Enhanced light extraction from textured surfaces with sub-wavelength size features: beyond ray tracing approximation

Spilios Riyopoulos, SAIC
Collaborators:
Prof T. D. Moustakas, Boston University

Work supported by DOE
Cooperative Agreement No. DE-FC26-04NT42275
Enhanced Extraction from Textured Surfaces

- Issue: Defeat the extraction cone limitation of flat surfaces
  \[ \text{GaN / Air:} \]
  \[ \text{Critical Angle} = \arcsin\left(\frac{1}{2.6}\right) = 22.6^\circ \]
  \[ \text{Extracted Fraction} = 4\% \]

- Use of textured surfaces greatly enhances extraction efficiency
  ✔️ 54\% extraction efficiency reported in textured GaAs / Air
  ✔️ >90\% extraction inferred in textured GaN / Air

**Ray Tracing theory**: Ray bounces around until it hits at sub-critical angle = extraction

Micro-Textured Surfaces


Extraction from micro-textured surfaces

- Ray tracing fails for small surface features $b \sim \lambda$

- INSTEAD: **Multiple Scattering** from plane wave incidence
  - Partial Transmission $T(\theta)$ for single incidence and for any angle $\theta$
  - Diffusion of internally reflected $R(\theta)$ over all angles
  - Effective single-pass transmission equals angle-averaged $< T(\theta) >$

- Extraction Computation via Spectral Decomposition
Transmission through textured surface

- For flat surface $k_x = k_x'$
  \[ \sqrt{\varepsilon} \frac{\omega}{c} \sin \theta = \sqrt{\varepsilon'} \frac{\omega}{c} \sin \theta' \]
  No solution (total reflection) unless $\sin \theta < \sqrt{\varepsilon'/\varepsilon}$

- For periodic textured surface
  $k_x' = k_x - n q = k_x - n \left(2\pi/D\right)$

Transmission up to $\sin \theta < \sqrt{\frac{\varepsilon'}{\varepsilon} \frac{c q}{\omega \sqrt{\varepsilon}}}$

Scattering vector $q$ sets diffraction / reflection angle

\[
\sin \theta'(q) = \sqrt{\frac{\varepsilon'}{\varepsilon}} \sin \theta - \frac{q}{k \sqrt{\varepsilon}}, \quad \sin \theta''(q) = \sin \theta - q/k
\]

- Random textured surface:
  Many scattering vectors
  $k_x' = k_x - q_n = k_x - \left(2\pi/D_n\right)$
Method of Effective Surface Current

Continuous

\[ E_{||} = E_{||}' \]

\[ D_{||} \neq D_{||}' \]

\[ \varepsilon E_{||} \neq \varepsilon' E_{||}' \]

Discontinuous

Ampere’s Law: Surface Displacement Current

\[ \nabla \times \nabla \times B = \frac{1}{c} \nabla \times \frac{\partial D_{||}}{\partial t} \]

\[ \nabla \times \nabla \times B = I_S \propto -i\omega \left( \varepsilon E_{||} - \varepsilon' E_{||}' \right) \]

Define \( I_k \) for any incident wavenumber to yield correct reflected / refracted for flat surface incidence!

Surface Current Computation

**Flat Surface**

Apply Boundary Conditions For Reflected / Refracted

**Corrugated surface**

Spectral amplitude $I(q)$:
Fourier transform of surface feature

$$I_o(q)^{TM}_{TE} = -i k \mathcal{D}(q) F(q) E_o$$

Scattered Field Components

Scattering vector $\mathbf{q}$: diffracted / reflected $k', k''$

Maxwell’s EQ: 
\[ E' \propto k' \times B \quad (TM) \]
\[ B' \propto -k' \times E \quad (TE) \]

Boundary Conditions:
\[ E_\parallel + E_\parallel'' = E_\parallel', \quad B_\parallel + B_\parallel'' = B_\parallel' \]
Transmission / Reflection Coefficients
\[ t = E'/E, \quad r = E''/E \]

\[
\begin{pmatrix}
  r(q_n) \\
  t(q_n)
\end{pmatrix}_{TE} =
\begin{pmatrix}
  \frac{\cos \theta - \sqrt{\epsilon'/\epsilon} \cos \theta'(q_n)}{\cos \theta'(q_n) + \sqrt{\epsilon'/\epsilon} \cos \theta'(q_n)} \\
  \frac{\cos \theta'(q_n) + \sqrt{\epsilon'/\epsilon} \cos \theta'(q_n)}{\cos \theta'(q_n) + \sqrt{\epsilon'/\epsilon} \cos \theta'(q_n)}
\end{pmatrix}
\]

\[
\begin{pmatrix}
  r(q_n) \\
  t(q_n)
\end{pmatrix}_{TM} =
\begin{pmatrix}
  \frac{\sqrt{\epsilon'/\epsilon} \cos \theta - \cos \theta'(q_n)}{\sqrt{\epsilon'/\epsilon} \cos \theta'(q_n) + \cos \theta'(q_n)} \\
  \frac{\sqrt{\epsilon'/\epsilon} \cos \theta'(q_n) + \cos \theta'(q_n)}{\sqrt{\epsilon'/\epsilon} \cos \theta'(q_n) + \cos \theta'(q_n)}
\end{pmatrix}
\]

Scattered Floquet Components

\[ E' = t(q_n, \theta) F(q_n) E \]
\[ E'' = r(q_n, \theta) F(q_n) E \]

\[ F(q_n) : \text{Fourier amplitude of surface geometry} \]

\[
F(q_n) = \sum_{n=1}^{N} f(q_n) \exp[iqR_n]
\]

\[
R_n = \sum_{k=1}^{n} D_n
\]
Reflected / Reflected Power Formula

Scattered Power in q-th Floquet component

\[ \langle F(q) F^*(q) \rangle = \langle f(q) f^*(q) \rangle \sum_n^n \exp[\imath q R_n] \]

Reflected / Transmitted vs. angle

Periodic Bragg scattering goes to uniform diffusion with increasing rms fluctuations \( \Delta D \)

NUSOD, 9/25/2007
Multiple scattering of reflected: Uniform distribution of incoming angles

Elementary example: Uniform scattering into cone

\[ \delta \theta \quad 10 \delta \theta \quad 20 \delta \theta \]

\[ \Lambda \theta \quad 10 \quad 10 \]

\[ n=1 \quad 64 \quad 8 \quad 2 \quad 4 \]

\[ f(\theta) \]
Extraction Efficiency Computation

- Partial Transmission $T(\theta)$ from single incidence and for any angle $\theta$
  
  Single-pass extraction $T(\theta)$ - plane wave incidence

- Scattering of internally reflected waves:
  uniform spreading of incidence angle

- Angle-averaged $\langle T(\theta) \rangle$ for single-pass extraction

$$\langle T(\theta) \rangle \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \ T(\theta) \sin \theta$$

Efficiency = Multiple-bounce extraction

$$\mathcal{T} = \frac{\langle T(\theta) \rangle}{1 - (1 - \alpha) \langle R(\theta) \rangle}$$

74% efficiency for 8% single-pass extraction and 3% absorption

NUSOD, 9/25/2007
Multiple Bounce Extraction \( \mathcal{T} \)

Textured surface:
- Partial Transmission Probability for any incidence angle
- If a photon is not absorbed, it will be eventually get out

Flat surface:
- Photon Trapped “for ever” above critical angle

74\% efficiency for 8\% single-pass extraction and 3\% absorption

NUSOD, 9/25/2007
Comparison with Experiment

- Measures Single Incidence Transmission
- Bottom Absorber Blocks Multiple Reflection (no ray-bouncing around)
- Also found: internal reflection 80% isotropic

\[ \lambda = 850\text{nm} \]
Average feature size: 350x150x180nm

Simulation: 1-D version
RECTANGULAR TEETH
**Prism-like 2-D Quasi-Random Surface**

**Triangular Teeth:**

Similar Shapes (angle $\phi$)

Gaussian Size distribution

$D_j$, $h_j = (1/2) \sin \phi_j D_j$

\[
\langle R_j^+ \rangle - \langle R_j^- \rangle = \langle D \rangle, \quad \langle \phi_j \rangle = \langle \phi \rangle
\]

\[
\Delta^2 = \langle D_j^2 \rangle - \langle D \rangle^2, \quad \sigma^2 = \langle \phi_j^2 \rangle - \langle \phi \rangle^2
\]

**Periodic Limit:** $\Delta = \sigma = 0$

**Born approximation:**
Use unperturbed incoming to compute induced source currents
Numerical Results, Single Pass $T(\theta)$

Extraction over $4\pi$ Incident Solid Angle

\[ \psi' = \tan^{-1}(\tan \psi \cos \phi) \]

\[ \frac{\Delta}{\lambda} = 0.355 \pm 0.050 \]

\[ \phi = \frac{\pi}{2} \]

\[ \phi = \frac{3\pi}{8} \]

\[ \phi = \frac{\pi}{4} \]

\[ \phi = \frac{\pi}{8} \]

\[ \psi = \frac{\pi}{16} \]

\[ \psi = \frac{\pi}{8} \]

\[ \psi = \frac{3\pi}{16} \]

\[ \psi = \frac{\pi}{4} \]
Effect of Index Contrast

Optimum feature size increases with decreasing index contrast

\[ q \approx \frac{2\pi}{D} \sim k \frac{n}{n'} \]

where

\[ k' = \epsilon' \frac{\omega}{c} \]
\[ k_x = k \sin \theta \]
\[ k = \epsilon \frac{\omega}{c} \]

The diagram shows a plot of \( T \) versus \( \frac{<D>}{\lambda} \) for different index contrasts: GaN / Al\(_2\)O\(_3\), GaAs / Al\(_2\)O\(_3\), GaN / Air, and GaAs / Air.
Characterization of GaN Textured Templates by Atomic Force Microscopy (AFM)

3D Image

Depth analysis of several GaN textured templates shows Gaussian distribution of surface roughness with rms depths ranging from 0.8 um to 3 um.

NUSOD, 9/25/2007
Non Co-planar Scattering

Scattering vector NOT on incidence plane
Scattered wavenumber NOT coplanar with incident
Monochromatic incident $\rightarrow$ Scattering into 3-D cone

\[
\int dq \langle S(q) \rangle \Rightarrow \iint d\phi dq q \langle S(q,\phi) \rangle 
\]
Conclusions

• **Beyond ray-tracing: Diffraction / Scattering**
• **Closed formula for random surface transmission**
• **Dependence on geometry vs. \( \lambda \)**
  – Maximum extraction for \( D \sim \lambda \)
  – Optimum \( D \) increases with decreasing index contrast
  – Extraction increases with increasing triangular angle
  – Extraction increases with increasing randomness
• **Formalism adaptable to**
  – 2-D texturing
  – Feature shapes
• **Issues:**
  – Short wavelength (ray optics) limit \( kD = 2\pi \left( \frac{D}{\lambda} \right) \gg 1 \),
  – Accuracy limits in spectral integration
Periodic limit: $\Delta, \sigma \rightarrow 0$

Power in $q$-th Floquet component

$$\langle \hat{f}(q)\hat{f}^*(q) \rangle = \left( e^{-q^2\sigma^2} + 1 - 2\cos(q_\varphi(b)) e^{-q^2\sigma^2/2} \right) \frac{\sin(q_\varphi(a)/2)}{q_\varphi(a)/2} \left[ \frac{\langle a \rangle}{\langle D \rangle} \right]^2 \langle S^2 \rangle$$

Screen Form Factor

$$\langle S^2(q_n) \rangle = \frac{1}{N^2} \frac{1 - e^{-q^2\Delta^2} + 2e^{-\frac{q_{n+1}^2\Delta^2}{2}} e^{-\frac{q^2\Delta^2}{2}} \left( \cos \frac{N-1}{2} q_n^2 \langle D \rangle - \cos \frac{N+1}{2} q_n^2 \langle D \rangle \right)}{1 - 2\cos q_n^2 \langle D \rangle e^{-\frac{q_{n+1}^2\Delta^2}{2}} + e^{-q^2\Delta^2}}$$

Reflected / Transmitted vs. angle

$$\langle T \rangle_{TE}^{TM} = \left[ 1 + \langle \hat{R}(0) \rangle \right] \cos \theta' + \frac{1}{2\pi} \int d\varphi \langle \hat{f}(q)\hat{f}^*(q) \rangle \cos \theta'(q) \left[ \frac{\sqrt{\epsilon'}}{\epsilon} \frac{1}{\cos \theta} \right] |t|^2$$

$$\langle R \rangle_{TE}^{TM} = \left[ 1 + \langle \hat{R}(0) \rangle \right] \cos \theta + \frac{1}{2\pi} \int d\varphi \langle \hat{f}(q)\hat{f}^*(q) \rangle \cos \theta'(q) \left[ \frac{1}{\cos \theta} \right] |t|^2$$
Reflected / Reflected Power Formula

Scattered Power in q-th Floquet component

\[
\langle f(q_n) f^*(q_n) \rangle = \left( \langle F(q_n) F^*(q_n) \rangle \right) \sum_n \exp[i q R_n]
\]

Screen Interference Factor

Reflected / Transmitted vs. angle

\[
\langle T \rangle^{TM}_{TE} = \left[ 1 + \langle \hat{R} \hat{f}(0) \rangle \right] \cos \theta + \frac{1}{2\pi} \int dq \langle \hat{f}(q) \hat{f}^*(q) \rangle \cos \theta(q) \sqrt{\varepsilon} \frac{1}{\varepsilon \cos \theta} |t|^2
\]

\[
\langle R \rangle^{TM}_{TE} = \left[ 1 + \langle \hat{R} \hat{f}(0) \rangle \right] \cos \theta + \frac{1}{2\pi} \int dq \langle \hat{f}(q) \hat{f}^*(q) \rangle \cos \theta(q) \frac{1}{\cos \theta} |r|^2
\]

Transition from Periodic Bragg scattering to Uniform light diffusion with increasing rms fluctuations $\Delta D$

NUSOD, 9/25/2007