Quantitative assessment of diffusivity and specularity of surface-textured reflectors for light extraction in light-emitting diodes

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Surface-textured reflectors fabricated by natural lithography and ion beam etching have a specular and a diffusive component of the reflectivity. The diffusely and specularly reflected powers of surface-textured reflectors are measured and analyzed quantitatively in terms of a theoretical model. The diffusive-power-to-total-power ratio is determined and shown to strongly depend on the surface texture. The light extraction efficiency from a waveguide clad by a partially diffuse reflector is analyzed and shown to be enhanced. © *2006 American Vacuum Society.* [DOI: 10.1116/1.2194924]

I. INTRODUCTION

The light extraction efficiency in light-emitting diodes (LEDs) is one *important* parameter in determining the external quantum efficiency, power efficiency, maximum power, and junction temperature. The large difference between the refractive indices of semiconductor and the surrounding medium results in light being trapped by total internal reflection inside the semiconductor.[1–6] Light extraction of waveguided optical modes can be increased by diffusive optical elements such as roughened or textured surfaces.[2–9] Other means of enhancing the light extraction efficiency include patterned sapphire substrates,[10] arrays of micro-LEDs,[11] and chip shaping.[12]

II. THEORETICAL MODEL

For *specular* reflectors, the angle of reflectance is equal to the angle of incidence. In contrast, ideal *diffuse* reflectors follow the $\cos\theta$ dependence of Lambert's reflection law which is independent of the angle of incidence. In this article, the reflectance pattern of textured reflectors fabricated by natural lithography is measured and shown to strongly depend on the surface structure. Although it has been assumed that surface-textured reflectors have diffuse characteristics, it is shown that such reflectors have *both*, a diffusive and a specular component of the reflectivity. Because the light extraction efficiency from waveguide clad by specular and diffusive reflectors is markedly different, it is highly desirable to quantify the specularity and diffusivity of reflectors. A theoretical model is developed to quantitatively assess the reflection characteristics of mixed diffuse-specular reflectors. The light extraction from LED structures having mixed diffuse-specular characteristics is analyzed quantitatively.

Consider a waveguide with a flat top surface and a diffuse omnidirectional reflector on the bottom side, as shown in Fig. 1(a). Assume that the reflected light includes a specular component and a diffusive component. If light is reflected diffusively, part of the diffusively reflected light can be extracted out of the waveguide. If light is reflected specularly, guided modes propagate (are trapped) in the waveguide. A simplified structure of a GaN LED having a surface-textured p-type contact is shown in Fig. 1(b). The probability of extraction of a guided mode following a reflection event is given as

$$p = R\frac{P_{\text{diff}}}{P_{\text{diff}}+P_{\text{spec}}}\frac{\int_0^{\theta_c} I_{\text{diff}}\cos(\theta)\sin(\theta)2\pi d\theta}{\int_0^{\pi/2} I_{\text{diff}}\cos(\theta)\sin(\theta)2\pi d\theta}, \tag{1}$$

where R is the mirror reflectivity and P_{diff} and P_{spec} are the powers of diffusive and specular reflections, respectively. I_{diff} is the intensity of diffusive reflection along the normal direction. Using $R=1.0$ and Snell's law for the critical angle of total internal reflection θ_c, we obtain

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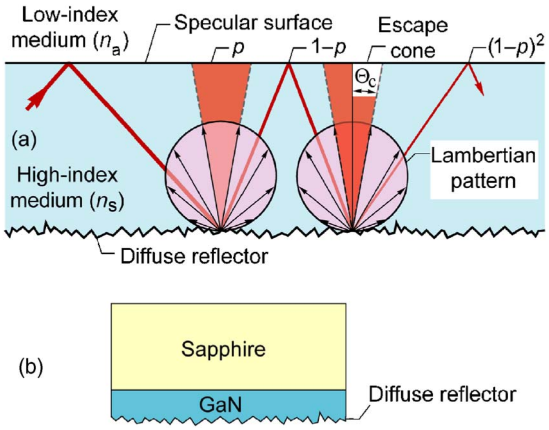

FIG. 1. (a) Propagation of light in a waveguide clad by a diffusive reflector. (b) Simplified structure of GaN LEDs with an omnidirectional diffuse reflector.

$$p = -\frac{1}{2}\frac{P_{\rm diff}}{P_{\rm diff}+P_{\rm spec}}\cos\left[2\arcsin\left(\frac{n_1}{n_2}\right)-1\right] = \frac{P_{\rm diff}}{P_{\rm diff}+P_{\rm spec}}\frac{n_a^2}{n_s^2}, \quad (2)$$

where n_a and n_s are the refractive indices of the surrounding ambient and the semiconductor waveguide core, respectively. After each reflection, $(1-p)$ of the incident light remains trapped in the waveguide. After N reflection events, the light power has decreased to $1/e$, that is,

$$(1-p)^N = 1/e. \quad (3)$$

Using Eq. (2), N is given by

$$N = -\left[\ln\left(1-\frac{P_{\rm diff}}{P_{\rm diff}+P_{\rm spec}}\frac{n_a^2}{n_s^2}\right)\right]^{-1}. \quad (4)$$

For high extraction efficiencies, low values of N are desirable to minimize absorption losses. Equation (4) shows that this can be achieved by maximizing the diffusive component of the reflectivity.

We express the intensity of the light reflected by a reflector having a specular and a diffusive component by

$$I(\theta,\phi) = I_{\rm diff}\cos(\theta) + I_{\rm spec}\cos(\theta)\frac{1}{\sigma^2 2\pi} \times\exp\left[-\frac{1}{2}\left(\frac{\theta-\theta_i}{\sigma}\right)^2\right]\exp\left[-\frac{1}{2}\left(\frac{\phi-\phi_i}{\sigma}\right)^2\right], \quad (5)$$

where $I_{\rm diff}$ and $1/(2\pi\sigma^2)I_{\rm spec}\cos\theta_i$ are the maximum intensities of diffuse and specular reflections, respectively, ϕ and θ are the azimuthal and polar angles, and ϕ_i and θ_i are the corresponding angles of incidence, respectively. The diffusive reflectance is represented by the first summand on the right-hand side of Eq. (5), i.e., the cosine function. The specular term is assumed to be broadened and given by a Gaussian function. The angular standard deviation of Gaussian-broadened specular reflection is given by σ. $I_{\rm diff}$, $I_{\rm spec}$, and σ can be obtained by measuring the angular distribution of the reflected light at different azimuthal angles and subsequent fitting of Eq. (5) to the experimental data.

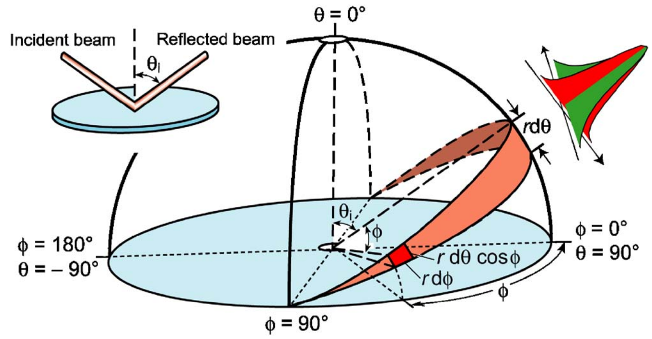

FIG. 2. Geometry of slice and surface area element.

Next we quantify the diffusively and specularly reflected powers. The diffusively reflected power is given by

$$P_{\rm diff} = \int_\theta 2\pi I_{\rm diff} r^2\cos\theta\sin\theta d\theta = \pi I_{\rm diff} r^2, \quad (6)$$

where r is the radius of the unit sphere. The specularly reflected power can be obtained by integrating over the top hemisphere shown in Fig. 2. The surface area of the shaded slice shown in the figure is given by $dS = rd\theta\cos\phi rd\phi$. The power emitted into one slice is given by

$$dP_{\rm slice} = \int_{\phi=-90°}^{90°} A\cos\theta\frac{1}{2\pi\sigma^2}\exp\left[-\frac{1}{2}\left(\frac{\theta-\theta_i}{\sigma}\right)^2\right] \times\exp\left[-\frac{1}{2}\left(\frac{\phi}{\sigma}\right)^2\right] rd\theta\cos\phi rd\phi. \quad (7)$$

For $\sigma \ll 90°$, the Gaussian function is confined to $\phi \ll 90°$, and thus $\cos\phi \approx 1$. Using $\cos\phi \approx 1$ in Eq. (7), one can solve the integral analytically and obtains

$$dP_{\rm slice} \approx A\cos\theta\frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{1}{2}\left(\frac{\theta-\theta_i}{\sigma}\right)^2\right] r^2 d\theta. \quad (8)$$

The total power can be expressed by the integral $P_{\rm spec} = \int_{\theta=-90°}^{90°} dP_{\rm slice}$ which can be solved numerically.

The ratio between $P_{\rm diff}$ and $(P_{\rm spec}+P_{\rm diff})$ affects light extraction [see Eq. (1)] and thus is an important quantity of a reflector. Figure 3 shows the calculated reflection pattern of a specular reflector, a diffusive reflector, and a mixed reflector with $P_{\rm diff}/(P_{\rm spec}+P_{\rm diff}) = 0.5$. A *high diffusivity* is desirable to improve the light extraction efficiency. But it is difficult to fabricate totally diffuse reflectors for a *limited* magnitude of the roughness. At the same time, the above model can help improve and optimize the fabrication process of diffuse reflectors by quantitatively evaluating the diffusivity.

III. EXPERIMENTAL

To demonstrate the viability of the model, the reflectance pattern of reflectors with silica substrate fabricated by natural lithography and ion beam etching is measured. Methanol solutions of nanopolystyrene balls with diameters of 445 and

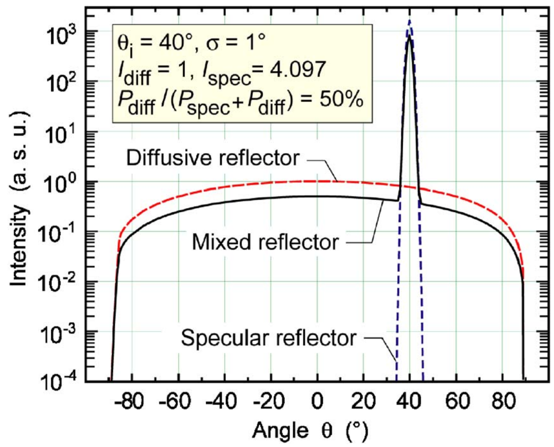

FIG. 3. Calculated reflection patterns of a broadened specular reflector, diffusive reflector, and mixed reflector. The mixed reflector has equal specular and diffusive reflection powers.

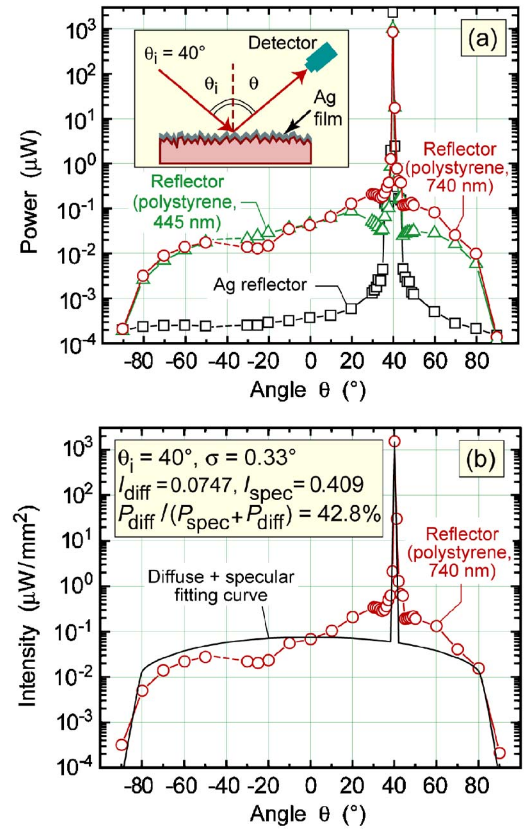

FIG. 4. (a) Reflectance power vs polar angle of a 445 nm reflector, a 740 nm reflector, and the Ag reflector. (b) Fitted curve of reflectance using Eq. (5) for the 740 nm reflector.

740 nm are dispersed on the sample surface by spin coating. Once the methanol has evaporated, the polystyrene balls on the surface serve as an etch mask for the initially planar samples. After lithography, ion etching is performed using a 600 VAr^+ beam. After the ion etching, the rms roughnesses are 14.7 and 21.2 nm for samples masked with 445 and 740 nm nanopolystyrene balls, respectively. Ag films of 1000 nm thickness are deposited on the roughened sample. The Fourier transform of the roughened surface gives bell-shape power spectra with full widths at half maximum of 0.48 and 0.35 μm^{-1} for samples masked with 445 and 740 nm nanopolystyrene balls, respectively. A 10 mW He–Ne laser emitting at 632.8 nm is used to measure the reflected power as a function of θ. The angular dependence of the reflectivity is measured with a pinhole with a diameter of 0.84 mm, giving an angular resolution of $\Delta\theta \approx 0.5°$ ($\Delta\theta \approx d/r$ with d=0.84 mm and r=13.5 cm). A Ag-coated flat sample, serving as a pure specular reflector, is measured for comparison.

IV. RESULTS AND DISCUSSION

Figure 4(a) shows the reflectance patterns of the samples fabricated with 445 nm polystyrene-ball natural lithography (445 nm reflector), 740 nm polystyrene-ball natural lithography (740 nm reflector), and the Ag-coated specular mirror (Ag reflector). The He–Ne laser beam, incident on the Ag surface, and the reflected beam are shown in the inset of Fig. 4(a). Inspection of Fig. 4 reveals that the reflectors with roughened surface clearly have a specular as well as a diffusive component of the reflectivity, thereby justifying our contention of mixed diffusive-specular characteristics. Note that the surface textured reflectors have a much higher diffusive component of the reflectance than the Ag reflector.

The theoretical expressions of the reflected intensity [see Eq. (5)] are used to fit the experimental reflectance-versus-angle curve of the 740 nm reflector, and the result of the fit is shown in Fig. 4(b). Three parameters are used in the simulation: I_{diff} for the diffusive part fitting and I_{spec} and σ for the specular part fitting. From the simulation, the diffusive ratio is obtained: 42.8% for the 740 nm sample and 38.1% is for the 445 nm reflector. For the planar Ag reflector, the ratio is 0.35%, which is consistent with the expectation of low diffusivity for this reflector. The different reflectances are summarized in Table I. The sum of the simulated diffuse and specular powers agrees with the incident power, as shown in Table I. From the reflectance-pattern measurements on samples with different etching times and polystyrene-ball concentrations, it is observed that the diffusivity increases with etching time and the concentration of the polystyrene balls.

Whereas the specularly reflected intensity can be measured directly with a single measurement, the diffusive power cannot. The directly measured specular power of the

TABLE I. Comparison of diffusive power ratio between simulation results and approximate measurement.

Sample	445 nm	740 nm	Silver
$P_{diff,simu.}$ (mW)	4.38	4.60	0.039
$P_{spec.,simu.}$ (mW)	7.12	6.14	11.07
$P_{total,simu.}$ (mW)	11.5	10.7	11.1
$P_{diff}/P_{total\ simu.}$	38.1%	42.8%	0.35%
$P_{spec,exp.}$ (mW)	4.89	4.01	9.40
$P_{diff}/P_{total\ exp.}$	51.1%	59.9%	6.0%

reflectors, shown in Table I, is in good agreement with the results obtained from the above analysis. Note that the experimental results and the analysis presented here have significant implication for (nonreflective) surface-textured structures that have been used in LEDs.[10] In analogy to textured *reflective* surfaces, it should be concluded that textured *transmissive* surfaces have a diffuse scattering component and a specular refraction component. The ratio of the two components depends on the surface texture. The quantitative analysis presented here should be applicable to such transmissive surfaces as well.

V. CONCLUSIONS

In conclusion, surface-textured reflectors have been fabricated by natural lithography and ion beam etching using 445 and 740 nm polystyrene balls. We show that the reflectors have diffusive and specular components of their reflectivity. The power ratio depends on the surface nanostructure. A theoretical model of the reflectance pattern of a mixed reflector is developed. The theoretical model closely matches the experimental reflectance pattern. The experimental results show that the diffusivity of reflectors depends on the nanostructure on the surface. The diffusive-to-total-power ratio of 42.8% is obtained in the reflector fabricated with 740 nm polystyrene balls.

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