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Research paper

Comparative Study of Optical Response of Semiconductors Using FDTD Method

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Abstract

Materials exhibit different properties at nanoscale than at visible-scale due to predominance of quantum effects. For solar cell applications, a nanostructure of particular interest is the nanowire. Free and open-source FDTD (Finite-Difference Time-Domain) software is used to simulate and study optical response of semiconductor materials both in the absence and presence of metal nanowires in 400 nm - 500 nm wavelength range. The results indicate enhancement in optical response of semiconductors in the presence of nanowires. Best enhancement for silicon can be obtained by using combinations of silver and gold nanowires, and this result can be used to improve the efficiency of solar cells.

Keywords: *FDTD; Nanowire; Semiconductor*

1. Introduction

Testing of optical response of materials is a fundamental step in designing solar cells. Experimentation with fabricated samples is a very reliable method for testing, but it poses some obvious challenges, like access to fabrication facilities, cost and availability of materials, imitation of the expected environmental conditions in lab, and controlling experimental errors. An alternative is to simulate the materials to be studied using an effective computational algorithm, that avoids all the above problems, and gives the desired results under the required conditions each time it is executed. The challenges in this case include inherent limitations of the algorithm and the system it is run on, and feeding accurate data to the algorithm for simulating the materials as perfectly as possible. Computational electrodynamics offers various methods for calculating the behaviour of materials in the presence of electromagnetic fields in different conditions, of which the finite-difference time-domain (FDTD) method is one of the most popular methods for simulating electromagnetic phenomena [1]. It has been implemented before and shown to give results that are in good agreement with experimental results [2].

The purpose of this work is to simulate various materials in use today in the photovoltaics industry, and to compare their absorption characteristics, which is an important factor in selection of materials for building solar cells. Nanostrucures made of noble metals have been previously shown to enhance the performance of these materials, by acting as nanoantennas or electrodes that effectively increase the light available for absorption in semiconductors due to their excellent plasmonic and scattering properties [2]-[4]. Absorption in semiconductors in the presence of metal nanowires is simulated. We also study the effect of different metal nanowire combinations on a single semiconductor block.

2. Computational Modelling

Meep, a free and open-source FDTD software package for simulating electromagnetic systems, is used to model the semiconductors and metal nanowires [5]. In FDTD method, Maxwell's equations are solved by implementing second-order accurate central difference approximations in space and time [1]. In Maxwell's equations, the electric field in a medium is described by specifying the material's relative permittivity, given by ϵ. Material dispersion renders the sole use of frequency-independent real part of ϵ insufficient to model absorption in a material, because polarization does not respond instantaneously to an applied field. This is accounted for, by including the polarization term, $\boldsymbol{P}$, in the electric field equation, so that the electric displacement, $\boldsymbol{D}$, is expressed as $\boldsymbol{D} = \epsilon\boldsymbol{E} + \boldsymbol{P}$. The imaginary part of ϵ for narrow bandwidth is incorporated in Meep through the conductivity term σ_D, chosen such that $\mathrm{Im}(\epsilon) = \mathrm{Re}(\epsilon)\sigma_D/2\pi f$, where f is the frequency of interest [6]. For modelling semiconductors, data for complex relative permittivity is used from various sources [7]-[11]. Lorentz-Drude model from [12] is used for describing metals. The expression for ϵ in Lorentz-Drude model is:

$$\epsilon(\omega) = 1 - \frac{\Omega_p^2}{\omega(\omega - i\Gamma_0)} + \sum_{j=1}^{k} \frac{f_j \omega_p^2}{(\omega_j^2 - \omega^2) + i\omega\Gamma_j},$$

where ω_p is the plasma frequency, k is the number of oscillators with frequency ω_j, strength f_j, and lifetime $1/\Gamma_j$, while $\Omega_p = \sqrt{f_0}\omega_p$, is the plasma frequency associated with free-electron transitions with oscillator strength f_0 and damping constant Γ_0. Values for all these parameters were obtained from [12] and normalized for use in Meep as unitless numbers.

To compare the absorption quantitatively, absorption cross-sections are calculated for each simulation and plotted. Absorption cross-section, σ_a, can be expressed as:

$$\sigma_a = \frac{P_{abs}}{S_{inc}},$$

where P_{abs} is the power absorbed by the material and S_{inc} is the incident power per unit area. The absorption cross-section has units of area.

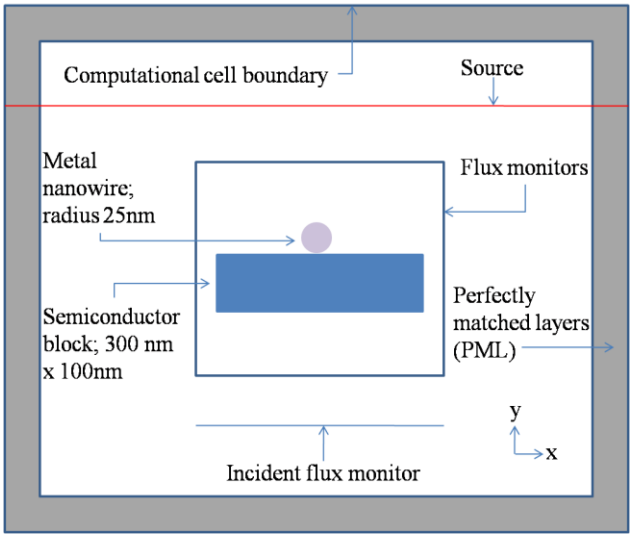

Fig. 1: Schematic diagram of computational cell.

Semiconductor blocks of width 300 nm and thickness 100 nm are simulated. Absorption cross-sections of silicon, germanium, gallium arsenide, and cadmium telluride are obtained. The simulations are repeated for these semiconductor blocks in the presence of Ag, Au, and Cu nanowires of radius 25 nm. The cross-sections are obtained in the two-dimensional x-y plane at z = 0, and the z-axis dimensions for these structures are chosen as infinity, assuming ideally long nanowire and semiconductor block. Fig. 1 shows the schematic diagram for an arrangement of a semiconductor block and a nanowire with a linear source on top, which represents the incoming electromagnetic radiation.

Our analysis of the model performance will be focused for the particular source radiation wavelength range of 400 nm - 500 nm, which is the sun's peak irradiation range as calculated from Wien's Displacement Law.

3. Simulation Results and Discussion

After defining the basic structure within the computational cell, simulations are performed for comparing absorption cross-sections of various semiconductor materials, both in the absence and presence of metals. Simulation results are followed by a discussion on solar cell applications of the simulated materials.

3.1. Absorption in silicon in the presence of metal nanowire

We compute the absorption cross-section of silicon in the presence of Ag, Au, and Cu nanowires.

In the wavelength range of 400 nm - 500 nm, the presence of silver, gold, or copper nanowires (AgNW, AuNW, CuNW) is observed to enhance the absorption cross-section of intrinsic silicon (Fig. 2). Gold and copper nanowires show similar and slightly better enhancement than that by silver nanowire, especially at wavelengths above 440 nm, as can be inferred from Table 1. From Fig. 3, it is observed that scattering cross-section of AgNW is higher than those of both AuNW and CuNW. Good scattering properties are desirable because this increases the light available to semiconductors for absorption.

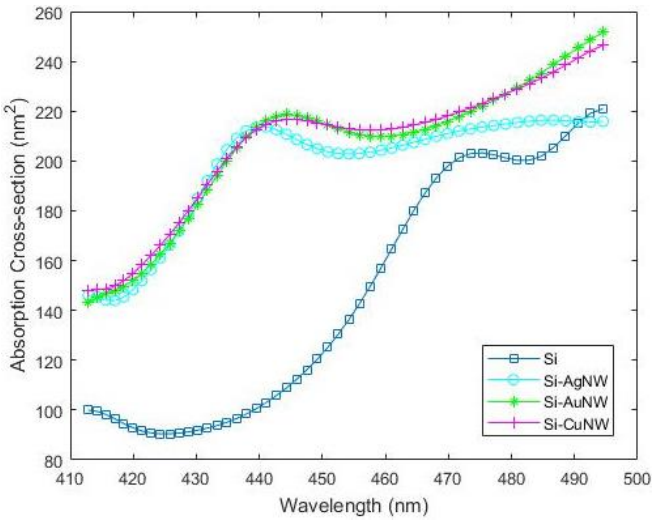

Fig. 2: Absorption cross-section plot of intrinsic silicon, and of silicon in the presence of AgNW, AuNW, and CuNW, respectively.

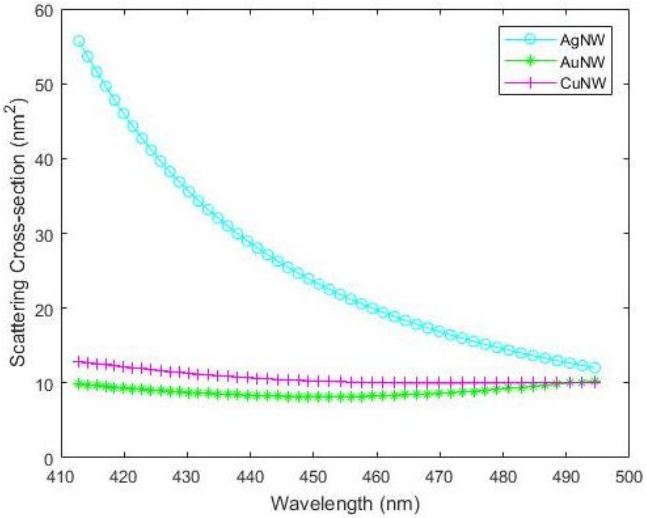

Fig. 3: Scattering cross-section of AgNW, AuNW, and CuNW.

Table 1: Percent improvement in absorption cross-section of Si-AgNW, Si-AuNW, Si-CuNW, compared to Si.

Wavelength (nm)	Percent improvement in absorption cross-section over intrinsic silicon		
	Si-AgNW	Si-AuNW	Si-CuNW
431.8	107.1	102.9	105.5
450.8	62.8	71.4	71.4
475.3	5.1	9.2	9.7

The study of copper nanostructures is a popular subject of research, because not only the performance of copper nanostructures is observed to be comparable to that of noble metals, the manufacturing processes are also simpler because silver and gold are much more inert to reactions.

3.2. Absorption in silicon in the presence of different metal nanowire combinations

We now replace the single nanowire in the computational cell with two nanowires of different metals, with their centres 100 nm apart. Below 430 nm, best absorption cross-section is obtained when both nanowires are silver (Fig. 4). From 430 nm to 460 nm, the gold-copper combination of nanowires performs best. At wavelengths above 460 nm, all combinations show similar performance, more or less.

However, when we replace two nanowires with three, spacing their centres 100 nm apart and varying the number of silver and gold

nanowires, gold is observed to enhance the absorption better at the higher end of the wavelength range under analysis (Fig. 5).

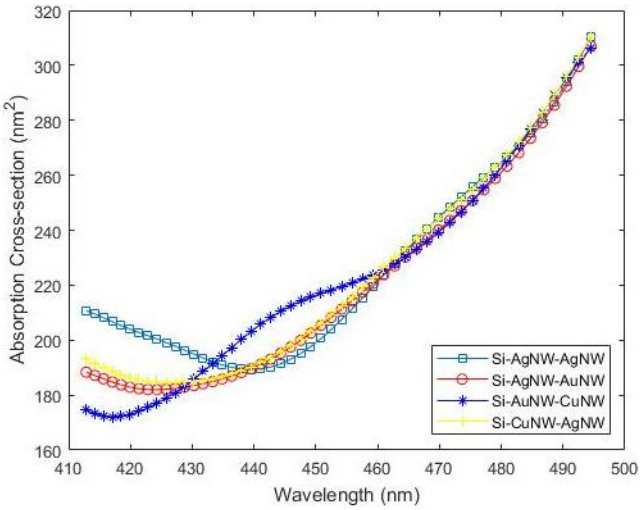

Fig. 4: Absorption cross-section of Si with two nanowire combinations of different metals.

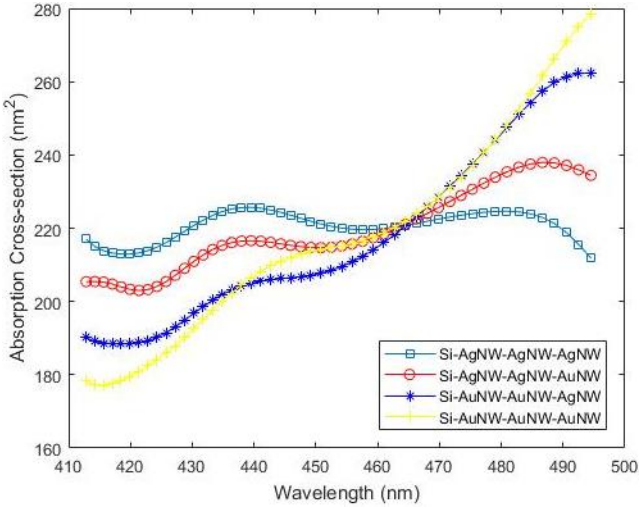

Fig. 5: Absorption cross-section of Si with three nanowire combinations of Ag and Au.

Higher concentration of silver shows better performance at the lower end of the wavelength range. The cooperative plasmonic effect due to dual resonance enhancement of Ag and Au nanowires shows improvement in absorption over a wider bandwidth than that over which either metal enhances absorption separately [13].

3.3. Comparison of absorption in semiconductors: Si, Ge, GaAs, and CdTe

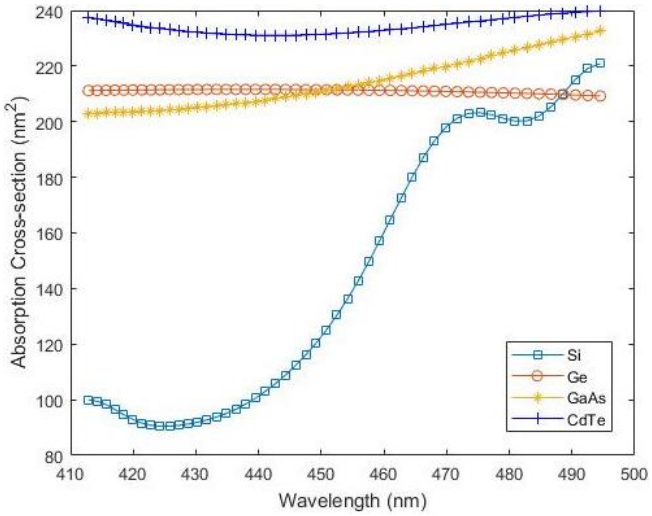

Fig. 6: Absorption cross-section plot of Si, Ge, GaAs, and CdTe.

Fig. 6 shows the absorption cross-section plot of Si, Ge, GaAs, and CdTe. CdTe shows the best absorption characteristics.

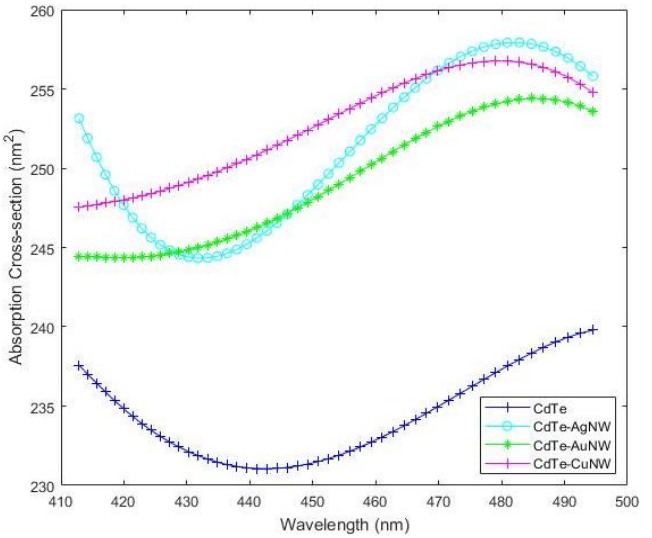

Fig. 7: Absorption cross-section plot of CdTe, and of CdTe in the presence of AgNW, AuNW, and CuNW, respectively.

Table 2: Font Percent improvement in absorption cross-section of CdTe-AgNW, CdTe-AuNW, CdTe-CuNW, compared to CdTe.

Wavelength (nm)	Percent improvement in absorption cross-section over CdTe		
	CdTe-AgNW	CdTe-AuNW	CdTe-CuNW
417.1	5.8	3.6	5.0
450.8	7.6	7.2	9.2
475.3	8.8	7.2	8.6

CdTe photovoltaics represent a significant segment of commercial thin-film module production worldwide, due to improvements in manufacturing processes in terms of feasibility and economy [14]. Though concerns have been raised regarding the impact of cadmium telluride on the environment, a CdTe cell as such is not toxic, and reuse and recycling of such materials is being actively investigated to mitigate potential threats to the environment. GaAs solar cells on Ge substrates have been a commercial product in the space satellite industry, where efficiency, not cost, is the most important factor that influences the choice of solar cells [15].

Fig. 7 shows the improvement in performance observed in a CdTe block in the presence of single metal nanowire. Silver nanowire gives the best enhancement in absorption cross-section at the lower and higher ends of the wavelength range, whereas copper shows the best enhancement over most of the range.

4. Conclusion

Despite the availability of more suitable materials for solar cell applications, silicon continues to drive research interest for improvement and modifications to achieve ever higher efficiencies. This is attributed to silicon's abundance, low cost, non-toxicity, high and stable efficiency of silicon solar cells, and comprehensive knowledge and expertise available in the production of silicon based devices [16]. Noble metal nanowires enhance the absorption in a semiconductor. In the 400 nm - 500 nm range, combination of Ag and Au nanowires can be used for improving absorption in silicon over a wide bandwidth.

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