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Graphene-sandwiched silicon structures for greatly enhanced unpolarized light absorption

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ABSTRACT

Based on the attenuated total reflection configuration, a multi-layer graphene (MLG) sandwiched silicon structure is proposed for greatly enhancing light absorption over a broad spectral range (1000–2000 nm). At specific incident angles, the electric field in the sandwiched graphene can be simultaneously enhanced for both transverse electric (TE) and transverse magnetic (TM) polarized light. Numerical analysis and finite-difference time-domain simulation demonstrate over 80% and 70% light absorption for TE- and TM-polarized light, respectively. Owing to the unique optical properties of graphene, the absorption of any photon by graphene may give rise to an electron–hole pair. Thus, the greatly enhanced absorption of unpolarized, broadband light may find significant applications in future photovoltaic devices. However, the excess energy carried by the electron–hole pair can dissipate within a sub-picosecond due to the ultra-fast intraband carrier relaxation, which is the challenge for photovoltaic application and will also be discussed.

1. Introduction

Graphene has long been investigated for optoelectronic application due to its extraordinary properties [1,2]. For example, it has an excellent electron mobility of 2×10^5 $cm^2\,V^{-1}\,s^{-1}$ at room temperature [3,4], which makes it a desirable material for nanoelectronics [5]. Graphene has high transparency, and monolayer graphene can absorb $\pi\alpha=2.293\%$ light over a broad spectral range [2]. As a result, it can serve as transparent conducting electrodes in solar cells [1,6,7], or active material in LEDs and photodetectors [8–13]. Graphene is a very strong light absorber considering its single atom thickness. Many novel approaches have been explored to enhance light absorption of graphene. For example, by introducing a microcavity structure integrating with graphene, over 60% light absorption can be achieved [14]. Others also suggest enhanced light absorption by integrating graphene with plasmonic nanostructures [15] or nanoparticles [16]. A recent work suggests monolayer graphene-based photodetector with ultrahigh photoresponsivity relying on band structure engineering [17]. Despite the strong light-matter interaction achieved in previous works, these approaches are either limited by working bandwidth [16,18] or require complicated, time-consuming fabrication processes [14,17].

To overcome this, our group has proposed a simple three-layer structure based on the attenuated total reflection (ATR) method, which experimentally realizes up to 43% light absorption by monolayer graphene over a broad spectral range, from visible (650 nm) to near-infrared (1620 nm) [19]. Multi-layer graphene (MLG) is also under investigation for the same purpose. In our work, we also suggested 93% light absorption by 5-layer graphene based on the same configuration. More recently, a method utilizing graphene-based hyperbolic metamaterial has achieved perfect (100%) light absorption [20]. Unfortunately, both works are restricted to a specific incidence polarization (i.e. the former only works for TE mode and the latter is limited to TM polarization), so it is necessary to develop new approaches.

2. Graphene-sandwiched Si structure and attenuated total reflection

The structure utilized in our previous work was essentially graphene sandwiched in superstrate (BK7 glass) and substrate (index liquid with a slightly smaller index than that of superstrate) [19]. In this work, we replaced the superstrate (n_1) and substrate (n_3) by two types of silicon, e.g. *p*-Si and *n*-Si, with n_1 being slightly larger than n_3. This is the typical case where the superstrate is crystalline Si and the substrate is amorphous Si. As illustrated in Fig. 1(a), although materials are replaced, the working mechanism

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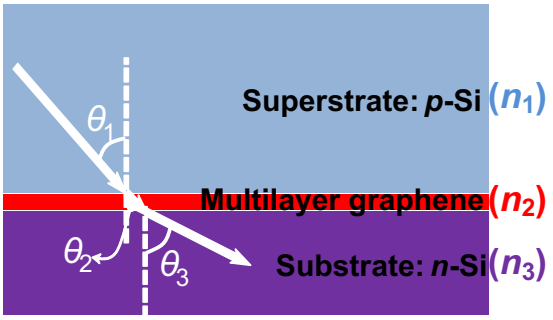

Fig. 1. The illustration of the proposed MLG-sandwiched silicon structure.

is quite analogous: light wave is obliquely incident into the three-layer structure and the corresponding propagation angles to the normal direction are θ_1, θ_2, and θ_3, respectively. According to Snell's law, $n_q \sin\theta_q = n_1 \sin\theta_1$ ($q=2, 3$). Based on the transfer matrix method (TMM) [21], the amplitude reflectance can be calculated by

$$r = \frac{(\tilde{n}_3 - \tilde{n}_2)(\tilde{n}_2 + \tilde{n}_1)e^{+j\tilde{\varphi}_2} + (\tilde{n}_3 + \tilde{n}_2)(\tilde{n}_2 - \tilde{n}_1)e^{-j\tilde{\varphi}_2}}{(\tilde{n}_3 - \tilde{n}_2)(\tilde{n}_2 - \tilde{n}_1)e^{+j\tilde{\varphi}_2} + (\tilde{n}_3 + \tilde{n}_2)(\tilde{n}_2 + \tilde{n}_1)e^{-j\tilde{\varphi}_2}} \quad (1)$$

where $\tilde{\varphi}_2 = n_2 k_0 d \cos\theta_2$ (k_0 is the wavenumber of the light wave in free space; $d \approx N \times 0.335$ nm is the thickness of N-layer graphene). Also, $\tilde{n}_q = n_q \cos\theta_q$ ($q=1, 2, 3$) for TE-polarized light (i.e. electric field is parallel to the three-layer structure), and $\tilde{n}_q = n_q / \cos\theta_q$ ($q=1, 2, 3$) for TM-polarized light [19].

The power reflectance can be calculated by $R=|r|^2$, which is a function of incident angle θ_1. Similarly, we can obtain the power transmittance T. Thus, the absorption $A=1-R-T$. Note that when the incident angle is larger than the critical angle, T will equal zero, so light will be either reflected back or absorbed by graphene. That is why it is called attenuated total reflection (ATR). ATR configuration has been used to measure the graphene absorption spectra [22], analyze terahertz surface plasmons on graphene [23], estimate number of carbon layers in an unknown graphene sample [24], and also, enhance coherent light absorption by graphene [25].

3. Analytical calculation and numerical simulation

In our structure, we assume $n_1=3.5$ and $n_3=3.4$ for all examined wavelengths, and 30-layer graphene with overall thickness of only 10.05 nm is sandwiched between the superstrate and substrate. The surface conductivity of pristine graphene $\sigma_g(\omega, \mu_c, \Gamma, T)$ is a complex number depending on the light angular frequency ω, chemical potential μ_c, charged particle scattering rate Γ and temperature T, however, in a broad range of photon energies, its real part can be universally approximated as $\sigma_g = \pi e/2h = 6.084 \times 10^{-5}$ S, where h is the Planck's constant and e represents the elementary charge [26–28]. Thus, the refractive index of graphene is a complex number and can be calculated by $n_2 = \sqrt{1 + j\sigma_g/\varepsilon_0\omega d}$, where ε_0 is the vacuum permittivity, ω is the angular frequency of the incident light, and d is the graphene thickness. In the previous research, people have found that epitaxially grown MLG exhibits consistency with monolayer graphene in characteristics such as high carrier mobility and infrared transmission [29–31]. Therefore, here we adopt the optical constant of monolayer graphene for calculating our MLG sandwiched structure.

We analytically calculated the reflection and transmission of the proposed structure based on the TMM described in the previous section, and also numerically simulated the structure by the finite-difference time-domain (FDTD) method with mesh size down to 0.1 nm for the MLG. In the numerical simulation, we set the same parameters as in analytical calculation, and also collected the reflection and transmission data. In the analysis and calculation, we spanned the working wavelength from 1000 nm to 2000 nm. Fig. 2 plots the absorption of TE- and TM-polarized light as a function of incident angle θ_1 obtained by the two methods at $\lambda_0=1000$ nm and $\lambda_0=2000$ nm, respectively. As can be seen, analytical and numerical results match quite well. At $\theta_1 \approx 80°$, maximum absorption near 100% can be achieved for TM-polarized light at $\lambda_0=1000$ nm and it drops to about 70% at $\lambda_0=2000$ nm. On the other hand, for TE polarized light, the maximum absorption (at $\theta_1 \approx 76°$) for the two wavelengths keeps above 80%. As a result, absorption of both polarizations of light, or unpolarized light absorption, can be greatly enhanced.

To further investigate the absorption spectral response of the structure, we plot the maximum absorption obtained as a function of wavelength for both TM and TE polarizations, as shown in Fig. 3 (a). According to the figure, the proposed structure (with 30-layer graphene) can absorb over 70% of incident power all the way from $\lambda_0=1000$ nm to $\lambda_0=2000$ nm, regardless of the incidence polarization. Therefore, the structure has a broadband performance. Besides, here we also investigate the influence of the number of graphene layers on the absorption-spectrum response. We can see that the number of layers does not greatly affect the maximum absorption for TE polarization; however, it does make a big difference for TM polarization at larger wavelengths: if large absorption is desired at wavelengths toward the mid-infrared regime, more graphene layers would be necessary. In addition, by comparison, absorption under TM polarization is much more sensitive to wavelength.

As can be seen in Fig. 2, light absorption strongly depends on the incident angle. In order to illustrate what level of absorption can be achieved at a specific angle θ_1, we plot the absorption-wavelength relation for both polarizations at $\theta_1=76°$, 77°, 78° and 79°, respectively (Fig. 3(b)). Note that still 30-layer graphene is applied in the calculation. From the figure, over 80% unpolarized light absorption can only be achieved at $\theta_1=76°$ for shorter wavelengths ($\lambda_0 < 1280$ nm). For high absorption over a large spectrum, $\theta_1=76°$ and $\theta_1=77°$ may be desired incident angles, at which we can see over 64% light absorption anywhere between $\lambda_0=1000$ nm and $\lambda_0=2000$ nm.

The power density distribution of the simulated structure, when the maximum absorption is reached, is shown in Fig. 4, which also includes TE and TM polarizations at $\lambda_0=1000$ nm and $\lambda_0=2000$ nm, respectively. From the figure, most power is confined in the MLG or its vicinity. This has further verified the enhanced light absorption.

For the proposed structure, the incident angles that allow maximum absorption to appear are near the critical angle between the superstrate and the substrate, which are quite large ($>76°$). A larger index contrast between the n_1 and n_3 will make the critical angle smaller. However, this would bring a considerable absorption drop especially for TM-polarized light at longer wavelengths. For example, if the index of the substrate changes to 3.3, ~55% could be achieved for 2000 nm TM-polarized light. On the other hand, for TE mode or TM mode at shorter wavelengths, the maximum absorption decreases very slowly with larger index contrast.

4. Qualitative explanation for the enhanced light absorption

The reason why light absorption can be enhanced for both polarizations can be explained qualitatively as follows. Thirty