar cells, providing efficiency, open circuit voltage, and short circuit current density of 4.39%, 0.56 V, and 14.26 mA/cm^2, respectively [11]. There is a comparative study using Personal Computer One Dimensional (PC1D) software between the GaAs-Si and InP-Si based solar cells, reporting their efficiency of 18 and 20%, respectively, after optimizing the doping and the thickness of materials [12]. Other researchers proposed the InP nanoresonator on 2 μm silicon substrate with the addition of anti-reflective coating (ARC) compared to Si nanodisk/Si structure, showing the absorption value of 47.5% compared to normal Si absorption value, which was 18.2% [13]. Some researchers fabricated an advanced InP-based tunnel junction solar cells, demonstrating that the device could reach up to 495 mA/cm^2 and 9.3×10^{-4} Ωcm^2 for current density and resistivity, respectively, permitting the device to operate under the 30000 suns exposure [14]. Si/InP thin-film tandem solar cell was equipped with a black silver reflector and silver nanowires on the top of device, indicating 52% greater efficiency and short current density of 41.62 mA/cm^2, due to the improvement of light trapping in the solar cell [15].

However, the development of advanced heterostructure InP-based solar cells is a time-consuming, complex and expensive process. Therefore, we simulated and optimized the simple structure of heterojunction InP/Si solar cells by investigating the electrical characteristics and efficiency of various device designs. The relationship between the thickness and doping of layers was explored in this work. PC1D, is widely used to design and analyse the effectiveness of solar cells before it can be fabricated in the laboratory [16-19]. This simulation software was developed at the University of South Wales in Sydney, Australia [20]. PC1D offers faster results and an inexpensive method. It can predict the device performance without the need to fabricate devices in the laboratory. The electrical characteristics for various InP-based solar cells, such as maximum output power (P_{max}), open-circuit voltage (V_{oc}), short-circuit current (I_{sc}), fill factor (FF), and efficiency (η) were evaluated in this work. To assist the understanding of light absorption and trapping process in the device structure, we combined results from PC1D simulation with the results from wafer ray tracer simulation. Open-source wafer ray tracer simulation can be freely assessed from the PV lighthouse website, containing a Monte-Carlo algorithm and selected materials optical properties. By inserting a specific parameter for absorption and refractive index from the available library, one can investigate the photo-generation and loss of optical characteristics for the developed model, which help the researcher to get the best condition or the optimized device structure. The rationale of using these softwares in this work is that they are widely used to simulate solar cells device or design without needing to fabricate it in the laboratory, thus saving the budget and helping the researcher find the best structure and design before proceeding to the real fabrication work. When running the simulation, we considered the actual parameters, such as absorption, reflection, refracting index, and material properties to avoid false or inaccurate results, and then, compared our results with other simulations or experimental works.

2. Methodology

The simulated structure included bandgaps of 1.35 eV for InP and 1.124 eV for Si. The active area of the heterojunction InP/p-Si based-solar cell heterojunction was configured as shown in Figure 1. The electrical and optical characteristics of such solar cells were studied using the PC1D numerical simulation. In the PC1D simulation program, silicon was designated as the p-region layer, and indium phosphide was designated as the n-region layer. The performance of the heterojunction InP/p-Si based-solar cell was examined in this study with respect to the different n-region and p-region thicknesses and doping concentrations.

The model parameters used in this investigation are listed in Table 1. The goal of the PC1D simulation was to determine the maximum output power (P_{max}), open-circuit voltage (V_{oc}), and short-circuit current (I_{sc}). Based on these results, the efficiency (η) and the fill factor (FF) were calculated using the following formulas respectively:

$$Efficiency: \frac{P_{max}}{0.1\ X\ Device\ Area} x100\% , \quad (1)$$

$$Fill\ Factor = \frac{P_{max}}{I_{sc}\ X\ V_{oc}} x100\% , \quad (2)$$

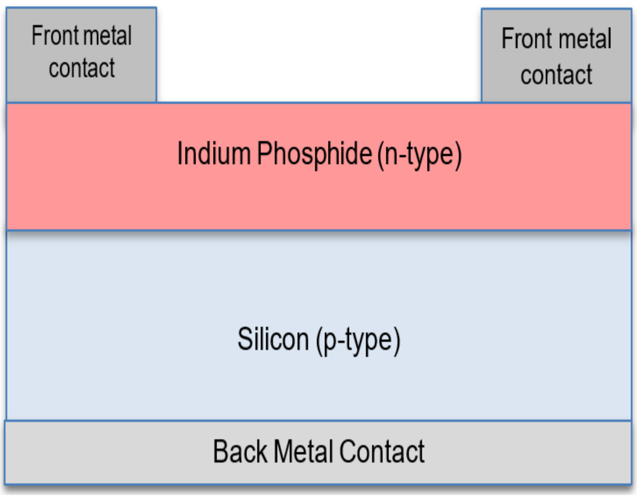

Fig. 1. The schematic structure of the heterojunction InP/p-Si based-solar cell

Table 1. List of the fundamental variables used in the heterojunction InP/p-Si based-solar.

Parameter	Value	
Device area	$100\ cm^2$	
Region	**n-InP**	**p-Si**
Band gap	1.35 eV	1.124 eV
Intrinsic conc. (300K)	$8\times10^6\ cm^{-3}$	$1\times10^{10}\ cm^{-3}$
Bulk recombination lifetime	1000 µs	1000 µs
Excitation mode	One-sun (transient; 16 timesteps)	
Spectrum	AM1.5G	
Intensity	$0.1 W/cm^2$	
Temperature	25°C	

Ray tracing in optical simulations for solar cells refers to the computational process of modelling the propagation of individual light rays, where the intensity I, of each ray diminishes in accordance with the Beer-Lambert law (equation (3)) as it traverses an optically thick region.

$$I(z) = I_0\, exp(-\alpha z) \quad (3)$$

With z being the propagation depth, I_0 the light intensity at z = 0 and α the extinction coefficient of the material. At material interfaces and thin passivation layers, a physical model was applied to the ray tracer to enable the calculation of the beam's interaction. For well-defined interface structures, such as pyramidal or planar surfaces, and with known optical constants of the materials, the Fresnel equation could be utilized through the transfer matrix formalism [21]. As this was a physical model, it provided adequate precision [22]. Generally, physical models are preferred for optical simulation as they offer predictable reflection and transmission characteristics at material interfaces.

The optical properties, including: reflection, absorption, and transmission, were determined and analysed. A transverse matrix method was employed for the theoretical analysis of the proposed models. This method is a well-established technique for calculating the optical properties of solar cells [23-26]. Given the solar spectrum's wide wavelength range of 300 to 1200 nm, calculating the average reflection is necessary. When the light ray travels from air and transmits into the cells, reflection, R, and transmission, T, can be determined using following equations.

$$R = \frac{1-n}{1+n} \quad (4)$$

$$T = \frac{2}{1+n} \quad (5)$$

The absorptance A is given by applying the law of conservation of energy as stated in equation (6):

$$A = 1 - R - T \quad (6)$$

3. Results and Discussion

Fig. 2 shows the impact of varying InP layer thickness on heterojunction InP/p-Si based-solar cells. The efficiency of the heterojunction InP/p-Si solar cell decreased as the thickness of the p-region increased from 30 µm to 150 µm. The sample with 30 µm thickness exhibited the lowest current value, while the one with 150 µm thickness exhibited the highest current value. Power decreased when the p-region thickness exceeded 300 µm. Table 2 presents The electrical characteristics of all the samples. It shows that the efficiency decreases as the InP thickness increases, dropping from 23.9% (η) at 5 µm to 22% (η) at 30 µm. This indicates that the changes in InP thickness affectes all cell parameters.

The maximum efficiency of 23.9% was achieved with the thinnest n-region layer, 5 µm, where the V_{oc} was 0.7528 V, the I_{sc} was 0.379 A, the P_{max} was 0.0239 W, and the FF was 0.837. As the layer thickness increases, these outcomes decreased, causing the efficiency to gradually decline. Figure 2 illustrates the influence of different InP substrate thicknesses on the solar cell's efficiency. The results showed that varying the InP substrate thickness in heterojunction InP/p-Si based-solar cells affected their efficiency. The highest current value was obtained with a 5 µm thickness, while the lowest value was observed at a 30 µm thickness, as shown in Table 2. Optimal efficiency was achieved with a thinner InP layer, specifically at 5 µm, where the solar cell exhibited the highest efficiency and electrical parameters. As the thickness increased, both the efficiency and performance metrics declined, indicating that thinner InP layers were more effective in enhancing the overall efficiency of heterojunction InP/p-Si based-solar cells. Thin layers may experience higher surface recombination effects, limiting the overall efficiency of the solar cell. Thicker layers may face increased bulk recombination, where carriers recombine within the bulk of the material. The electrical characteristics of the n-type indium phosphide substrate at different doping doses are displayed in Figure 3. The n-region doping concentration varies over six orders of magnitude, ranging from 1×10^{14} cm^{-3} to 1×10^{17} cm^{-3}. As shown in Table 3, the heterojunction InP/p-Si based-solar cell achieved a comparable efficiency of 23.9% when the n-type doping concentrations were adjusted to 1×10^{14} cm^{-3} and 1×10^{15} cm^{-3}. Increasing the doping concentration beyond the optimal values of 1×10^{14} cm^{-3} and 1×10^{15} cm^{-3} did not improve efficiency and, in many cases, led to a decline. This decline is primarily due to the increased recombination rates at higher doping concentrations, which reduce I_{sc}. Additionally, recombination in the heavily doped emitter layer began to reduce solar efficiency at doping level of 1×10^{19} cm^{-3}. For comparison, the ideal doping concentration for the n-region in heterojunction InP/p-Si based-solar cells was 1×10^{18} cm^{-3}.

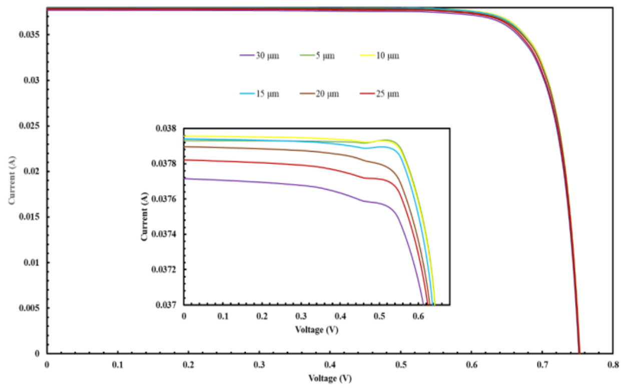

Fig. 2. The impact of different n-region thicknesses at heterojunction InP/p-Si based-solar cells.

Table 2. The electrical characteristics of all the samples.

Thickness (µm)	I_{sc} (mA)	V_{oc} (V)	*FF* (%)	η (%)
5	37.9	0.7528	0.837	23.9
10	37.7	0.7526	0.835	23.7
15	37.4	0.7521	0.835	23.5
20	36.9	0.7517	0.829	23.0
25	36.3	0.7511	0.825	22.5
30	35.6	0.7505	0.823	22.0

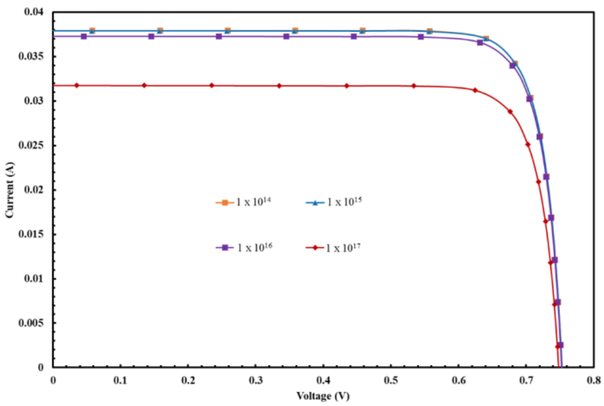

Fig. 3. The results of the influence of doping concentration on the InP substrate.

Table 3. The electrical characteristics of InP layers with different dopant concentrations.

Dopant (cm^{-3})	I_{sc} (mA)	V_{oc} (V)	*FF* (%)	η (%)
10^{14}	37.9	0.7529	0.837	23.9
10^{15}	37.7	0.7531	0.841	23.9
10^{16}	37.3	0.7532	0.836	23.5
10^{17}	31.8	0.7483	0.832	19.8

The optimal efficiency of the heterojunction InP/p-Si solar cell, achieved with an n-region doping concentration of 1×10^{15} cm^{-3}, included the following parameters: efficiency of 23.9%, V_{oc}=0.7531V, I_{sc}= 0.3777A, P_{max}=0.239W, and *FF*= 0.841. Similarly, the highest efficiency of 23.9% was attained with the thinnest n-region layer (5µm), resulting in V_{oc}= 0.7528V, I_{sc}= 0.379 A, P_{max}= 0.0239 W, and *FF*= 0.837. Figure 4 illustrates the PV and IV characteristics, demonstrating the highest efficiency achieved by varying the doping concentration and the thickness of the indium phosphide layer. These results indicate that InP/p-Si solar cells can achieve higher efficiency under these optimal conditions.

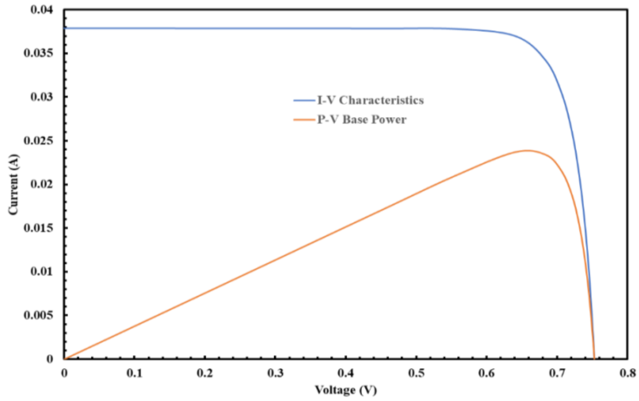

Fig. 4. Graph of IV and PV curves.

Fig. 5 shows the reflection of heterojunction InP/Si layers in the wavelength range of 300-1200 nm. Between 450 and 700 nm wavelengths, 50 nm InP sample showed the lowest reflection compared with all the other samples. Additionally, for wavelengths between 700 and 1200 nm, 50 nm and 100 nm InP layer were lower reflection characteristics compared than the 3000 nm InP layer. However, the reflection characteristic of the 10 nm InP layer being higher than the 3000 nm layer remained unpredictable. Advanced physics models are required to accurately simulate reflections from specimens with layer thicknesses below 50 nm. It is well-established that a thinner n-layer and a thinner overall wafer can lead to higher open-circuit voltage (V_{oc}) due to a reduction in bulk recombination, which is often more pronounced in thicker wafers. The lower thickness enhances the collection efficiency of photo-generated electron-hole pairs, as it reduces the distance for carrier diffusion, allowing for more effective extraction at the electrodes. Additionally, thinner wafers exhibit a higher carrier lifetime and reduced Auger recombination, further contributing to an increase in V_{oc} [26-28].

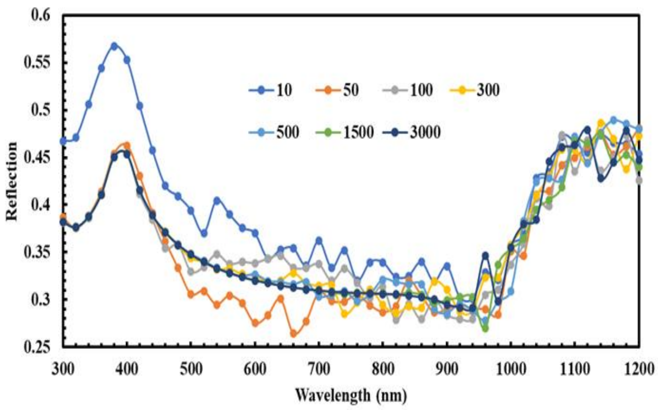

Fig. 5. Reflection vs wavelength of all the samples

Similarly, Figure 6 illustrates the absorption spectra all the samples over the wavelength range of 300–1200 nm. The trends showed the absorption values decreased with the increase of InP layer thickness around the 300 to 920 nm wavelengths. The results from Figure 6 were consistent with those from Figure 2, where the decrease in

InP layer thickness led to an increase in absorption, which, in turn, resulted in higher current due to more photons being absorbed and more excess electron carriers being produced. At a longer wavelength, i.e., 920 nm, the absorption of all the InP layers decreased drastically due to the wafer's low absorption of light at wavelengths above ~900 nm [29]. Meanwhile, Figure 7 represents the transmission spectra for heterojunction InP/Si layers. It is clearly observed from this figure that all the specimens have almost the same the transmission behaviours over the 800-1200 nm wavelength. Incident light with longer wavelengths had a lower absorption coefficient in solar cells, meaning that the photon energy was less efficiently absorbed within the material. As a result, a longer-wavelength light required a greater path length to be fully absorbed, as the probability of photon absorption decreased with increasing wavelength. This phenomenon is governed by the material's band gap and the nature of the absorption spectrum, which dictates that photons with lower energy (longer wavelength) are absorbed less efficiently.

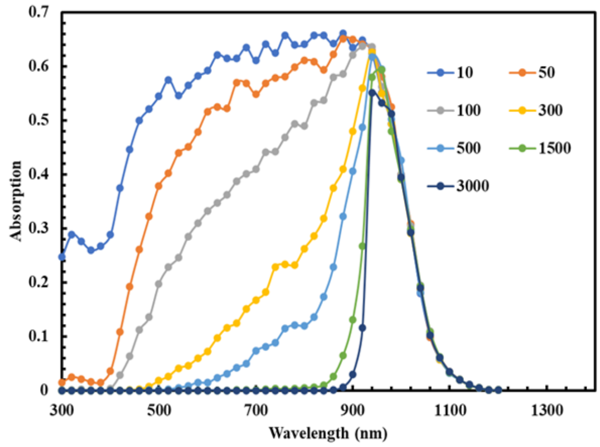

Fig. 6. Absorption vs wavelength of all the samples.

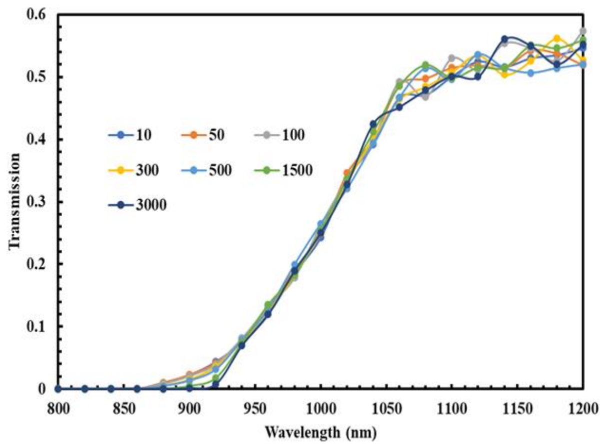

Fig. 7. Transmission vs wavelength of all the samples.

The overall trend showed that InP layer thickness played an important role in reducing the optical losses in the solar cell and increasing the path length of the incident light within the solar structure, which increased the amount of light absorption in the p-Si absorber layer. A large portion of the radiation was absorbed by the specimen top surface. By thinning the top layer, a large fraction of the charge carriers produced by the incoming light was created within a diffusion length of the *p-n* junction. It was noticeable that this light could traverse the wafer multiple times until it generated free carriers unless it was coupled out again at an interface. The latter meant that a thicker silicon wafer was able to absorb more long wavelength light compared to a thinner one. However, a thicker wafer also led to higher bulk recombination rates.

The substrate's interfaces and optical characteristics are key to allowing multiple indecent light passes through the boundary, and the light confinement process occurs within the interlayer. Surface texturing and anti-reflective coating (ARC) are typical methods to enhance light trapping amount inside the substrate. Random pyramids or periodic holes are examples of surface texturing on the top of substrate surface to significantly boost light trapping by increasing the light path around the sample, reducing reflections and improving light absorption [30, 31]. Another process to reduce reflection and maximize light absorption is by applying ARC on the top surface of the sample, which can improve the external quantum efficiency and conversion efficiency [32]. The other alternative methods that can be used to maximize light absorption are by using plasmonic structures, intermediate reflectors and back reflectors. In future work, the implementation of MgF_2 and SiO_2 ARC thin films will be our focus to enhance the performance of heterojunction InP/Si based-solar cell due to the improvement of transmission spectra [33].

4. Conclusions

Using PC1D simulation software, this study thoroughly examined the performance of InP/p-Si solar cells, focusing on the impacts of doping concentration and n-region thickness. The optimal efficiency of 23.9% was achieved with a doping concentration of 1×10^{15} cm^{-31} and n-region thickness of 5μm. Increasing the thickness of the InP layer beyond 5μm or the doping concentration beyond 1×10^{15} cm^{-3} resulted in reduced efficiency due to elevated recombination losses. The study highlights the importance of balancing both the thickness and doping concentration to achieve an effective trade-off between the I_{sc} and V_{oc}, minimizing recombination losses, and maximizing overall efficiency. Fine-tuning these parameters is essential for improving the performance of InP/p-Si solar cells. These findings provide valuable insights into the design and optimization of high-efficiency solar cells, contributing to advancements in renewable energy technology. Future research could focus on exploring cutting-edge materials, such as metal III-nitrides, and enhancing surface characteristics to further boost solar cell performance.

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Conflicts of Interest

The authors declare no conflicts of interest.

Authors Contribution Statement

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Data analysis and interpretation: N.A.S. Mohamed Azman, M.Y. Bermakai

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