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Simulation analysis of GaN microdomes with broadband omnidirectional antireflection for concentrator photovoltaics

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Microdome structures are analyzed as surface topology to reduce surface reflection over a broad spectral range and wide light incidence angle for concentrator photovoltaics application. Three dimensional finite difference time domain method was used to accurately calculate the surface reflection and transmission for surface topologies with different feature sizes and aspect ratios. Studies show that the use of GaN microdomes will lead to a significant reduction of the surface reflection over a broad wavelength range and wide incidence angle range. The surface reflection significantly depends on the surface structure feature size and geometrical shape. The design of the GaN microdomes provides flexibility to tune the structure in order to obtain the minimum surface reflection for different designs of concentrator optical systems. The surface reflections of the GaN microdomes are compared with that of the conventional flat surface as well as the one with antireflection coating. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4870714]

I. INTRODUCTION

III-nitride (In, Al, Ga, -N) semiconductors cover a wide spectral range in solar spectrum from ultraviolet to near infrared, which provides a great promise to be used as tandem multi-junction (MJ) cells for the next generation high efficiency concentrator photovoltaics (CPVs). Due to the higher refractive index of III-nitride semiconductors (~2.5) as compared to that of the air, more than 20% of the normal incidence (θ = 0°) light is reflected back into the air. The surface reflectance is even higher when the light incident angle increases. Thus, the incident photon energy loss due to the reflection and scattering at the interface between semiconductor and free space becomes one of the main challenges that limit the total conversion efficiency of solar cells. Current approaches used for surface antireflection include: (1) single layer or multiple layer anti-reflection coatings (ARCs) and (2) sub-wavelength surface topology. Single layer ARC is used for suppression of reflectance for a particular incidence wavelength at normal incidence. The selection of material is challenging due to the specific requirement of the refractive index of ARC. Multiple layer ARCs are used for broadband anti-reflection. However, the trade-off between a larger bandwidth and overall reflectivity still remains a challenge. In addition, the uniformity of the ARCs highly determines the effectiveness of the antireflection, and it is challenging to achieve sustainable and highly uniform multiple layer ARCs. The development of the surface topology was essentially triggered by the requirement of omnidirectional broadband antireflection. However, desirable surface topology for omnidirectional broadband antireflection with low cost and scalable fabrication approach is still challenging.

Recently, the surface texturing has been demonstrated as an effective approach to suppress the surface reflection and thus to enhance device efficiency of solar cells. The reduced surface reflection from the textured surface is due to the modification of the effective refractive index profile between the ambient medium and the bulk material. The studied surface texturing for antireflection in solar cell devices include surface roughness, inverted pyramids texturing, microspheres, nanopillars, nanocones, and photonic crystals. These different surface texturing structures provide different effective refractive index profiles that significantly affect the propagation, reflection, and transmission of electromagnetic fields.

In this study, we propose to form GaN microdomes in the range of sub-micron to micron as a broadband omnidirectional antireflection structure for concentrator solar cells. Simulation studies on the surface reflection and transmission were based on the three-dimensional finite difference time domain (3D-FDTD) method. Comprehensive studies of the dependence of the surface reflection on the geometrical sizes and shapes of the GaN microdomes were performed. The fabrication of the GaN microdomes was based on a low cost and scalable self-assembled approach, which was presented in Ref. 33.

II. III-NITRIDE MICRODOME STRUCTURE

III-nitride microdome structures were analyzed as surface topology with significantly reduced surface reflection to enhance light collection efficiency in III-nitride based solar cell devices. Here, the surface reflection of GaN microdomes with a periodic hexagonally close-packed array was studied and analyzed. The schematic of the 3D microdomes on top of GaN substrate is shown in Fig. 1(a). Specifically, the surface reflection of the following three structures were studied and compared with that of the conventional flat surface: (1) GaN micro-hemispheres [Fig. 1(b)], where the diameter D is two times of the height H (D = 2H); (2) GaN micro-hemispheres

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(D ≠ 2H) [Fig. 1(c)]; and (3) GaN flat surface with ideal antireflection coating [Fig. 1(d)]. In this study, the effect of the size and shape of the GaN microdomes with varied diameter D and height H on the surface reflection was analyzed. The studies of the surface reflection on the microdomes were compared with that of the flat surface as well as flat surface with ideal antireflection coating. Recently, the III-nitride microdomes have also been studied as surface topology for enhancing the light extraction efficiency in both InGaN based visible light-emitting diodes (LEDs) and AlGaN based ultraviolet LEDs.

III. NUMERICAL SIMULATION METHOD

In this study, 3D-FDTD method was utilized to calculate the surface reflectance of the incident light. Plane wave was used as the incident light source for the calculation of the reflection and transmission for the hexagonally close-packed GaN microdomes as compared to that of the conventional GaN with flat surface as well as the GaN flat surface coated with antireflection coating. Surface reflectance and transmission of the plane wave source with P polarization and S polarization were calculated separately. In the calculation, we took into account the material refractive index properties of both the wavelength dependence of the refractive index and material absorption loss. The plane wave source wavelength ranges between 300 nm and 1200 nm, and light incidence angle ranges between 0° and 80°, where light incidence angle of 0° represents the case of normal incidence.

To accommodate the requirement of large computing resources from the 3-D simulation, the simulation region was reduced to a unit cell as shown in Fig. 1(e), where \( a \) represents the center-to-center distance of the close-packed microdomes array. Perfectly matched layers (PML) boundary condition was used in the normal direction (growth direction) to absorb all incident energy. Bloch boundary condition was used at interface of the in-plane directions.

The FDTD calculation utilized the commercial software Lumerical FDTD simulator. The minimum mesh step in the calculation was set as 0.25 nm. The distance between the power source and the top of the microdomes structure was 60% of the microdome height. The simulation area is based on the unit cell of microdome hexagonal close-packed pattern, \( a \times \sqrt{3} a \).

IV. RESULTS AND DISCUSSION

To investigate the effect of the GaN microdome size on the surface reflection, Fig. 2 plots the surface reflection comparison as a function of the light incidence angle for GaN micro-hemispheres with different diameter (D) and the conventional GaN flat surface for both P [Fig. 2(a)] and S [Fig. 2(b)] polarizations. The incident light wavelength is fixed at 500 nm. Note that the 500 nm wavelength represents the wavelength region with the highest irradiance power in the solar spectrum, and thus the optimization of the antireflection based on this wavelength is representative and useful for solar cell application. The surface reflectance of GaN micro-hemispheres with diameters (D) of 100 nm, 200 nm, 300 nm, 500 nm, 750 nm, and 1000 nm was calculated. From the simulation results, the surface reflection strongly depends on the size of the micro-hemispheres. The reflection of the incident light increases with the increase of the diameter of the micro-hemispheres.

![FIG. 1. Schematics of (a) 3D hexagonally close-packed GaN microdomes on GaN substrate; (b) GaN microdomes with micro-hemisphere geometrical shape; (c) GaN microdomes with micro-hemiellipsoid geometrical shape; (d) GaN flat surface with antireflection coating layer for a particular wavelength; and (e) unit cell used for the 3D-FDTD simulation.](image)

![FIG. 2. Surface reflection of GaN micro-hemispheres with incident light wavelength of 500 nm as a function of the incidence angle for (a) P polarization and (b) S polarization.](image)
light with P polarization form the conventional GaN flat surface shows the Brewster angle at around 68° - 70°, as shown in Fig. 2(a). The surface reflection is significantly reduced for the P polarization with incidence angle between 0° and 60°. The reflection of the P polarization with incidence angle >60° does not show reduction with GaN micro-hemispheres due to the shift of the Brewster angle to smaller angles as compared to that of the GaN flat surface. From Fig. 2(b), the general trend indicates that the surface reflection increases as the light incidence angle increases. As compared to the GaN flat surface, the use of GaN micro-hemispheres leads to significant reduction of the reflection at different incidence angles for S polarization and P polarization with incidence angle between 0° and 60°.

In order to evaluate the dependence of the surface reflections on the micro-hemisphere size, angle-averaged surface reflection of unpolarized light was obtained by averaging reflections over incidence angles from 0° up to 80° with both P and S polarizations. Figure 3 plots the angle-averaged surface reflectance as a function of the micro-hemisphere diameter, which indicates the reflectance has strong dependence on the micro-hemisphere diameter. The surface reflectance decreases as the micro-hemisphere increases from 0 to 200 nm, and then saturates as the micro-hemisphere diameter further increases. Based on this study, diameter D = 200 nm was selected for further study of the reflectance on the geometrical shape of the GaN hemi-ellipsoids with different heights. Considering for experimental implementation, surface structure on the 200 nm scale or smaller is preferable due to the restriction on the top p-type GaN layer thickness of ~300 nm. Based on a self-assembled microsphere lithography approach, the experimental formation of the GaN microdomes on the 200 nm scale is still feasible.

Figure 4 plots the reflection of GaN micro-hemiellipsoid structures with D = 200 nm and H = 25 nm, 75 nm, 100 nm, 125 nm, 175 nm, 225 nm, 250 nm, 300 nm, 350 nm, and 400 nm, respectively. The incident wavelength was fixed at 500 nm. Surface reflections of both P [Fig. 4(a)] and S [Fig. 4(b)] polarizations were calculated and compared. Results shown in Fig. 4 indicate a significant dependence of the microdome geometrical shape on the surface reflectance. The general trend indicates that the surface reflectance reduces at different incidence angle as the GaN microdome height increases for both P and S polarizations. The GaN micro-hemisphere (D = 2H) is obviously not the optimized structure for antireflection. Thus, the tuning of the micro-dome height is critical in order to obtain the lowest surface reflection at different incidence angle. For the case of GaN microdomes with D = 200 nm, the Brewster angle of P polarization shifts to smaller angles as compared to the case of GaN flat surface with Brewster angle of 68° - 70°. The GaN microdomes with D = 200 nm and varied H leads to a significant reduction of surface reflection for P polarization (with \( \theta < 60° \)) and S polarization (for all incidence angles). With D = 200 nm and H = 250 nm – 400 nm, the surface reflection at the normal incidence angle is reduced to <0.5% for P polarization and <1% for S polarization, as compared to the surface reflection of ~20% for GaN flat surface. The reduction of the surface reflection for the GaN microdomes with varied height is compared to that of the conventional flat
surface is due to the rotation of the surface normal as the surface curves, which reduces the effective incidence angle for the incident light.

Similar to Fig. 3, Fig. 5 plots the angle-averaged surface reflection of unpolarized incident light as a function of the microdome height with fixed microdome diameter of $D = 200 \text{ nm}$. The angle-averaged reflection was obtained by averaging reflections over range from $0^\circ$ to $80^\circ$. The trend as shown in Fig. 5 indicates that the reflection decreases as the GaN microdome height increases up to $H = 250 \text{ nm}$. When the microdome height increases further, i.e., $H > 250 \text{ nm}$, the angle-averaged surface reflection saturates. For device applications with limited top layer thickness, such as in InGaN based solar cell devices, microdomes with relative low height is preferred. In this study, the GaN microdomes structure with diameter $D = 200 \text{ nm}$ and height $H = 250 \text{ nm}$ could be considered as an optimized structure for antireflection for solar cell devices.

From this study, the size and geometrical shape of the GaN microdomes have a great impact on the surface reflection with different incidence angle and source polarization. In concentrator solar cells, the design of concentrator optical system requires the flexibility of the surface topology tuning in order to obtain the largest light collection efficiency. Note that the study of the effect of the GaN microdomes on the surface reflection is based on the experimental feasibility to fabricate these structures. In Ref. 14, we have demonstrated the controllability of the reactive ion etching process to tune the shape and aspect ratio of the GaN microdomes.

In order to compare the surface reflection from the microdome structure with that from ideal homogeneous antireflection coating, we studied and compared the following three structures: (1) conventional GaN flat surface [Fig. 6(a)]; (2) GaN microdomes with $D = 200 \text{ nm}$ and $H = 250 \text{ nm}$ [Fig. 6(b)]; and (3) GaN with quarter wavelength antireflection coating [Fig. 6(c)]. The corresponding effective refractive index profile for the three structures is plotted in Fig. 6. Ideally, for a single homogeneous layer as antireflection coating, the refractive index of the material should be

![FIG. 5. Surface reflection of GaN micro-hemiellipsoids with incident light wavelength of 500 nm as a function of hemiellipsoid height for angle-averaged unpolarized light. The micro-hemiellipsoid structure diameter is $D = 200 \text{ nm}$, and heights $H = 0$ (GaN flat surface), 25, 75, 100, 125, 175, 225, 250, 300, 350, and 400 nm, respectively. The angle-averaged reflection is obtained by averaging the reflections for $0^\circ$ to $80^\circ$.](image)

![FIG. 6. 3D-FDTD simulation of the surface reflection of the three structures (1) conventional GaN flat surface; (2) GaN microdomes ($D = 200 \text{ nm}$, $H = 250 \text{ nm}$); and (3) GaN flat surface with antireflection coating layer ($n = 1.56$, $t = 80 \text{ nm}$) as a function of the light incidence angle for both (d) P and (e) S polarizations with light incidence wavelength $\lambda = 500 \text{ nm}$). The corresponding refractive index profiles of the three structures are shown in (a), (b), and (c).](image)
The thickness of the antireflection coating should be \( t = \lambda / (4 n) \). The schematic of the effective refractive index profile for the GaN microdomes was obtained based on the effective medium theory. Note that the design of the single antireflection coating layer is targeting for the suppression of surface reflection of a particular wavelength. Here, the study focused on the incidence wavelength of 500 nm. Thus, the designed single antireflection coating thickness is \( t = 80 \text{ nm} \).

Figures 6(d) and 6(e) plot the surface reflection as a function of the incidence angle for the three structures with fixed incidence wavelength \( \lambda = 500 \text{ nm} \) for both P [Fig. 6(d)] and S [Fig. 6(e)] polarizations. For P polarization, the surface reflection from the GaN microdomes is lower with incidence angle larger than 32°, as compared to that of the GaN flat surface with antireflection coating (\( n = 1.56, t = 80 \text{ nm} \)). With incidence angle smaller than 32°, the surface reflection from the GaN surface with antireflection coating is lowest (<0.2%). For S polarization, the surface reflection from the GaN flat surface with antireflection coating shows the lowest among the three structures, especially with the incidence angle smaller than 50°. At incidence angle of 80°, the surface reflections from GaN microdomes and GaN flat surface with antireflection coating are 47% and 40%, respectively, as compared to 73% of the conventional GaN flat surface.

Based on Eq. (2) in Ref 37, angle-averaged surface reflections for the conventional GaN flat surface, GaN microdomes with \( D = 200 \text{ nm} \) and \( H = 250 \text{ nm} \), and GaN with quarter wavelength antireflection coating are 24.9%, 8.9%, and 7.0%, respectively. Note that the antireflection coating material thickness is designed based on the incidence wavelength of 500 nm.

The comparison of the surface reflection from the three structures as a function of the incidence wavelength from 300 nm to 1200 nm with fixed incidence angle of \( \theta = 25^\circ \) is plotted in Fig. 7 for P and S polarizations. Note that the selection of incidence angle of 25° does not lose the generality of the wavelength dependence analysis. From the above results on the angle dependence surface reflection calculations, the surface reflection for S polarization shows the general trend of increase as the incidence angle increases, and the surface reflection for P polarization decreases as the incidence angle increases to the Brewster angle and then increases as the incidence angle increases further. These trends are true regardless of the wavelength. From Fig. 7, the surface reflection from the GaN surface with antireflection coating is lowest at around \( \lambda \sim 500 \text{ nm} \) for both P and S polarizations, due to the antireflection coating thickness was optimized for 500 nm incident wavelength. When the incidence wavelength is away from 500 nm, the surface reflection increases significantly. In contrast, the surface reflection from the GaN microdomes stays relatively low across the whole wavelength range for both P and S polarizations. The P polarization reflection from the GaN microdomes is reduced to <1% for wide wavelength range from 300 nm to 1100 nm. For the S polarization, the reflection is lower than 5% for the broadband wavelength range.

The results from this study indicate that GaN microdomes provide a uniform and controllable surface texturing for reducing reflection over a broad wavelength range and a wide incidence angle. This design has great potential to be applied in III-nitride based concentrator solar cell devices to enhance the light collection efficiency. In addition, the proposed design is transformable to be applied in different material system and devices including the traditional III–V solar cells.

V. SUMMARY

In summary, GaN microdomes have been analyzed as surface topology to enhance the light collection efficiency in concentrator photovoltaics. The size and geometrical shape of the GaN microdomes are critical in order to obtain the minimal surface reflection. GaN microdomes (\( D = 200 \text{ nm}, H = 250 \text{ nm} \)) leads to significant reduction of the surface reflection over a broad wavelength range and wide light incidence angle for both P and S polarizations. The surface topology design based on microdomes is transformable to be applied in the III–V concentrator solar cell devices. Our recent experimental exploration demonstrated the feasibility to fabricate the GaN microdomes with tunable size and aspect ratio by using a low cost, scalable self-assembled approach.
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