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Dielectric gratings for wide-angle, broadband absorption by thin film photovoltaic cells

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Optical management is essential to increase absorption in thin photovoltaic cells. In this article, full electromagnetic simulations show that a back mirror and a one-dimensional front SiC sawtooth grating of ~1 μm dimensions can significantly increase absorption in a thin layer under light concentration. A 50 nm thick GaSb active layer in the described configuration absorbs ~66% of the incident solar photons above the band gap for a concentration equivalent to a numerical aperture NA=1/√2. This absorption represents a ~76% or 26% increase over the same structure but with the grating removed or substituted by an ideal antireflection coating, respectively. © 2010 American Institute of Physics. [doi:10.1063/1.3512898]

Reducing the thickness of the active material in a photovoltaic (PV) cell is a means to reduce fabrication costs and also to improve carrier collection efficiencies. This reduction of active material usually entails a weaker absorption of photons. As high absorption is required to achieve optimal cell efficiencies, optical management of the thin cell is becoming a key issue.

Light absorption in thick, typically Si, PV cells has been widely studied, see Ref. 1 and references therein. Considering absorption in thin layers, different solutions exist in the monochromatic regime, and total absorption is indeed possible using, for example, simple Fabry–Perot structures. To obtain an increase in absorption over the full spectral width and wide angular range of interest in solar applications is considerably more problematic.

Recently, much work has been devoted to the study of submicrometer metallic structures for PV applications. For example, metallic gratings supporting surface plasmons can result in strong absorption for adequate conditions. Randomly distributed particles make efficient light trapping possible, can work as antireflection layers and, when sufficiently large, exhibit a total cross-section mostly determined by the scattering. For thin layers, the effect of waveguide modes on the scattering should be included. While metallic structures are promising, inevitable absorption in the metal instead of in the active layer constitutes a fundamental challenge when attempting to reach full absorption in the latter. For example, it has recently been discussed how dielectric particles can outperform metallic ones.

Hence, dielectric gratings and photonic crystals that can excite resonant modes without introducing significant additional absorption are a promising alternative. Further, solar concentration allows larger achievable efficiencies and can lower costs. For proposed hot-carrier solar cells, the large energy density in the thin active layer should help reducing thermalization speed and increasing the cell efficiency above the limit for a standard one-junction cell. The behavior of the structure changes as the incidence angle is varied, which will affect systems working under light concentration.

In this paper, we demonstrate significantly increased absorption in a thin active layer for PV systems working under solar concentration. We consider a metal back mirror and front sawtooth grating made of SiC together with a thin GaSb layer.

The proposed asymmetric configuration considers a one-dimensional crystalline SiC sawtooth grating. A 900 nm thick and with dielectric constant ε_{SiC} situated directly over a 50 nm thick crystalline GaSb active layer, characterized by ε_{GaSb}. The effect of doping in the latter is not included. A silver substrate with dielectric constant ε_{Ag} serves as a back mirror and completes the structure, which has a period T=1100 nm in the horizontal direction along the x axis. We choose GaSb because of its potential for hot-carrier solar cells but it should be possible to apply similar structures to other, more common, semiconductors. The dielectric grating is made of crystalline SiC because the large

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refractive index \( n_{\text{SiC}}^i = \text{Re}(\sqrt{n_{\text{SiC}}}) \) (and low extinction coefficient \( n_{\text{SiC}}^s = \text{Im}(\sqrt{n_{\text{SiC}}}) \)) seemed favorable. We use the values for the 6H–SiC form and, for simplicity, ignore the slight anisotropy and consider the ordinary component. All dielectric constants used are bulk values.

The incident light after concentration is described by an incoherent superposition of plane waves of wavelength \( \lambda \), azimuthal \( \phi \) and polar \( \theta \) angles of incidence (Fig. 1), and both \( p \) (TM) and \( s \) (TE) polarizations. A rigorous coupled wave analysis (RCWA) \(^{27,28} \) code for one-dimensional gratings and conical incidence gives the absorption \( a'(\theta, \phi, \lambda) \) in the GaSb layer for these plane waves; the index \( i = p, s \) refers to \( p \) or \( s \) polarization and values are normalized so that \( a'(\theta, \phi, \lambda) = 1 \) for full absorption. To be able to account for the sawtooth shape of the grating, we always decompose it into ten layers of identical thickness, each uniform along the direction \( z \) normal to the substrate. To reach convergence, we typically calculate the absorption for \( \lambda, \theta, \phi \) steps equal or smaller than 20 nm, 3°, and \( \sim 13° \), respectively. We define the average proportion of photons absorbed in the GaSb layer \( \beta(\text{NA}) \) as a function of the concentrator numerical aperture, NA, by computing

\[
\beta(\text{NA}) = \frac{\int_{\lambda_1}^{\lambda_2} \int_{0}^{\Omega} d^4 \Omega a'(\theta, \phi, \lambda) \frac{dN_p}{d\lambda d\Omega}}{\int_{\lambda_1}^{\lambda_2} \int_{0}^{\Omega} \frac{dN_p}{d\lambda d\Omega} d\lambda d\Omega},
\]

The integral over \( \lambda \) extends from the shorter wavelengths of the solar spectrum \( \lambda_1 = 280 \) nm up to the region of the GaSb gap \( \lambda_2 = 1800 \) nm, while the solid angle \( \Omega \) takes values over \( \phi = [0, 2\pi] \), \( \theta = [0, \arcsin(\text{NA})] \). Finally \( dN_p/d\lambda d\Omega(\lambda) \) is the isotropic and unpolarized solar AM=1.5 (Ref. 29) photon density per solid angle and wavelength of the concentrated solar illumination.

To be able to assess the performance of the proposed structure, it is important to compare it with reference configurations. For a simple 50 nm GaSb layer over a silver substrate, without any further structure, we obtain \( \beta(1/\sqrt{2}) \approx 0.375 \). Adding to this simple configuration a 40 nm thick SiC layer over the GaSb as a simple antireflection layer, we find \( \beta(1/\sqrt{2}) \approx 0.445 \). Last, \( \beta(1/\sqrt{2}) \approx 0.525 \) after substituting this SiC layer by an idealized perfect antireflection coating that varies only along \( z \), perfect in the sense that it is lossless and serves to avoid any reflection (except at the GaSb–Ag interface).

Figure 2 demonstrates the large absorption under concentration for the proposed configuration (Fig. 1), which is only weakly dependent on polarization and numerical aperture. The obtained \( \beta(1/\sqrt{2}) \approx 0.66 \) value is \( \sim 76\% \) larger than in the simple case with only the GaSb layer and the Ag substrate. It is also significantly larger (\( \sim 26\% \)) than for the perfect antireflection coating.

The proposed dielectric periodic structure can be beneficial for solar applications both as an antireflection mechanism \(^{22,24,36} \) and as a path to excite resonant modes. \(^{12,231} \) An unambiguous separation of both effects is difficult and not even necessarily possible. It seems nonetheless clear that the antireflection mechanism cannot account alone for the obtained results, since the absorption in the thin GaSb layer is more efficient for the thick grating structure than for the ideal antireflection coating. We thus consider the existence of resonant modes \(^{32} \) to be critical to explain the large absorption. To better understand the behavior of the proposed system, we show in Fig. 3(a) how the absorption \( a'(\theta, 0, \lambda) \) in the GaSb layer varies with the angle \( \theta \) and the wavelength, for \( p \) polarizations and \( \phi = 0 \). Significant absorption is indeed

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**FIG. 2.** (Color online) Average absorption in the GaSb layer for the proposed structure as a function of numerical aperture, according to Eq. (1), for both \( p \) \( (\beta(\text{NA})) \) and \( s \) \( (\beta(\text{NA})) \) polarizations and after averaging both polarizations \([\beta(\text{NA})]\).

**FIG. 3.** (Color online) (a) Fraction of the incident power absorbed in the GaSb layer of the proposed structure as a function of wavelength \( \lambda \) and angle \( \theta \) for \( \phi = 0 \) and \( p \)-polarization \( a'(\theta, 0, \lambda) \). (b) Same quantity for a thinner SiC grating (100 nm).

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achieved for a large spectral range as far as \( |\theta| \) is not close to 90\(^\circ\). The absorption decreases at large wavelengths due to the strongly diminishing GaSb extinction coefficient \( n_{\text{GaSb}} = Im(\sqrt{\varepsilon_{\text{GaSb}}}) \) near the gap.

The excitation of the modes results in enhanced localized fields in the structure and therefore in an enhanced absorption in the film. The modes are characterized by a dispersion relationship that appears as absorption maxima along lines in the \((\lambda, \theta)\) plane in Fig. 3(a). The pattern of overlapping multiple lines illustrates how the periodic structure supports the excitation of a large number of modes that allows to cover most of the spectrum over a broad range of angles. For the proposed geometry, the large density of modes cannot be explained by only considering the very thin GaSb layer.\(^2\) We must take into account the modes of the full structure, including the thick grating. We discuss the field distribution in the supplementary information (Ref. 33). To illustrate and further emphasize the importance of the grating thickness, we show in Fig. 3(b) the absorption when using a thinner SiC grating. It is seen that the number of lines is reduced so that the absorption is significantly less efficient for many different illumination conditions.

The relatively simple structure described in this article makes it promising for experimental fabrication. With respect to the grating, this paper only considers crystalline SiC but amorphous SiC may be an interesting alternative as long as the absorption in this material is kept sufficiently low. In addition, if a perfect sawtooth grating is too challenging or expensive to fabricate, two-layer asymmetric gratings may serve as an alternative for which we still found significant absorption \( \beta(1/\sqrt{2}) \sim 0.6 \). Finally, for a solar cell the silver substrate serves as a convenient back contact but the lack of front contacts in the described structure needs to be addressed. The most direct approach is to substitute the grating at certain areas by metal digits sufficiently sparse to affect the optical behavior only weakly. A promising alternative is to include conducting wires into the periodic structure itself.

In conclusion, we have designed a structure that exhibits a high optical absorption over a large wavelength and angular range for PV applications. \(~66\%\) of the solar spectrum photons between 280 and 1800 nm are absorbed under a \( 1/\sqrt{2} \) numerical aperture concentration. While the choice of GaSb as absorbing layer was motivated by its interest for hot electron solar cells, the principles are quite general, and thus this type of structure is promising for other thin PV cell configurations.

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