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Design of broadband absorber using 2-D materials for thermo-photovoltaic cell application

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ABSTRACT

Present study is done to analyze a nano absorber for thermo-photovoltaic cell application. Optical absorbance of two-dimensional materials is exploited to achieve high absorbance. It is found that few alternating layers of graphene/transition metal dichalcogenide provide high absorbance of electromagnetic wave in visible as well as near infrared region. Four transition metal dichalcogenides are considered and found that most of these provide perfect absorbance for almost full considered wavelength range i.e. 200–1000 nm. Demonstrated results confirm the extended operating region and improved absorbance of the proposed absorber in comparison to the existing absorbers made of different materials. Further, absorber performance is improved by using thin layers of gold and chromium. Simple geometry of the proposed absorber also ensures easy fabrication.

1. Introduction

Absorbers are indeed a very important part of energy harvesting device i.e. solar cell [1]. It also has application in opto-electronics [2] and other fields. For an ideal absorber a very high absorbance must be achieved from approximately 100 to 1500 nm for solar cell application. Solar thermo-photovoltaic (STPV) cell is one of the types of solar cell, which uses absorber as an inseparable part of its structure. In STPV cells optimized absorbance is very important because it collects the solar radiation which further used for electron–hole pair generation. Based on the geometry and structure, solar absorber can be of different types i.e. intrinsic, textured, layered etc. Textured absorbers provide sufficiently optimized absorbance of solar radiation, thus a lot of research is going on this type of absorbers. In 2002, a report submitted by C.E. Kennedy [3], which had the detailed analysis for different solar absorbers. It observed that various researchers are working in this field facing varied problems. Some have issues with high temperature tolerance, some with low absorbance, and others are facing complex material issues. After this detailed report, several research groups start working to improve the performance of absorbers [4–6] to get better radiation collection using metamaterial and other complex material [7]. Although metamaterial absorbers have high absorbance and extended wavelength range than the natural metals, because of their tunability for the impedance matching [5]. But the complex geometry and small feature size of metamaterial requires highly advanced fabrication facilities. Moreover, absorbance of metamaterial absorbers is not smooth which reduces the overall absorbance [5,6]. Two-dimensional (2-D) materials can minimize these problems, due to their high electromagnetic (EM) absorbance properties.

Breakthrough publication on graphene (2-D material) by R. R. Nair et al. in 2008 [8] proved that monolayer graphene with a thickness of 0.35 nm has better absorption i.e. 2.3% in visible region, than any other existing material till then, due to coupling between light and relativistic electrons, associated with quantum electrodynamics. Despite being only one atom thick, graphene is found to absorb a significant fraction of incident light. Moreover, synthesis of graphene is much easier than the fabrication of metamaterial. Afterward various studies are done, theoretically and experimentally by using graphene with the other materials such as metamaterial [4–6]. These absorbers smoothen the absorbance curve but the fluctuations are not removed completely. To enhance the absorbance with high temperature stability and smoothen the absorbance curve, transition metal dichalcogenides (TMDs) can be used. Most interesting TMDs are molybdenum disulfide (MoS_2), molybdenum diselenide ($MoSe_2$), tungsten disulfide (WS_2), and tungsten diselenide (WSe_2), have direct band gap in visible region of EM spectrum [9] and it may absorb 5 to 10% of the incident light for thickness of 0.71 nm, 0.97 nm, 0.81 nm, and 0.76 nm respectively. The most interesting properties of TMDs which utilized here are stability, thinness, high absorption [10,11]. High absorbance of TMD materials

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is because of their thin layer (monolayer) has direct band gap in the visible wavelength region which is absent in bulk form.

In 2011, T. Korn et al. [12] experimentally presented that 2-D TMDs deliver much higher absorption in visible region based on the layer thickness and temperature. This study is done only for MoS_2. It observed that monolayer MoS_2 flakes provide very good photo luminescence at higher temperature which indicates the usefulness of MoS_2 as an STPV cell absorber material. After some time, in 2013, M. Bernardi et al. [10] demonstrated photovoltaic cell using MoS_2 and graphene. It suggested that the band gap of MoS_2 widely depends on the number of layers and thus it can be a good solar absorber. P. Bermel et al. [13] demonstrated experimentally a PhC absorber for STPV cells, but the efficiency was very low due to various losses. In the same year 2013, B. Shin et al. [14] proposed a complex thin film absorber for the improved efficiency of STPV cells up to 8.4%. After that in 2014, A. Lenert et al. [15] demonstrated nanophotonics-based STPV cell for increased efficiency. B. Mukherjee et al. [16] presented a Bragg stack EM absorber providing near to 100% absorbance from 350 to 670 nm wavelength range. In this study MoS_2 and SiO_2 layer set repeated 500 times to get 94.7% absorbance. 106.5 nm thick each SiO_2 layer used which made the proposed structure thick enough. Thus this absorber cannot be said as a nano-absorber and use of SiO_2 made it highly temperature dependent.

It is seen that there are many problems with existing absorbers either for STPV cells or conventional solar cells, such as complex geometry [4], low absorbance [11–16], tough fabrication [4–6] and temperature stability issue etc. Thus, to overcome these shortcomings, an absorber is proposed here with few alternating layers of graphene with different TMDs, to get the broadband absorbance.

This is an analytical study, Lumerical's FDTD simulation software is used to analyze the proposed absorber. FDTD method is used because of its small mesh size which ensures the better analysis of nano sized structures. Material modeling is done using Lorentz model. Upper layer of TMD material ensures the photo luminescence occurrence [12]. A brief synthesis process of 2-D material is also given in this section.

Used 2-D materials can easily be synthesized using chemical vapor deposition (CVD) method. For graphene synthesis copper foil can be used as the substrate in CVD method. Methane (CH_4), diluted hydrogen (H_2) gases are used in CVD chamber with argon (Ar) gas environment for approx 30 min which results the growth of graphene. Then the chamber is cooled at room temperature for the layer stabilization. For TMDs synthesis, CVD is the most popular method for large area growth. Sulfurization (MoS_2, WS_2) or selenization ($MoSe_2$, WSe_2) of MoO_3 or WO_3 is to be done in the presence of Ar–H_2 gases on Si substrate using standard procedure. Detailed synthesis procedure of graphene and TMDs is presented by A. Kumar et al. [17] and R. Lv et al. [18] respectively.

2. Mathematical modeling

All the materials are modeled mathematically using Lorentz Drude model. Following subsections have the details about the material modeling.

2.1. Natural metals (Au and Cr)

Au and Cr are modeled using Drude model. Refractive index (R.I.) of Au is defined as follows,

$$n_m(\lambda) = \sqrt{1 - \frac{\lambda^2 \lambda_c}{\lambda_p^2(\lambda_c + i\lambda)}} \tag{1}$$

where λ_c and λ_p represents the collision wavelength (8.9342×10^{-6} m) and plasma wavelength (1.6826×10^{-7} m) respectively [19]. Dielectric function ($\epsilon(\omega)$) of Cr is modeled using following mathematical relation,

$$\epsilon(\omega) = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\omega_\tau} \tag{2}$$

where ϵ_∞ is dielectric constant for air, $\omega_\tau = 1/\tau$ and $\omega_p = \sqrt{ne^2/(\epsilon_0 m_{eff})}$ are relaxation rate and plasma frequency respectively. ϵ_0 is the permittivity of vacuum, n is carrier concentration, τ relaxation time, and e is electron charge [20].

2.2. Graphene and its dispersion relation

Graphene is a semi transparent very thin layer of graphite. It is very efficient absorber layer because of its high surface to volume ratio, except this its coupling with light also supports high absorbance. For modeling, R.I. of graphene is calculated using following Eq. [9];

$$n(\lambda) = 3.0 + i\frac{C}{3}\lambda \tag{3}$$

where, C is constant i.e. 5.446 μm^{-1}, λ is the wavelength in μm. Through this dispersion relation graphene is modeled for the study.

2.3. TMDs and their dispersion relation

TMDs used in this study are modeled using Kramers–Kronig analysis for dispersion relation [21]. Dielectric constant of TMDs is also complex function of real and imaginary dielectric constant. Imaginary part of the dielectric function i.e. ϵ_2 can directly be obtained from the electronic structure calculation, using the joint total density of states and the optical matrix elements [22]. Since the imaginary part is partly related to the optical absorption, intense absorption attributes direct inter-band transition. Thus, dielectric function used for the material modeling as a function of photon energy E using a superposition of Lorentzian oscillators, is given as,

$$\epsilon(E) = 1 + \sum_{k=1}^{N} \frac{f_f}{E_k^2 - E^2 - iE\gamma_k} \tag{4}$$

where f_k and γ_k are oscillator strength and line width of the oscillator. E_k is the full spectral range. Here spectral range is varied from 1.5 eV to 3 eV for all considered TMDs. This is a combined relation for dielectric function, which can be factorized to get real and imaginary parts individually. Imaginary part (ϵ_2) can be expressed as [23],

$$\epsilon_2(\omega) = \frac{8\prod^2 e^2}{\Omega m^2 \omega^2} \sum_{n}^{unocc} \sum_{n'}^{occ} \int BZ(kn|p_i|kn')(kn'|p_j|kn) \times f_{kn}(1 - f_{kn'})\delta(E_{kn'} - E_{kn} - \hbar\omega)d^3k \tag{5}$$

where m, e, ω, Ω, and p_i are the electron mass, electron charge, EM pulsation, volume of unit cell, and momentum element respectively. f_{kn} is Fermi distribution function which ensures the counting of transition from the filled to the unoccupied states, $\delta(E_{kn'} - E_{kn} - \hbar\omega)$ shows the condition of total energy conservation. Real part (ϵ_1) can be expressed as,

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P\left(\int_0^\infty \frac{\omega'\epsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'\right) \tag{6}$$

where P is principle value of the integral [21].

2.4. Performance parameters

Two performance parameters are decided to evaluate the proposed absorber performance. These are, average absorbance and operating region. Average absorbance is the average of absorbance for all over the considered wavelength range, and operating region is the range where the absorbance is more than 75% for the scale from 0 to 100% [6]. For the systematic study, first the absorbance of individual TMDs and graphene is examined. After observing the absorbance of individual materials, pair of graphene with one TMD is studied. Afterward the base metal and intermediate layer is added for further improvement of absorbance and fabrication point of view. Results and comparison of the proposed absorber with the existing absorbers is done in next section.