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RESEARCH ARTICLE

# MODELING METAL NANOPARTICLES INFLUENCE TO PROPERTIES OF SILICON SOLAR CELLS

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## Abstract

Nanotechnologies are entering every field. Nanoparticles have been widely used in medicine and technology. We decided to study the behavior of nanoparticles under the influence of light and its effects on solar cells, based on a number of properties. How gold and silver nanoparticles are introduced into the optical layer of the solar cell has been studied enough to affect the properties of the solar cell. However, the effect of silicon-based solar cell metal nanoparticles in the n domain on the solar cell has not been sufficiently studied. In addition, in this study, the properties of solar cells, which included nanoparticles of various shapes, were modeled. Since the end of the last century, new methods of modeling have been introduced into scientific research. A lot of modeling software has been developed. They are based on a numerical method. Synopsys program of Sentaurus TCAD software package was used in the modeling to ensure the accuracy and reliability of the research. Using Sentaurus TCAD, a model of a silicon-based solar cell with simple and various shapes of platinum nanoparticles embedded in the n field was developed. The focus is on determining the effect of the shape of a nanoparticle introduced on solar cells on its properties. The effect of nanoparticles on the optical and I-V characteristics of a solar cell is also analyzed in depth.



## Introduction:-

The need for renewable energy sources is leading to more research in this area. Renewable energy sources account for 17% of the world's electricity generation. Renewable energy sources include wind, solar, biomass and geothermal energy (1).

Prospective work is underway on the use of solar energy. In the twentieth century, the efficiency of solar cells was 10%, but today it is 30% (2). One of the important tasks facing scientists is to further increase the efficiency of the solar cell and the invention of low-cost solar cells. When the first solar cell was invented, its efficiency was less than 1%. 38% of the light falling on the solar element is reflection. As a solution to this problem, the surface of the solar cell is covered with anti-reflective layers. However, this allowed the solar cells to absorb more light only in the visible field. However, most of the rays in the infrared field were not absorbed. We know that the main energy of light from the sun is in the infrared. Therefore, the efficiency of the solar cell covered with an anti-reflective layer

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has increased to only 19.6%. Tandem solar elements have been developed to absorb rays in a larger range of light. Their maximum efficiency is over 30% (3). But the technology of their production is complex and expensive. Most of the solar cells currently in production are silicon-based.Because silicon is one of the most common and inexpensive elements on the planet. That's why we do our research on silicon. It is preferable to increase the efficiency of silicon-based solar cells.

As the size of an object decreases, its properties change completely. Particles in nanometers are called nanoparticles. Nanoparticles are being used extensively in many fields. The nanoplasmonic effect occurs when electromagnetic waves are applied to nanoparticles (4-5). Nanoplasmonics is the process of emitting electromagnetic waves and emitting free electrons when nanoparticles are irradiated (6-7). Solar cells have a method of inserting nanoparticles, nanoparticles are inserted only on the surface of the solar cell, i.e. in the optical layer. In our study, we set ourselves the task of how a nanoparticle affects the properties of a solar cell when it is introduced into the n domain. Also, does the size of the nanoparticle matter? We used modeling to answer these questions.

Modeling is a big part of science today.Ensures the effectiveness of research. One of the programs used in the study of solar cells is PC1D (Personal Computer One Dimesional) (8-13). In addition, the Matlab / Simulink program, which is widely used in mathematical modeling, contains codes for modeling solar cells (14-16). TCAD (technology Computer Aided Design) software is used in 2D and 3D modeling. Silvaco-Atlas and Synopsys' Sentaurus TCAD software package are used to model semiconductor devices. There is little complexity in using these programs (17-23).Because they are managed via TCL (Tool Command Language). That is, we write code to create each model. However, it contains a high degree of reliability and accuracy of the values obtained, as well as many physical models of semiconductors. The Comsol Multiphysics program, which is used in engineering, also created a library of semiconductor theory in 2018 and made it possible to model solar elements.

## Method:-

The Sentaurus TCAD software package was used to develop the model. Sentaurus has 17 main tools and 7 additional tools. Basically, 4 tools were used for modeling. These are Sentaurus Structure Editor (SDE), Sentaurus Device (SDevice), Sentaurus Visual (SVisual) and Sentaurus Workbench (SWB).

The 2018.06 version of the Sentaurus TCAD provides the ability to model solar cells and provides a number of examples to study. However, MatPar used an additional tool to model solar cells in the samples. We didn't use any additional tools to create our model.Because we tried to study not only the physics side of the research, but also the programming side.

### Geometric model:

SDE was used to develop the geometric model. We developed a 2D model to make it easier to calculate and to obey the law of symmetry. First, we make all the layers of the solar cell into rectangles. And we also publish material types. All dimensions were multiplied by the nanoparticle size. Top and bottom contacts are provided. We know that modeling is based on numerical methods. So we compiled the whole geometric model for the calculation. The p-n junction, the contact areas, and the nanoparticle embedded areas are made smaller in grid size. This is mainly because the main events take place in those places. We can scale all the fields to the same size, but it takes a lot of time to calculate. Nanoparticles were obtained in 3 different forms. Circle, square and triangle.Two of these shapes were created in a standard style, and a triangle was created by coordinating through a polygon. A while loop was used to generate each nanoparticle without repeatedly writing code. All the nanoparticles were introduced into the n field in a series. We can see the geometric model developed from SDE (Fig. 1). The size and material types of each of its layers can be found in Table 1.

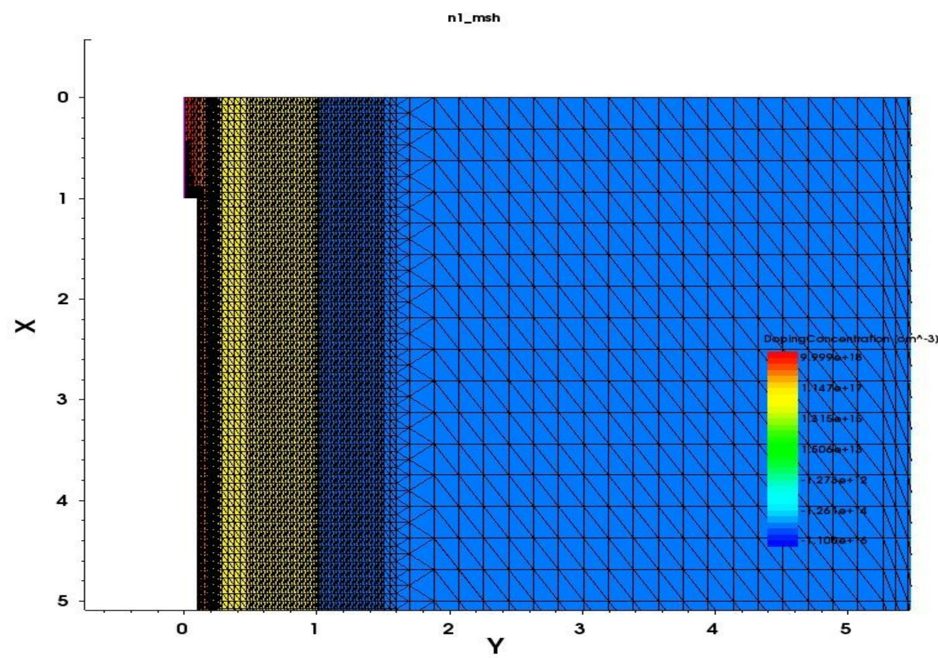


**Figure 1:-** Geometry model of silicon solar cell which is created by Sentaurus Structure Editor.

**Table 1:-** Parameters of a geometric model of a solar cell with a nanopartic.

| Layers | Material | Thickness | Width | Doping | Doping concentration |
|---|---|---|---|---|---|
| **Front contact side** | Monocrystalline silicon | 0.5d | 0.2 mkm | Phosphorus | 1e19 |
| **Optic layer** | $SiO_2$ | 2d | 1.8 mkm | - | - |
| **n++ domain** | Monocrystalline silicon | 3d | 2 mkm | Phosphorus | 1e18 |
| **n domain** | Monocrystalline silicon | 5d | 2mkm | Phosphorus | 1e17 |
| **Nanoparticles** | Platinum | d | d | - | - |
| **P domain** | Monocrystalline silicon | 37d | 2 mkm | Bohr | 1e15 |
| **P++ domain** | Monocrystalline silicon | 3d | 2 mkm | Bohr | 1e16 |

**Physical model:**

The geometric model made using Sdevice is given physical properties. Sdevice consists of File, Contact, Physics, Plot, Math and Solve parts. In the File section, the path of the files needed to calculate the physical properties of the solar element, such as the test generated file, the parameter file, the light source database file, and so on, is attached to the variable and directed to the Sdevice. In the Contact section, the voltage, current, types of materials and resistances applied to the anodes and cathodes formed in the geometric model are given. The Physics section comes in four different forms. It is divided according to the physical properties that apply only to the material, only to the area, only to the surface, and to the whole model. The Math section controls mathematical calculations, such as maximum error, number of cycles, and so on. In the solve part, mainly the Poisson equation is solved for electrons and cavities. There are basically two ways to do this. The first depends on the time, and the second depends on the change of a certain parameter. In the modeling of solar cells, we calculate mainly due to the change in voltage. The results are then output to a file. The parameters to be visualized are announced in the plot section.

We know that there are several models of each physical process. The great thing about Sentaurus TCAD is that there is a non-binding model of every physical process, and it works even if we don't publish any physical model for this process in the Physics section. We only choose physical models based on the device we are developing.

Because solar cells are optical and p-n diode devices, they have both optical and electrical phenomena. Since we have developed a 2d model, we will first give the value of the Areafactor. Then we introduce recombination models, depending on the type of solar cell. In our model, we included SRH, Auger,Radiative recombination because the solar cell is made of single crystal silicon. If we want to change the temperature of the solar cell, it is changed by assigning the desired value to the Temperature variable. If we do not change the temperature, it will normally take on a value of 300 K. The Transfer Matrix Method (TMM) was used to determine the optical properties of the solar cell. The solar element is given the polarity of the light incident through the optics, the coordinates of the incident surface, and the angle of incidence. In the process of modeling each device, it is important to choose the right physical models.

**Theory:**

The silicon-based solar cell absorbs most of the light in the visible field. This is because the band gap of silicon is 1.12 eV. There are two different theories of light, wave and particle theory. We use the wave theory of light to study the phenomena of refraction and refraction of light. The transfer matrix method is also based on the wave theories of light and Fresnel laws. It has no complexity. Only a combination is created by applying Burger's law and Fresnel's law to the layers. The absorption of light is analyzed directly by particle theory. If the energy of the photon is greater than the energy of the forbidden zone, then it is absorbed by the electron.

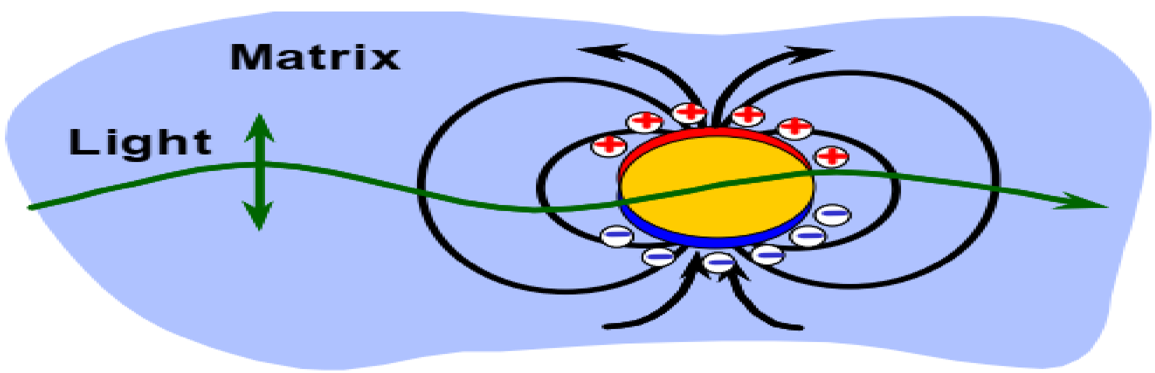


**Figure 2:-** The motion of electrons when a nanoparticle is exposed to light.

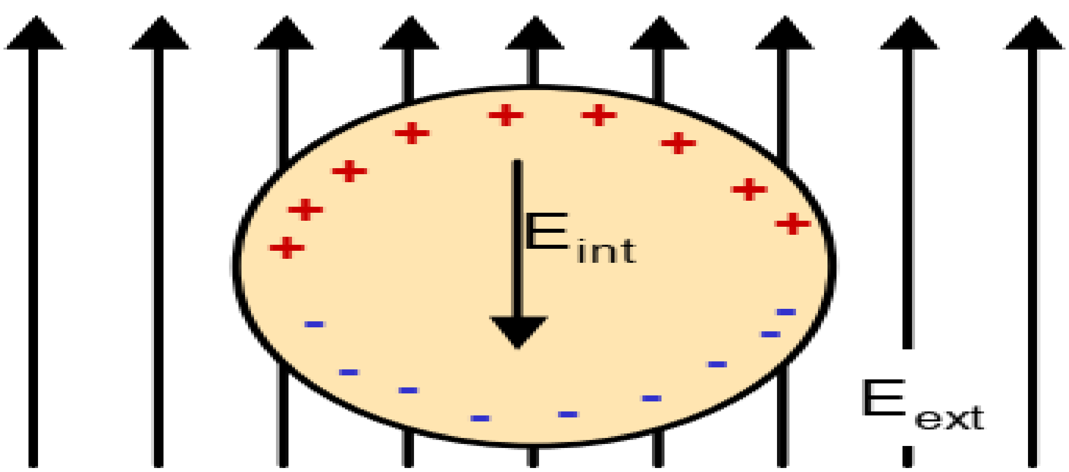


**Figure 3:-**Electrical field formation inside a nanoparticle .$E_{int}$ – internal electric field strength, $E_{ext}$ – external electric field strength

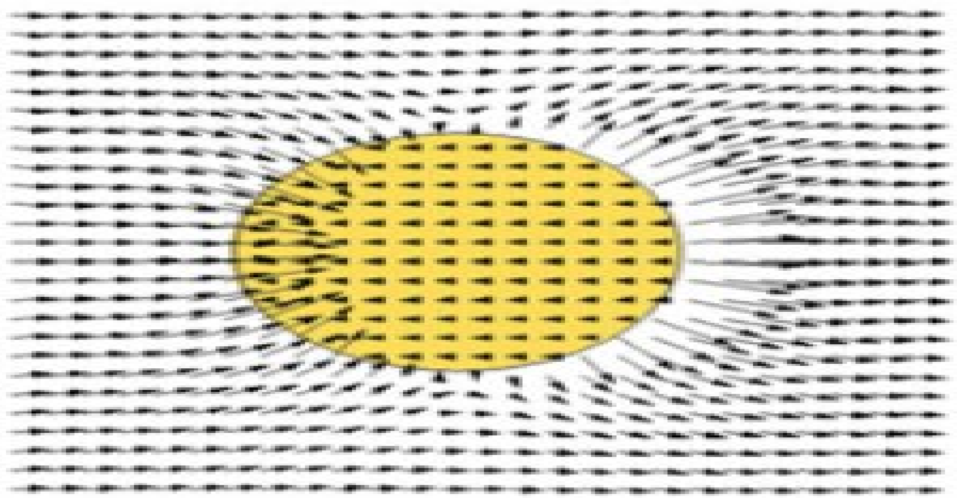

**Figure 4:-** Directions of the electric field around a nanoparticle.

Since the size of a nanoparticle is smaller than the wavelength of light, three different phenomena occur when light falls on it. Because light is an electromagnetic wave, it vibrates the electrons in a nanoparticle (Figure 2). Free electrons are formed on one side and ions on the other. This creates an internal area (Figure 3). The electric field around the nanoparticle changes (Figure 4). This is because of the internal space it contains. The electron vibrates with acceleration as it moves. This causes the nanoparticle to emit electromagnetic waves of a different frequency. Because it is a nanoparticle metal, it absorbs infrared light. If the energy of the photon absorbed by the nanoparticle is greater than the energy of the work done, then the nanoparticle emits electrons.

We use the theory of complex dielectric constant to determine the amount of radiation emitted by a nanoparticle. The amount of light emitted by a nanoparticle is strongly related to the size of the nanoparticle, the relative complex dielectric constant, and the wavelength of the incident light. Relative complex dielectric constant refers to the ratio of the complex dielectric constant of a nanoparticle to the complex dielectric constant of the medium in which it is located.

$C_{sc}(\omega)=k^4(3V)^2((\varepsilon_{r1}-1)^2+\varepsilon_{r2}^2)*((2+\varepsilon_{r1})^2+\varepsilon_{r2}^2)^{-1}*(6\pi)^{-1}$

$V$ – the volume of the nanoparticle

$k$ – wavenumber

$\varepsilon_{r1}$ – real part of relative permittivity of nanoparticles

$\varepsilon_{r2}$ – imaginary part of relative permittivity of nanoparticles

$C_{sc}$ – the ratio of the intensity of an electromagnetic wave emitted by a nanoparticle to the intensity of light incident on a nanoparticle.

Nanoparticles change not only the optical properties of a material, but also its electrical properties. This phenomenon is called nanoplasmonics.

We can think of nanoparticles as a means of converting light wavelengths. We must also note that if we say that the state is ideal, a free electron will appear due to the difference in the energies of the conversion. Ideally, part of the energy is converted into heat energy. That is, part of the light energy incident on the nanoparticle is converted into the vibrational energy of the ions at the node of the nanoparticle crystal lattice and increases the oscillation frequency. This causes the temperature around the nanoparticle to rise.

## Results:-

A simple single-crystal silicon-based solar cell has an increased absorption coefficient in the wavelength range of 360–420 nm. At temperatures greater than 420 nm, it is only reduced. Absorption coefficients decrease monotonically at values greater than 360 nm (Figure 5). Looking at Figure 1, the absorption, return, and transition coefficients are equal at 510 nm of wavelength. The maximum value of absorption is 420 nm and its value is 0.63.

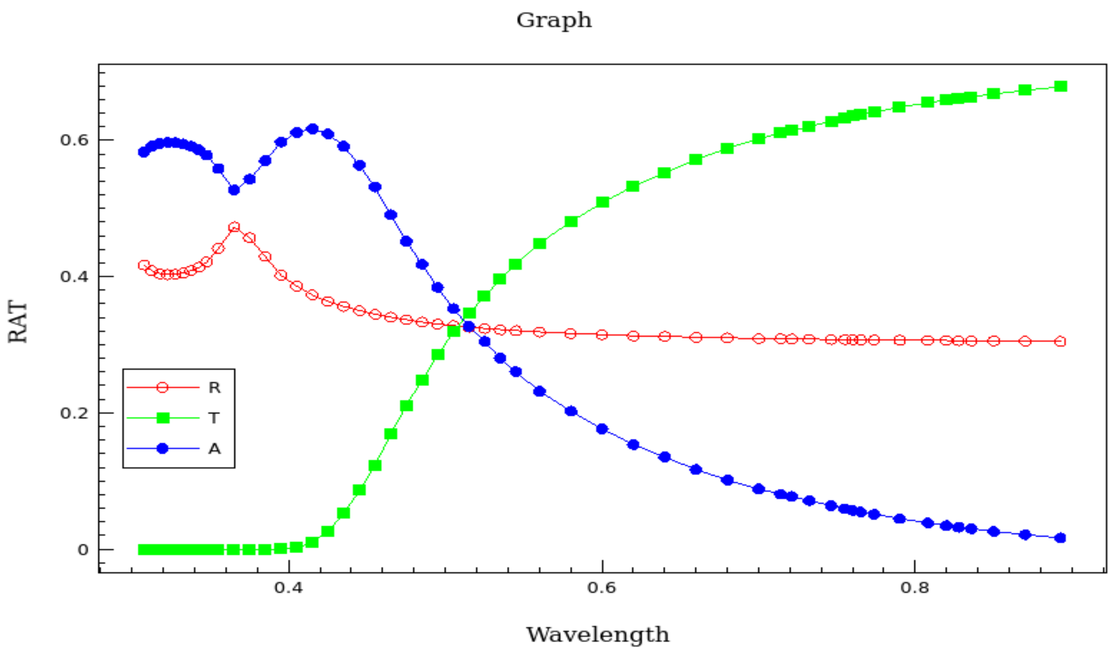


**Figure 5:-** The dependence of the absorption, reflection and transmission coefficients of a non-nanoparticles solar cell on the wavelength of light. R-reflection, A-absorption, T – transmission

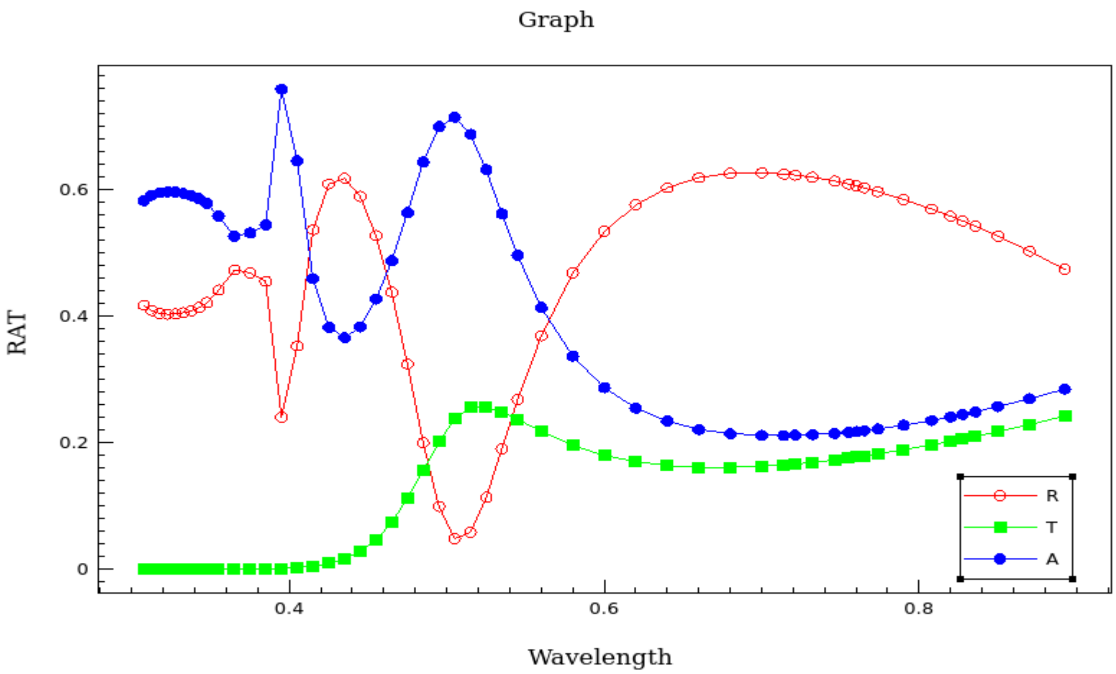


**Figure 6:-** Optical properties of a solar cell embedded in a spherical platinum nanoparticle with a diameter of 15 nm in the field n. R-reflection, A-absorption, T – transmission

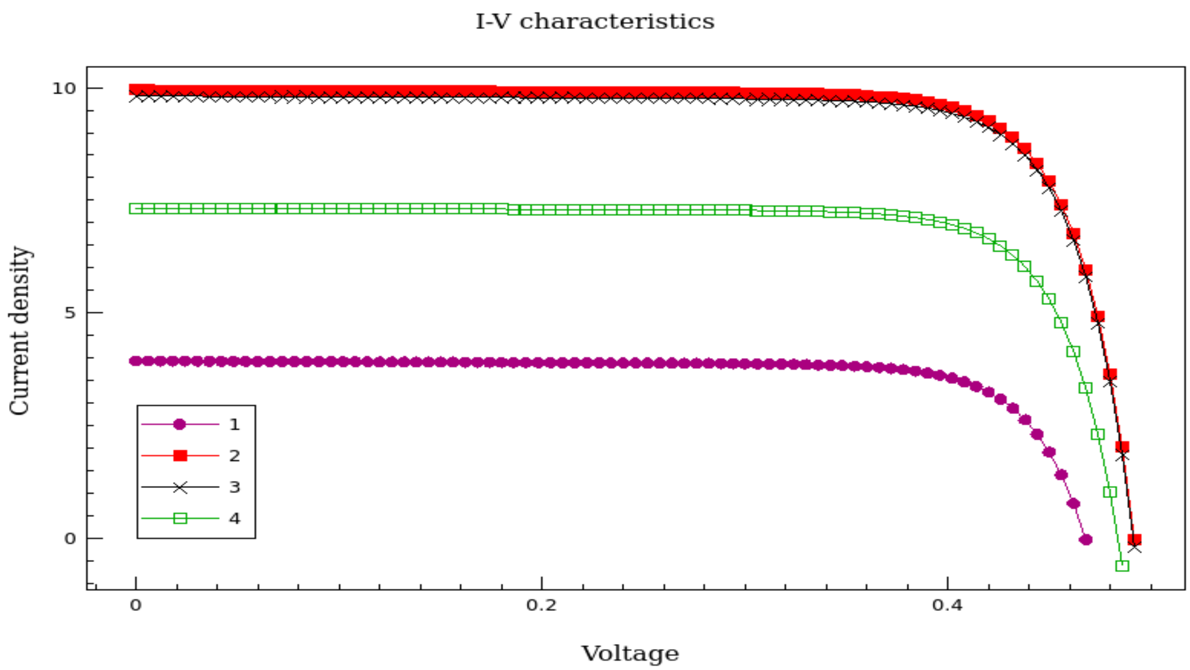


**Figure 7:-** I-V characteristic of a solar cell. 1 – A simple monocrystalline silicon-based solar cell, 2 – monocrystalline silicon-based solar cell embedded in a circular platinum nanoparticle with a diameter of 15 nm, 3 – monocrystalline silicon-based solar cell embedded in a square-shaped platinum nanoparticle with a length of 15 nm, 4 – monocrystalline silicon-based solar cell embedded in a triangular platinum nanoparticle with a side length of 15 nm

**Table 2:-** Basic photoelectric parameters of the solar cell.

| **Shape** | **$U_{oc}$, V** | **$I_{sc}$, mA/sm$^2$** | **$U_{mpp}$, V** | **$I_{mpp}$, mA/sm$^2$** | **$P_{mpp}$, mW/sm$^2$** | **FF** | **$\eta/\eta_0$** |
|---|---|---|---|---|---|---|---|
| **-** | 0.468 | 3.935 | 0.396 | 3.617 | 1.432 | 0.778 | 1 |
| **circle** | 0.492 | 9.948 | 0.42 | 9.262 | 3.89 | 0.795 | 2.72 |
| **square** | 0.492 | 9.81 | 0.42 | 9.12 | 3.83 | 0.793 | 2.7 |
| **triangle** | 0.486 | 7.33 | 0.408 | 6.88 | 2.8 | 0.787 | 1.95 |

When a nanoparticle with a diameter of 15 nm was introduced into the n domain of a solar cell, its optical properties changed significantly. Absorption was also increased in the infrared field. The maximum absorption value rose to 0.72. Absorption increased in some areas and decreased in others, reaching maximum and minimum values. The maximum values of absorption were found at wavelengths of 390 and 510 nm (Figure 6).

The most basic characteristic of a solar cell is the I-V characteristic. In our model, we analyzed a simple solar cell, a solar cell with a spherical nanoparticle, a solar cell with a triangular nanoparticle, and a solar cell with a square nanoparticle. The properties of a nanoparticle also depend on its shape. The efficiency of a solar cell with a circular nanoparticle was 2.72 times greater than the efficiency of a normal solar cell.

The square nanoparticle embedded in the solar cell was 2.7 times higher. However, the efficiency of the solar cell, which included a nanoparticle in the triangle, was 1.95 times higher. The difference between the Salt operating voltages is not very large.

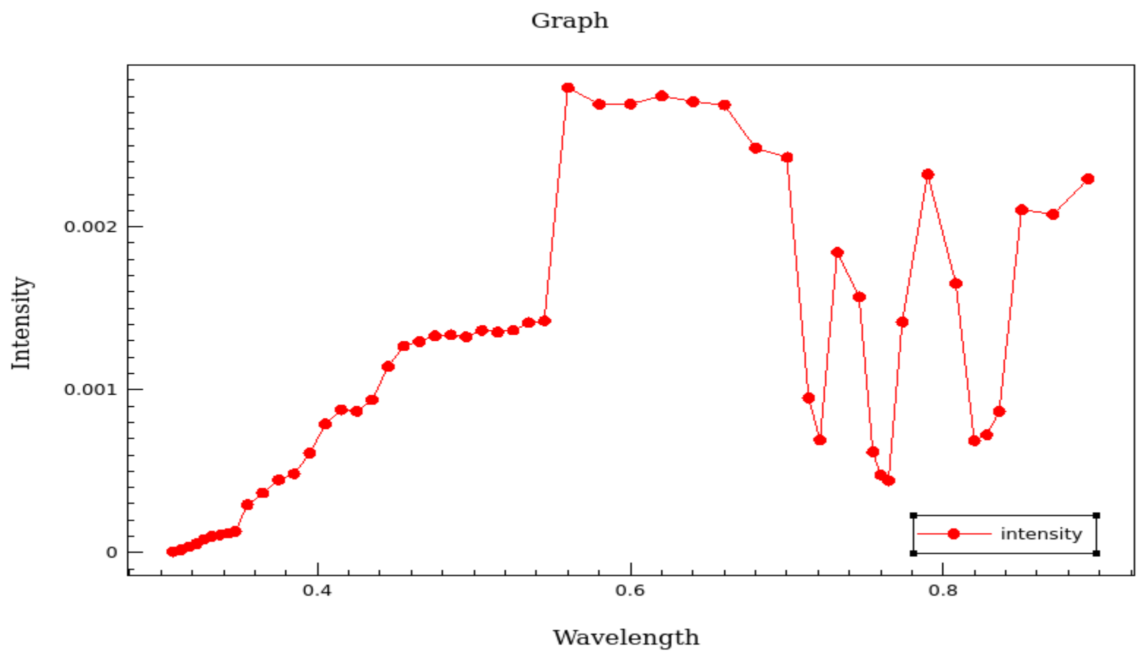


**Figure 8:-** Dependence of light source intensity on wavelength.

## Discussion:-

Each event process is explained by certain laws. The above results can be explained by nanoplasmonics. A nanoparticle introduced into the N field absorbs light and emits an electromagnetic wave in a visible field. The part with the highest intensity of sunlight falls in the range of 500 nm to 700 nm (Figure 8). However, if we pay attention to the optical properties of a simple solar cell (Figure 5), the absorption in the wavelength range from 500 nm to 700 nm decreased from 0.3 to 0.05. The absorption of the solar cell embedded in platinum nanoparticles decreased from 0.7 to 0.2 during this period (Figure 6). If the decrease is ideally linear, the average absorption of a normal solar cell in this range is 0.175, while that of a solar cell embedded in platinum nanoparticles is 0.45. The short-circuit current is directly proportional to the intensity, which means that as the absorption of light in a high-intensity area increases, so does the short-circuit current. Therefore, the short-circuit current of a solar cell with a nanoparticle was higher than that of a normal solar cell (Figure 7).

Nanoparticles of different shapes have led to different results. This is because, as we said in the theory above, the electrons inside a nanoparticle vibrate under the influence of an electromagnetic wave. Let us take two lines whose points of intersection are perpendicular to each other. The circle and the square are symmetrical about both axes. A triangle can be symmetrical about only one. Symmetric means that the concentration of electrons on one side is equal to the concentration of ions on the other side. And electrons vibrate periodically in an electromagnetic field. This causes it to emit electromagnetic waves of the same frequency. Without symmetry, the concentration of electrons and ions will not be equal. Electrons oscillate nonlinearly, and nanoparticles emit electromagnetic waves of different frequencies. Circular and square nanoparticles emit electromagnetic waves in a visible field, and triangles emit electromagnetic waves of different frequencies. Therefore, the efficiency of a solar cell with a circular and square nanoparticle is greater than the efficiency of a solar cell with a triangular nanoparticle.

## Conclusion:-

During the study of solar cells embedded in nanoparticles, I came to the following conclusions.

1. The optical properties of a solar cell embedded in a nanoparticle are better than the optical properties of a normal solar cell.
2. Nanoparticles cannot be introduced into the p field. It is preferable to include the nanoparticle in the n field.
3. The shape of the introduced nanoparticle is also important. The nanoparticles must be symmetrical.
4. We can think of a nanoparticle embedded in a solar cell as a means of converting wavelengths. Because it absorbs light from the infrared field and emits light from the visible field.

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**Disclosure and conflict of interest:**
To the best of our knowledge, the named authors have no conflict of interest, financial or otherwise.

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