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

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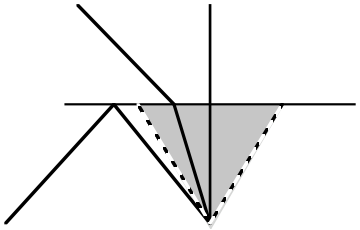
Enhanced Extraction from Textured Surfaces

- Issue: Defeat the extraction cone limitation of flat surfaces

GaN / Air:

Critical Angle = ArcSin(1/ 2.6) = 22.6°

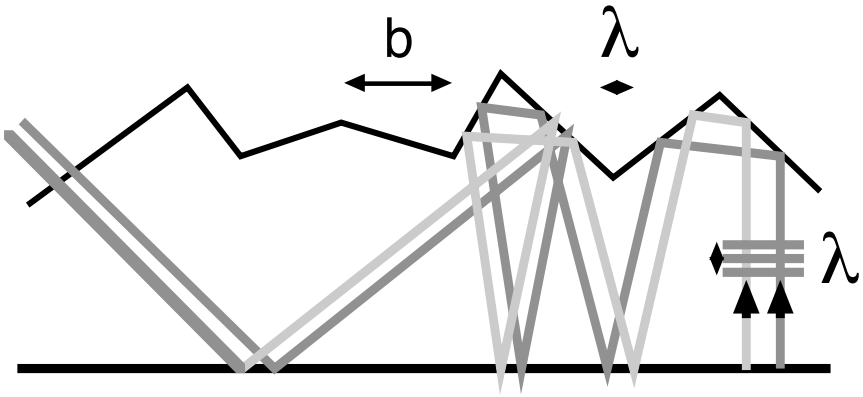
Extracted Fraction = 4%



- 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



• I. Schnitzer, E. Yablonovitch, C. Caneau, T. J. Gmitter, and A. Scherer, "30% external quantum efficiency from surface-textured, thin-film light-emitting diodes," Appl. Phys. Lett., vol. 63, 2174–2176, 1993.

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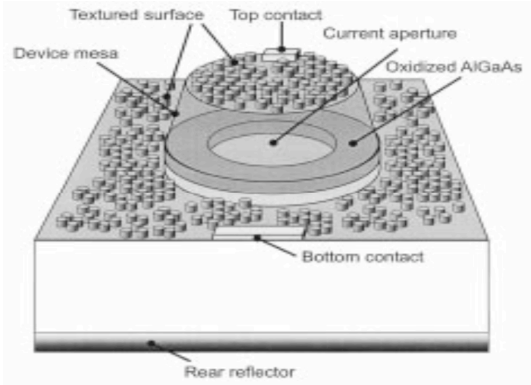
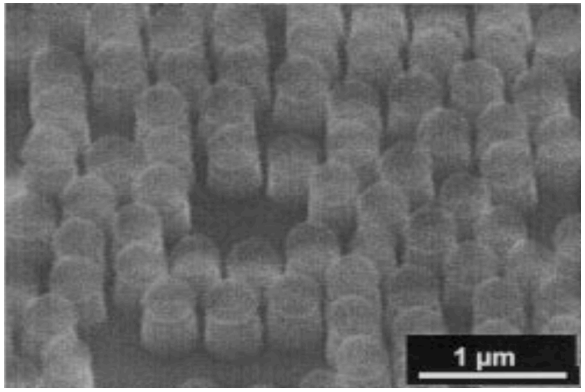
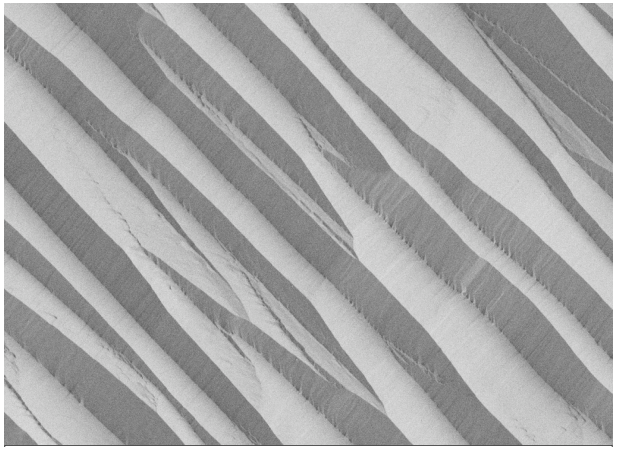
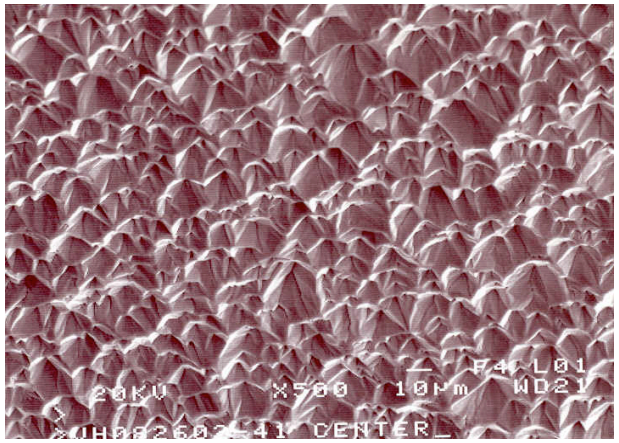
Micro-Textured Surfaces







— 5 µm



20 µm

** R. Windish, C. Rooman, B. Dutta, A. Knobloch, G. Borghs, G. H. Dohler and P. Heremans "Light-extraction mechanisms in high efficiency, surface textured LEDs", IEEE JSTQE **8**, 248-255 (2002).
*** J. S. Cabalu, C. Thomides, T. D. Moustakas, S. Riyopoulos, Lin Zhou and D. J. Smith "Enhanced internal quantum efficiency and light extraction efficiency from textured GaN/AlGaN quantum wells grown by molecular beam epitaxy", J. Applied Phys. **99** 064904 (2006)

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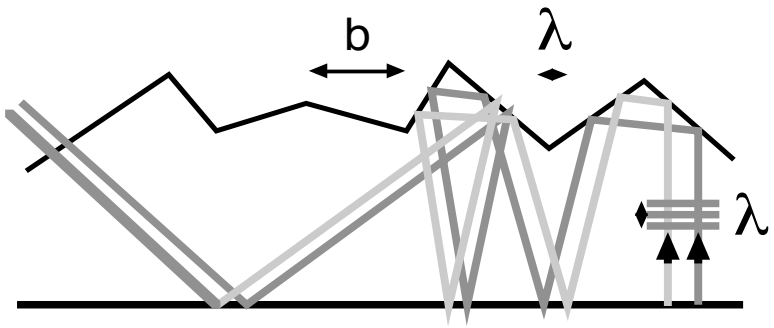
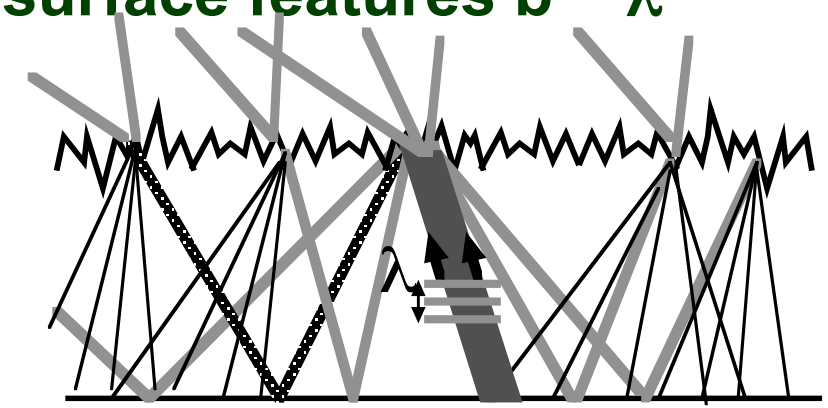
Extraction from micro-textured surfaces

- **Ray tracing fails for small surface features b ~ λ**





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

- **Extraction Computation via Spectral Decomposition**

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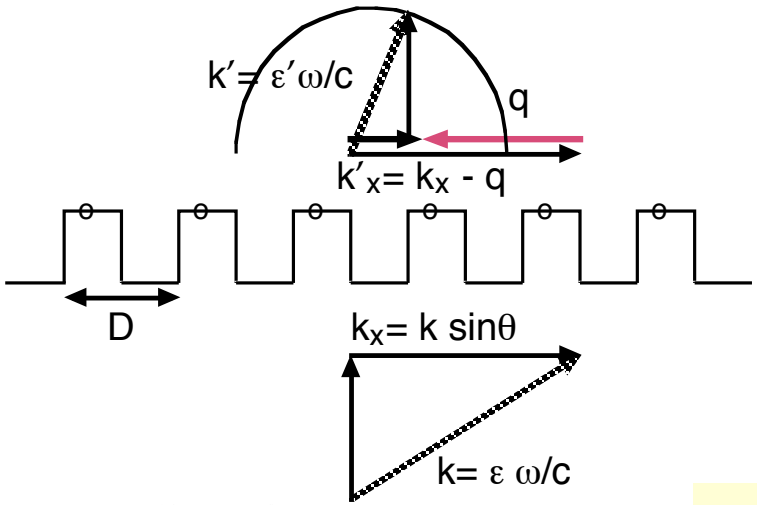
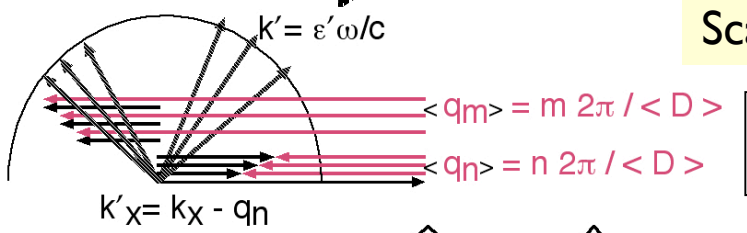
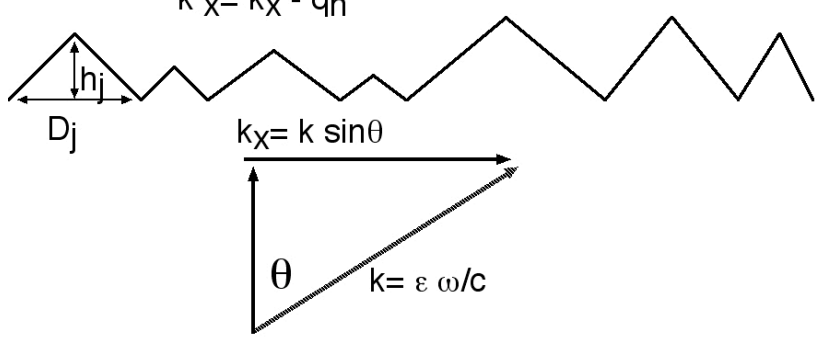
Transmission through textured surface







- For flat surface $k_x = k'_x$

$$\sqrt{\varepsilon}\frac{\omega}{c}\sin\vartheta = \sqrt{\varepsilon'}\frac{\omega}{c}\sin\vartheta'$$

No solution (total reflection) unless $\sin\vartheta < \sqrt{\varepsilon'/\varepsilon}$

- For periodic textured surface

$k'_x = k_x - n\,q = k_x - n\,(2\pi/D)$

Transmission up to $\boxed{\sin\vartheta < \sqrt{\frac{\varepsilon'}{\varepsilon}} + \frac{c\,q}{\omega\sqrt{\varepsilon}}}$

Scattering vector **q** sets diffraction / reflection angle

$$\boxed{\sin\theta'(q) = \sqrt{\varepsilon'/\varepsilon}\,\sin\theta - q/k\sqrt{\varepsilon}, \qquad \sin\theta''(q) = \sin\theta - q/k}$$

- Random textured surface:

Many scattering vectors

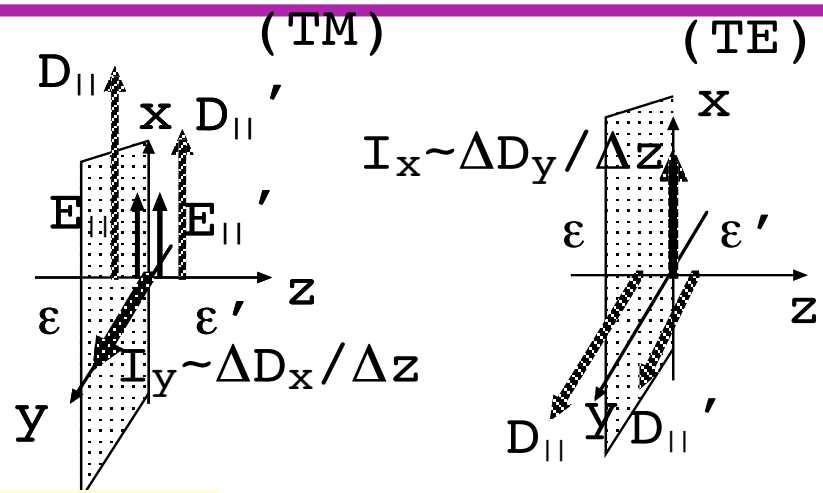
$k'_x = k_x - q_n = k_x - (2\pi/D_n)$

Method of Effective Surface Current

Continuous $E_{||} = E_{||}'$

Discontinuous $D_{||} \neq D_{||}'$

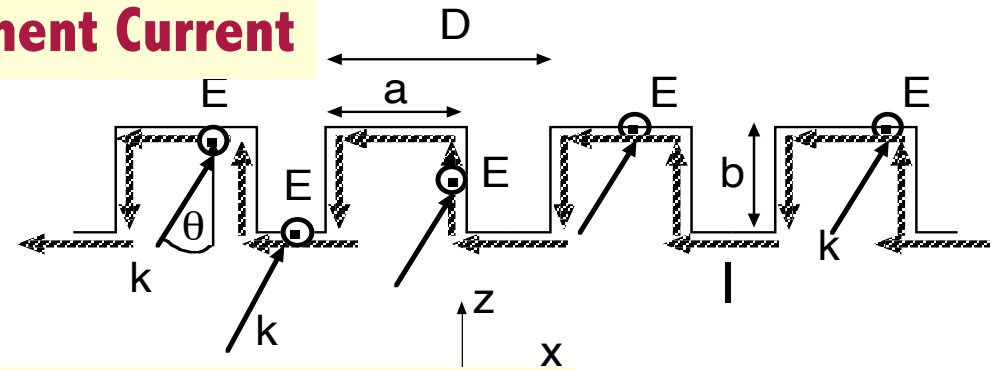
$\varepsilon E_{||} \neq \varepsilon' E_{||}'$



Ampere's Law: Surface Displacement Current

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

$$\nabla \times \nabla \times B = \mathrm{I}_S \propto -\frac{i\omega}{c}(\varepsilon E_{||} - \varepsilon' E_{||}')$$



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

S. Riyopoulos, "Supercritical angle transmission through quasi-random sub-wavelength feature interfaces: Integral approach via effective surface currents", JOSA A **22**, 2859-2871 (2005).

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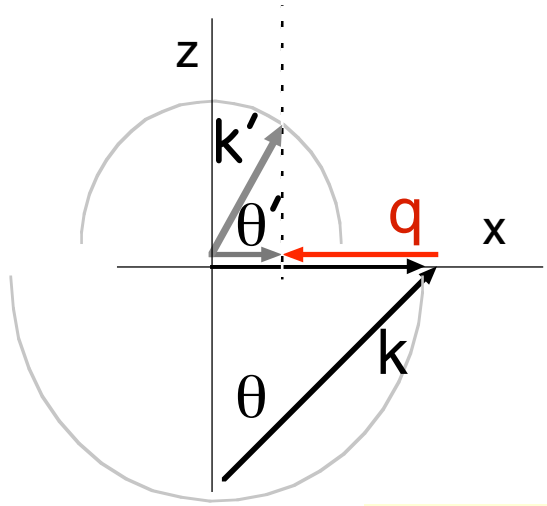
Surface Current Computation

Flat Surface

Apply
Boundary Conditions
For
Reflected / Refracted



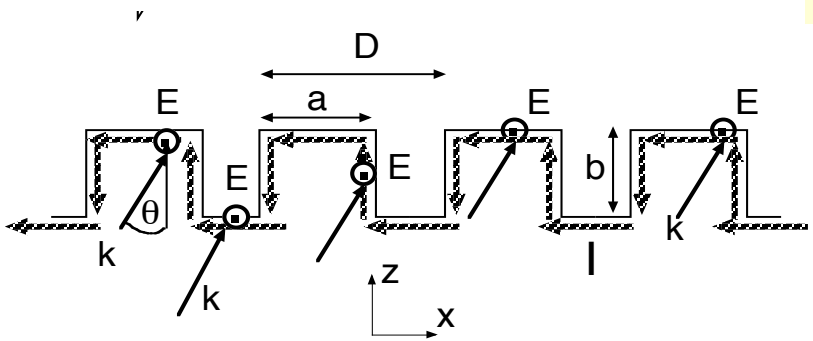
$$\mathbf{I_o}\big|(k-q)_{TE}^{TM} = -i\,k\,\mathcal{D}(q)\,E_o(k)$$

$$\mathcal{D}'(q)\big|_{TE}^{TM} = 2\varepsilon' t(\theta,q)\begin{pmatrix}\cos\theta'(q) & \hat{\mathbf{y}}\\ -\cos^2\theta'(q) & \hat{\mathbf{x}}\end{pmatrix}$$

$$\mathcal{D}''(q)\big|_{TE}^{TM} = 2\varepsilon r(\theta,q)\begin{pmatrix}\cos\theta''(q) & \hat{\mathbf{y}}\\ -\cos^2\theta''(q) & \hat{\mathbf{x}}\end{pmatrix}$$

Corrugated surface

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



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

S. Riyopoulos, "Supercritical angle transmission through quasi-random sub-wavelength feature interfaces: Integral approach via effective surface currents", JOSA A **22**, 2859-2871 (2005).

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Scattered Field Components

Scattering vector **q:**
diffracted / reflected k′, k′″

Maxwell's EQ:

$$\mathbf{E}' \propto \mathbf{k}' \times \mathbf{B} \quad \text{(TM)}$$

$$\mathbf{B}' \propto -\mathbf{k}' \times \mathbf{E} \quad \text{(TE)}$$

Boundary Conditions:

$$E_{\parallel} + E_{\parallel}'' = E_{\parallel}', \qquad B_{\parallel} + B_{\parallel}'' = B_{\parallel}'$$

Transmission / Reflection Coefficients

t = E′/E, r = E″/E

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

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

Scattered Floquet Components

$$E' = t(q_n, \theta)\, F(q_n) E$$

$$E'' = r(q_n, \theta)\, F(q_n) E$$

$F(q_n)$:
Fourier amplitude of surface geometry !

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

$$R_n = \sum_{k=1}^{n} D_n$$

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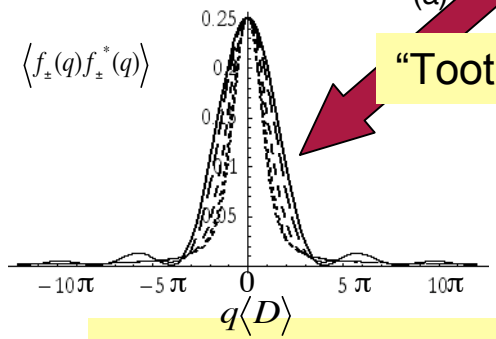
Refracted / Reflected Power Formula

Scattered Power in q-th Floquet component

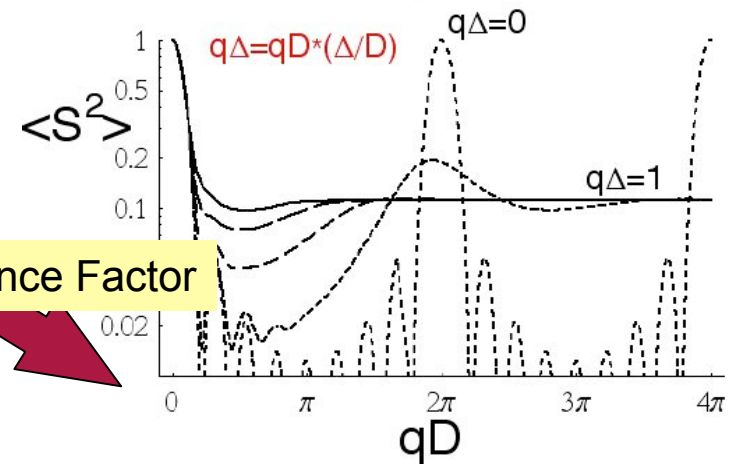
$$\left\langle F(q)F^*(q)\right\rangle = \left\langle f(q)f^*(q)\right\rangle \left\langle \sum_n^N \exp[iqR_n]\right\rangle$$

(a)



"Tooth" FT

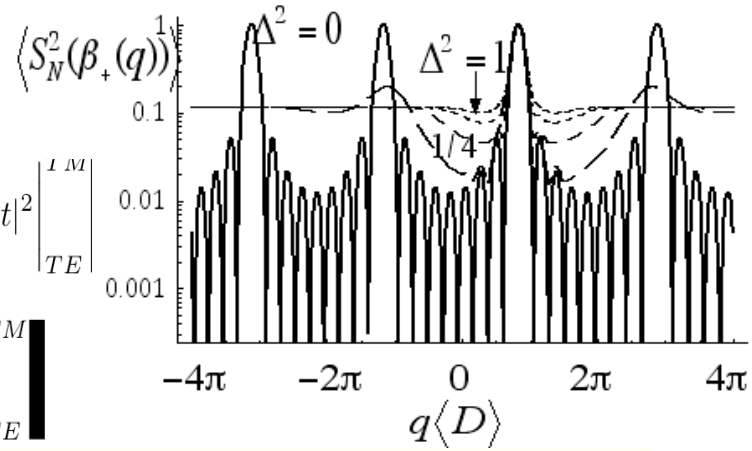
Screen Interference Factor



Reflected /Transmitted vs. angle

$$\langle T\rangle\Big|_{TE}^{TM} = \left\{\left[1+\left\langle \Re\hat{F}(0)\right\rangle\right] cos\theta' + \frac{1}{2\pi}\int d\bar{q}\left\langle \hat{F}(\bar{\mathbf{q}})\hat{F}^*(\bar{\mathbf{q}})\right\rangle cos\theta'(\bar{q})\right\}\sqrt{\frac{\epsilon'}{\epsilon}}\frac{1}{cos\theta}|t|^2\Big|_{TE}^{TM}$$

$$\langle R\rangle\Big|_{TE}^{TM} = \left\{\left[1+\left\langle \Re\hat{F}(0)\right\rangle\right] cos\theta + \frac{1}{2\pi}\int d\bar{q}\left\langle \hat{F}(\bar{\mathbf{q}})\hat{F}^*(\bar{\mathbf{q}})\right\rangle cos\theta''(\bar{q})\right\}\frac{1}{cos\theta}|r|^2\Big|_{TE}^{TM}$$



Periodic Bragg scattering goes to uniform diffusion

with increasing rms fluctuations ΔD

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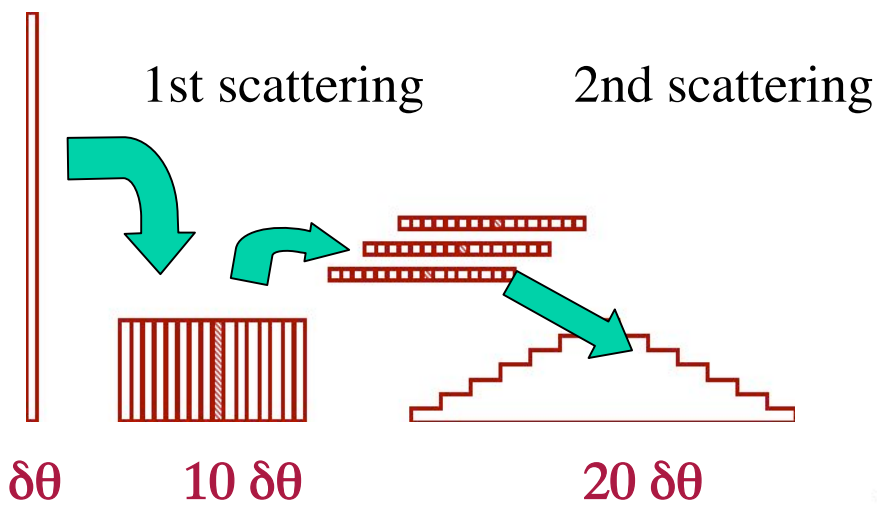
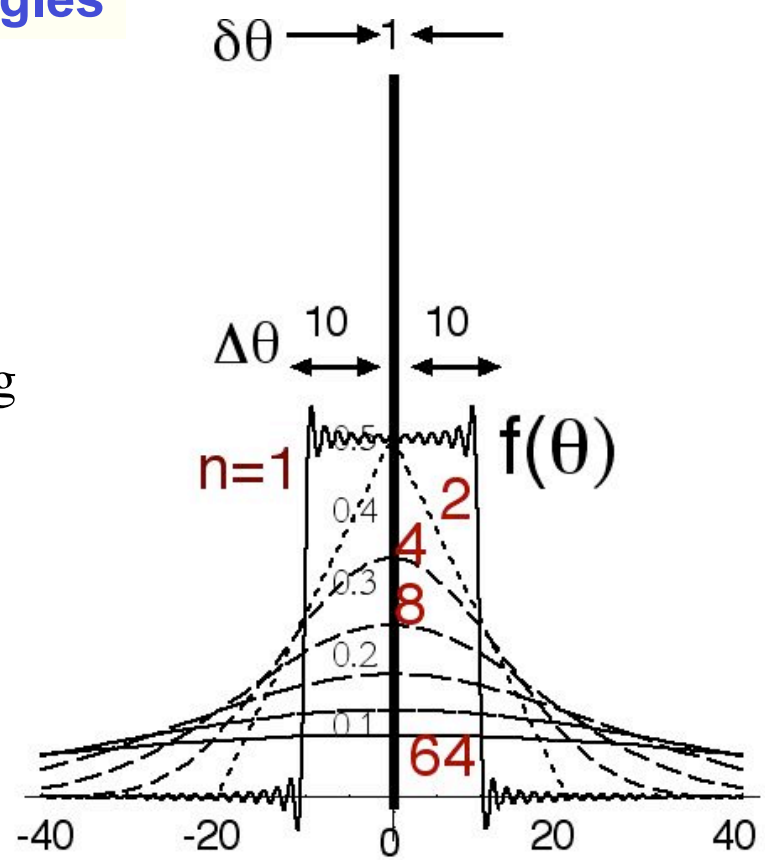
Spectral Diffusion of Reflected Radiation

Multiple scattering of reflected:
Uniform distribution of incoming angles

Elementary example:
Uniform scattering into cone





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Extraction Efficiency Computation

- **Partial Transmission T(θ) from single incidence and for any angle θ**

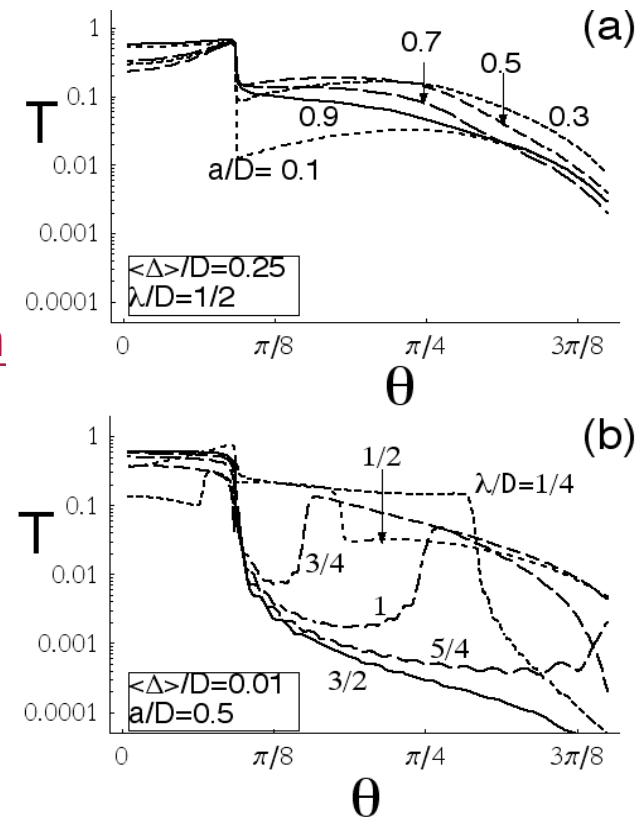
Single-pass extraction T(θ) - plane wave incidence

- **Scattering of internally reflected waves:**
  uniform spreading of incidence angle
- **Angle-averaged < T(θ) > for single-pass extraction**

$$< T(\theta) > \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \; T(\theta) \sin\theta$$

Efficiency = Multiple-bounce extraction

$$\mathcal{T} = \frac{< T(\theta) >}{1 - (1-\alpha) < R(\theta) >}$$



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

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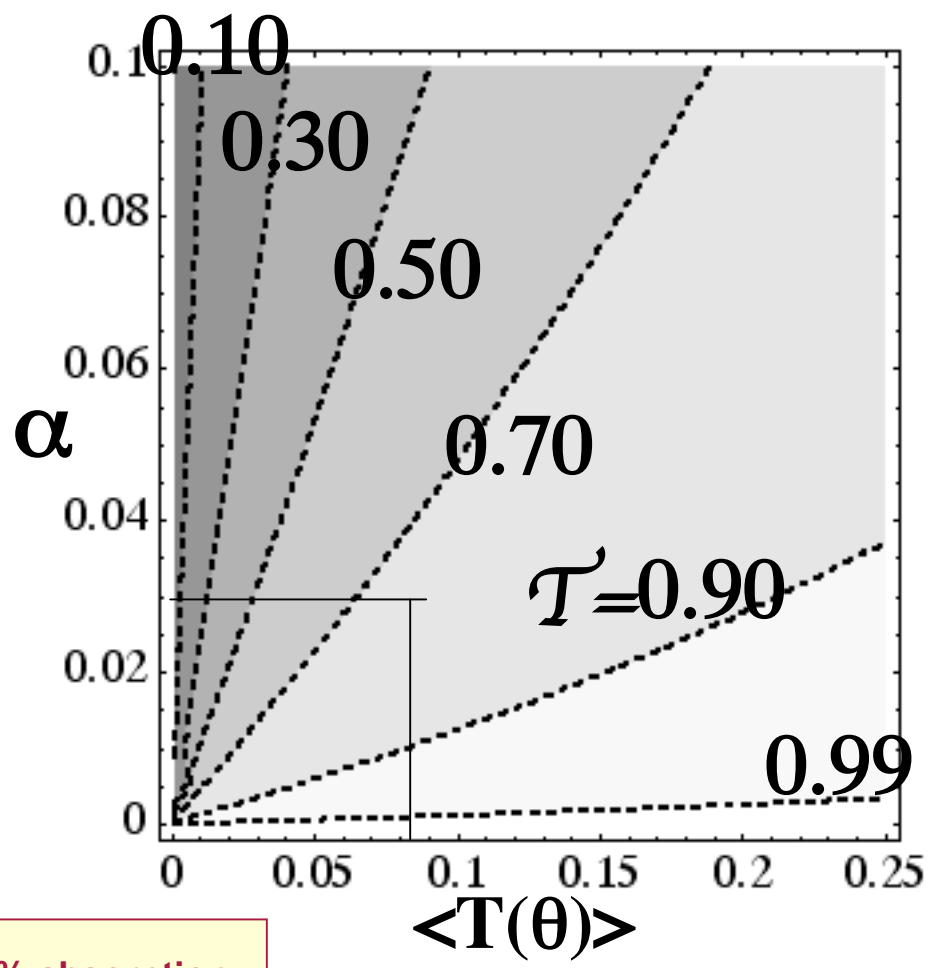
Multiple Bounce Extraction $\mathcal{T}$

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

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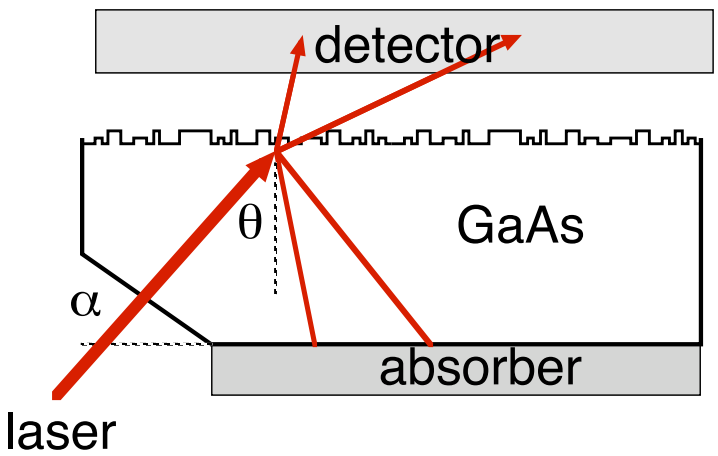
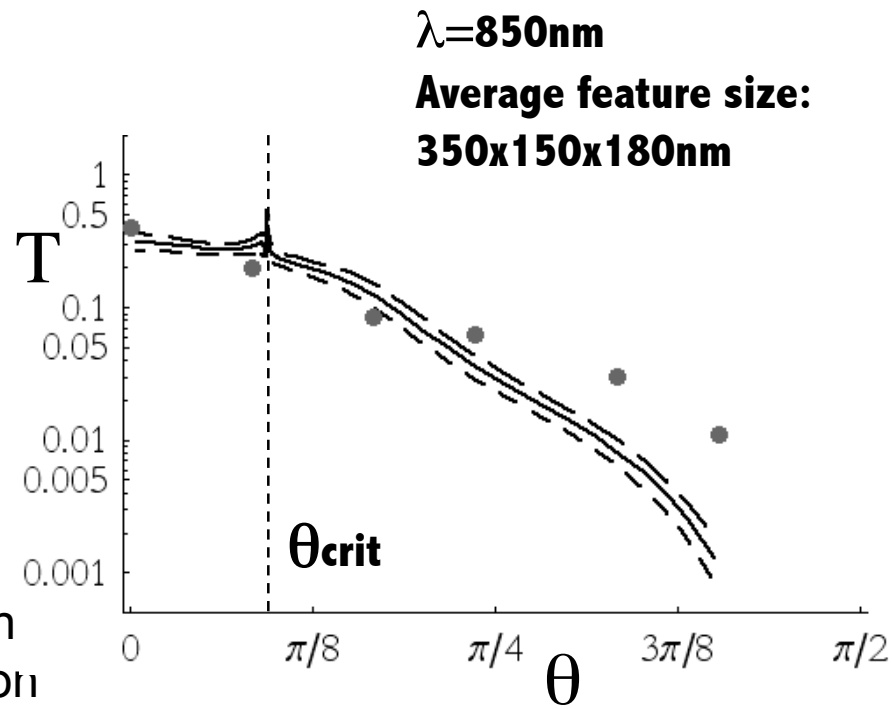
Comparison with Experiment

R. Windisch, C. Rooman, B. Dutta, Member, IEEE, A. Knobloch, G. Borghs, G. H. Döhler, and P. Heremans, IEEE JOURNAL ON SELECTED TOPICS IN QUANTUM ELECTRONICS, VOL. 8, 2p 84, 2002





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

Simulation: 1-D version
RECTANGULAR TEETH

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Prism-like 2-D Quasi-Random Surface

Triangular Teeth:

Similar Shapes (angle ϕ)

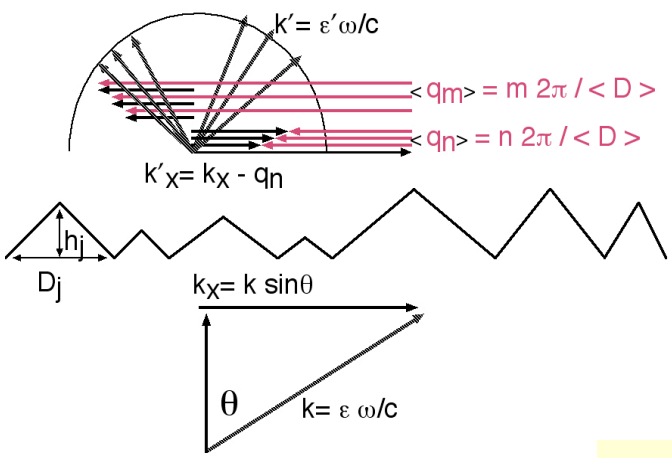
Gaussian Size distribution

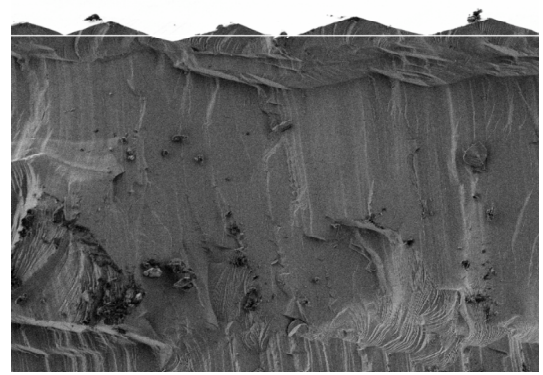
D_j , $h_j = (1/2)\sin\phi_j D_j$

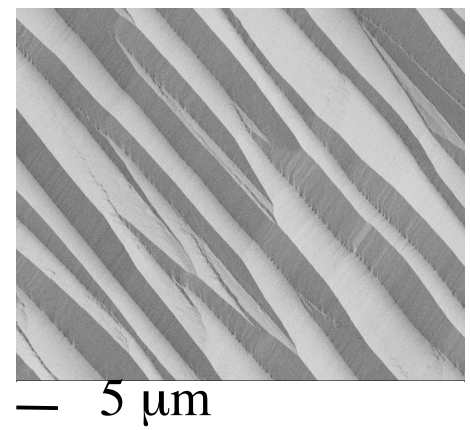
$$\langle R_j^+ \rangle - \langle R_j^- \rangle = \langle D \rangle, \qquad \langle \phi_j \rangle = \langle \phi \rangle$$

$$\Delta^2 \equiv \langle D_j^2 \rangle - \langle D \rangle^2, \qquad \sigma^2 \equiv \langle \phi_j^2 \rangle - \langle \phi \rangle^2$$

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







Born approximation:
Use unperturbed incoming
to compute induced source currents

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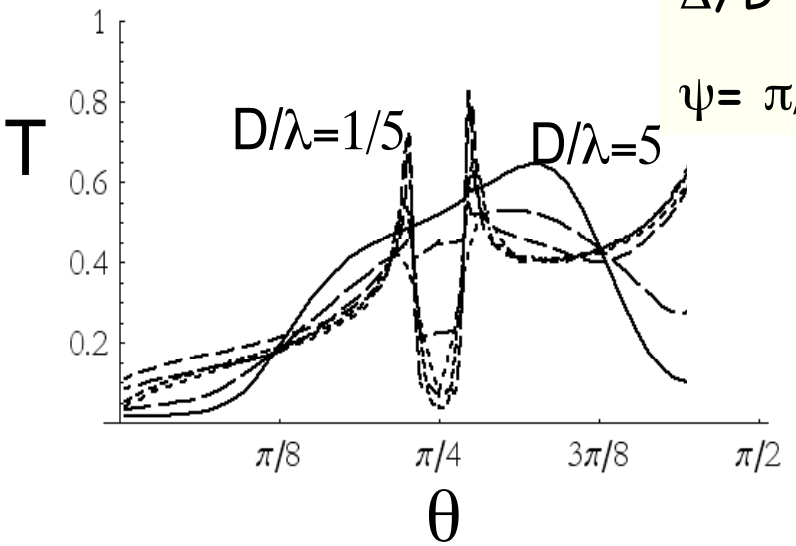
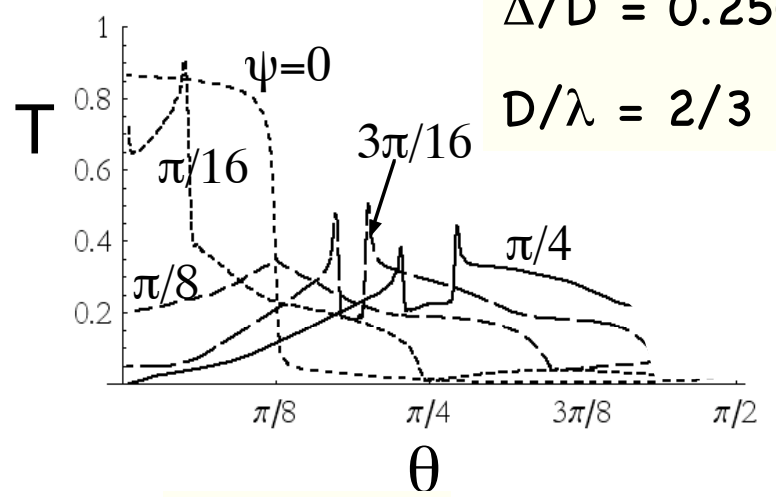
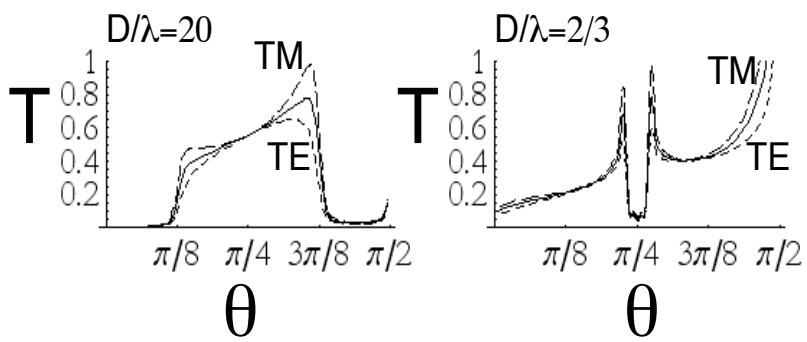
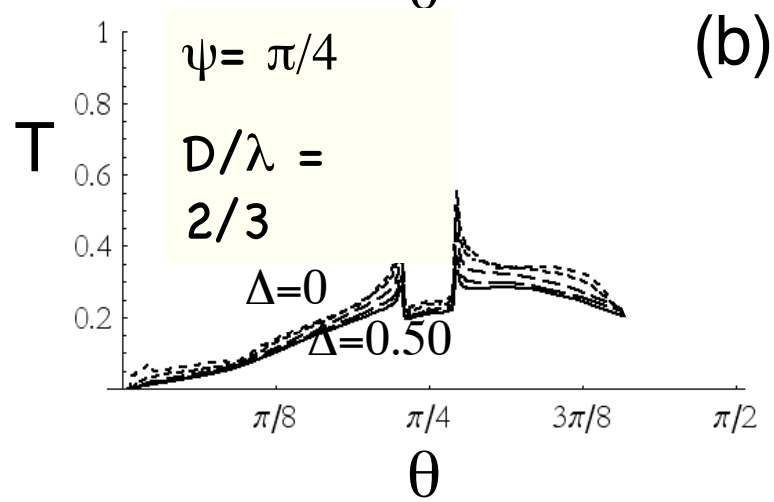
Numerical Results, Single Pass T(θ)









"Enhanced transmission through quasi-random nano-structured dielectric interfaces via supercritical angle scattering", S. Riyopoulos, T. D. Moustakas and J. S. Cabalu J. Appl. Phys. **102**, 043111 (2007).

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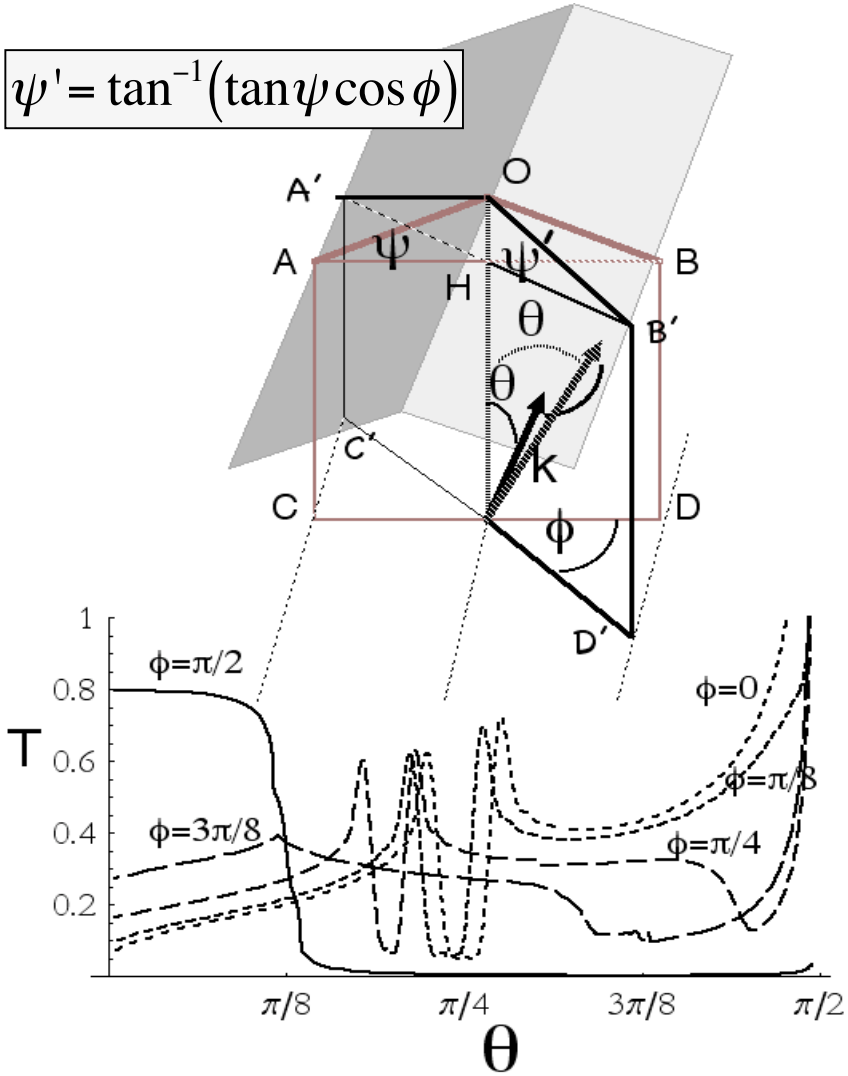
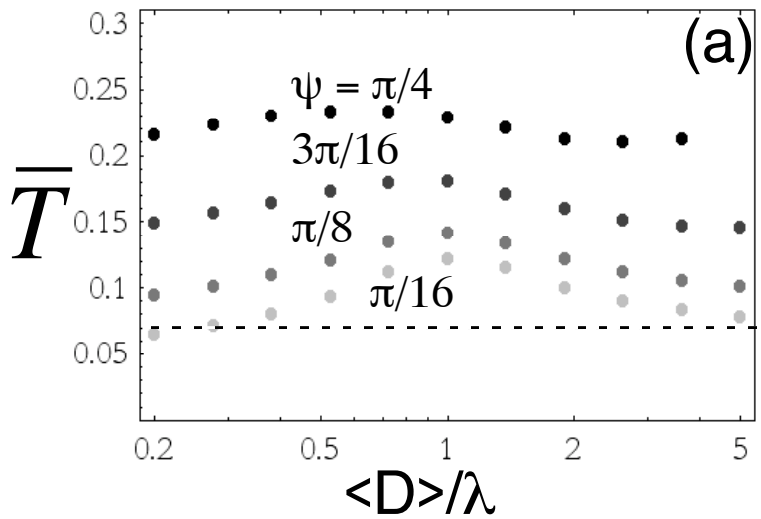
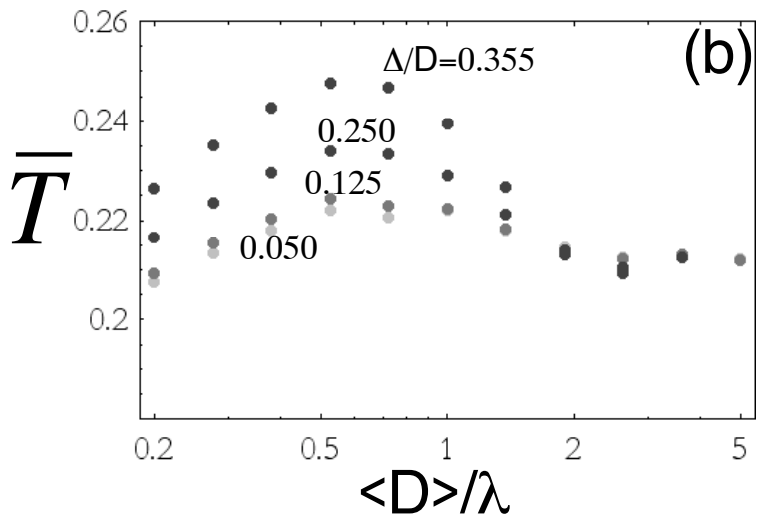
Extraction over 4π Incident Solid Angle

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







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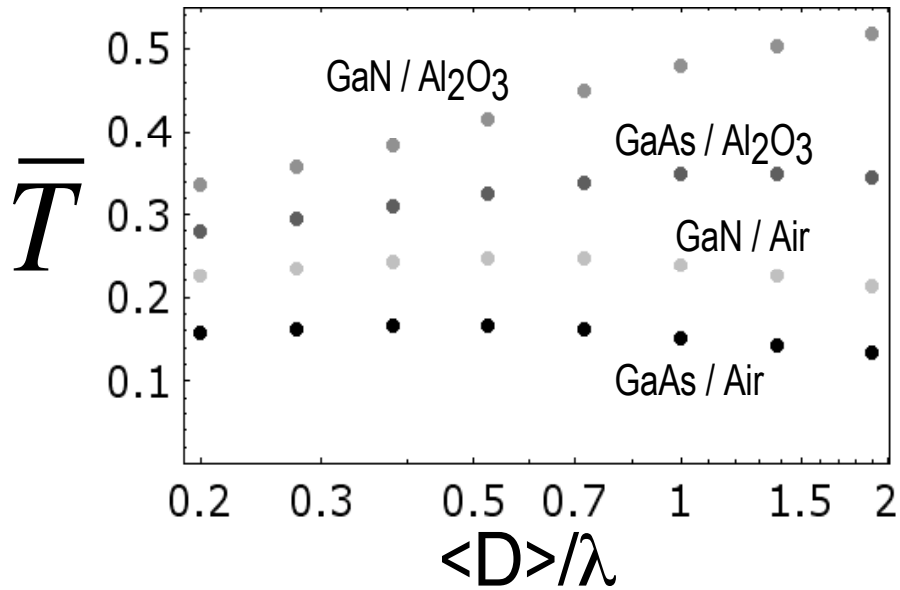
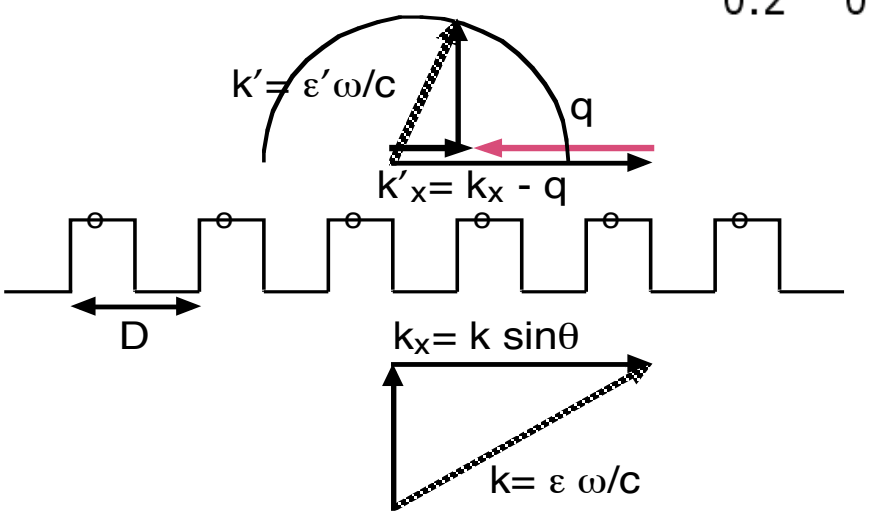
Effect of Index Contrast

Optimum feature size **increases** with **decreasing** index contrast

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





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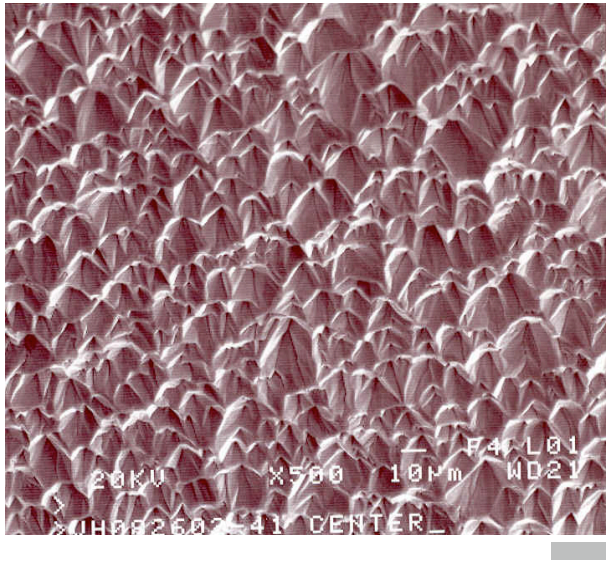
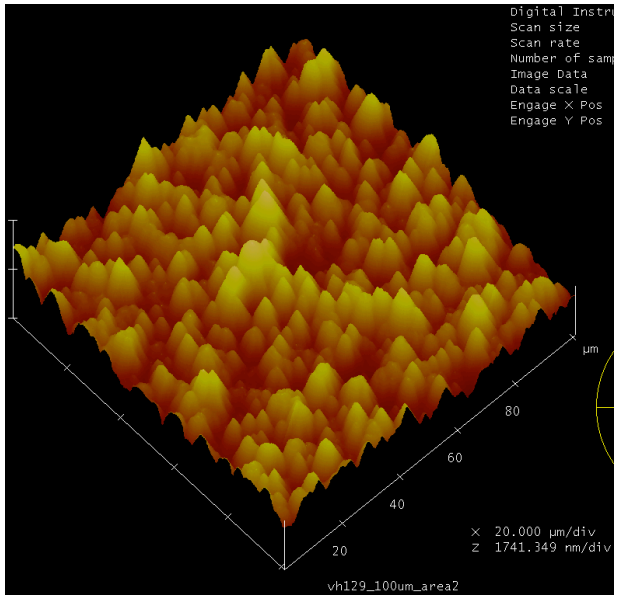
3-D Textured GaN Surface

Characterization of GaN Textured Templates by Atomic Force Microscopy (AFM)

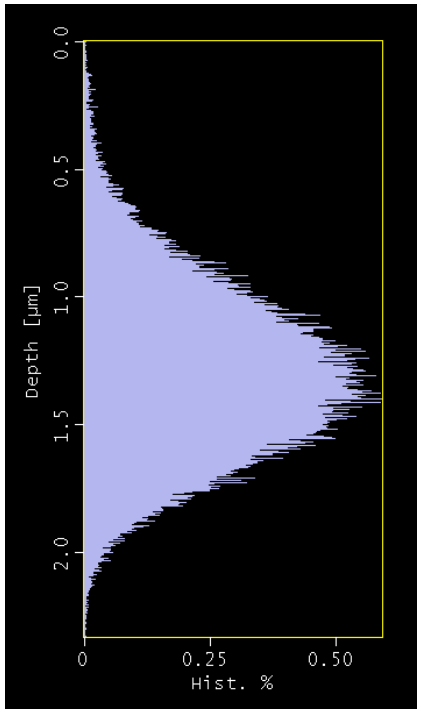


20 μm

3D Image



Depth Analysis



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

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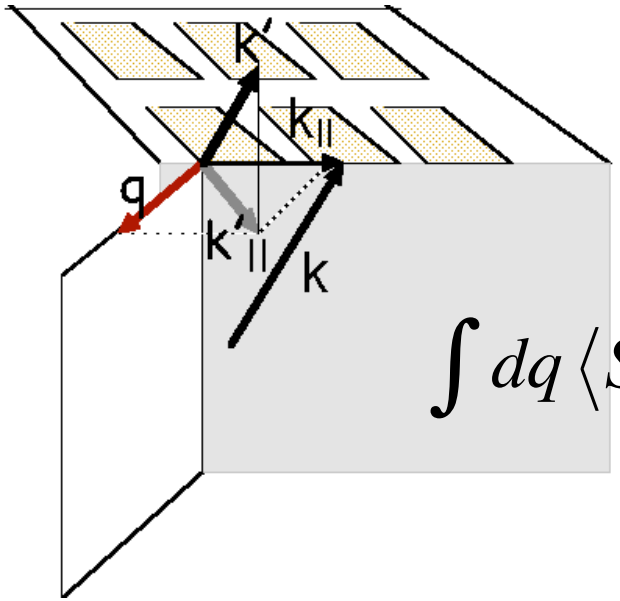
Non Co-planar Scattering

Scattering vector NOT on incidence plane

Scattered wavenumber NOT coplanar with incident

Monochromatic incident → Scattering into 3-D cone



$$\int dq \left\langle S(q)....\right\rangle \Rightarrow \iint d\phi\, dq\, q \left\langle S(q,\phi)....\right\rangle$$

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Conclusions

- **Beyond ray-tracing: Diffraction / Scattering**
- **Closed formula for random surface transmission**
- **Dependence on geometry vs. λ**
  - **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 $kD = 2\pi (D / \lambda) >> 1$,**
  - **Accuracy limits in spectral integration**

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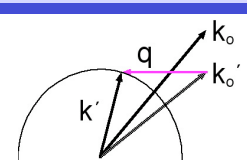
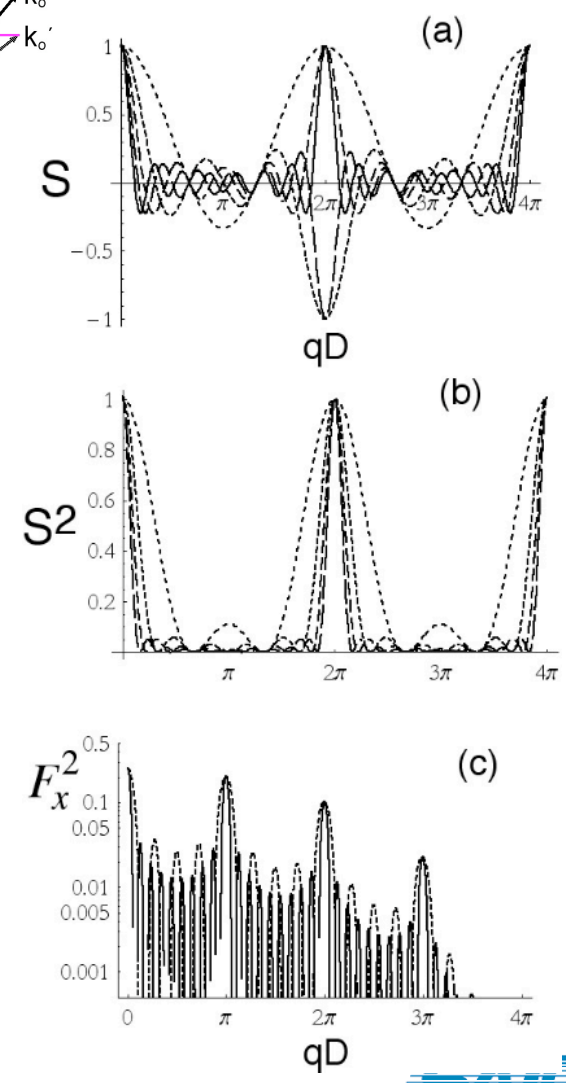
Periodic limit: Δ , σ ==> 0

Power in q-th Floquet component

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





Screen Form Factor

$$\langle \mathcal{S}^2(q_n)\rangle = \frac{1}{N^2}\,\frac{1 - e^{-q_n^2 2\Delta^2} + 2e^{-\frac{N+1}{4}q_n^2 2\Delta^2}\, e^{-\frac{q_n^2 2\Delta^2}{2}}\left(cos\frac{N-1}{2}q_n 2\langle D\rangle - cos\frac{N+1}{2}q_n 2\langle D\rangle\right)}{1 - 2cosq_n 2\langle D\rangle\, e^{-\frac{q_n^2 2\Delta^2}{2}} + e^{-q_n^2 2\Delta^2}}$$

Reflected /Transmitted vs. angle

$$\langle T\rangle\Big|_{TE}^{TM} = \left\{\left[1 + \left\langle \Re\hat{f}(0)\right\rangle\right] cos\theta' + \frac{1}{2\pi}\int d\bar{q}\left\langle \hat{f}(\bar{\mathbf{q}})\hat{f}^*(\bar{\mathbf{q}})\right\rangle cos\theta'(\bar{q})\right\}\sqrt{\frac{\epsilon'}{\epsilon}}\,\frac{1}{cos\theta}\,|t|^2\Bigg|_{TE}^{TM}$$

$$\langle R\rangle\Big|_{TE}^{TM} = \left\{\left[1 + \left\langle \hat{\Re}f(0)\right\rangle\right] cos\theta + \frac{1}{2\pi}\int d\bar{q}\left\langle \hat{f}(\bar{\mathbf{q}})\hat{f}^*(\bar{\mathbf{q}})\right\rangle cos\theta''(\bar{q})\right\}\frac{1}{cos\theta}\,|r|^2\Bigg|_{TE}^{TM}$$

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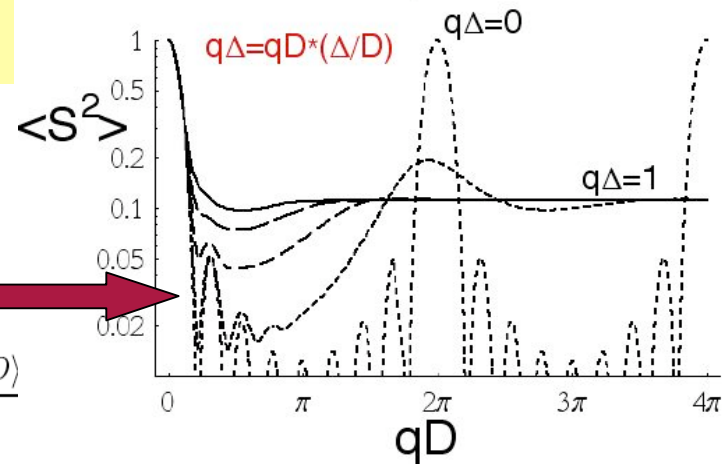
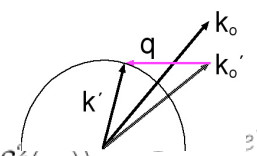
Refracted / Reflected Power Formula

Scattered Power in q-th Floquet component

$$\langle f(q_n) f^*(q_n)\rangle = \langle F(q_n) F^*(q_n)\rangle \left\langle \sum_n^N \exp[iqR_n] \right\rangle$$



Screen Interference Factor

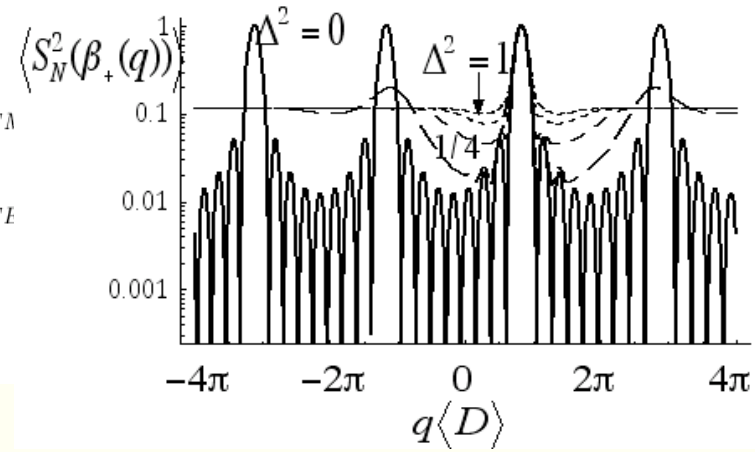


$$\langle S^2(q_n)\rangle = \frac{}{N^2} \frac{e^{-q_n^2 2\Delta^2} + 2e^{-\frac{N+1}{4} q_n^2 2\Delta^2} e^{-\frac{q_n^2 2\Delta^2}{2}} \left(\cos\frac{N-1}{2} q_n 2\langle D\rangle - \cos\frac{N+1}{2} q_n 2\langle D\rangle\right)}{1 - 2\cos q_n 2\langle D\rangle e^{-\frac{q_n^2 2\Delta^2}{2}} + e^{-q_n^2 2\Delta^2}}$$

Reflected /Transmitted vs. angle

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

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



Transition from

Periodic Bragg scattering to Uniform light diffusion

with increasing rms fluctuations ΔD

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