Modern PV-Technologies
3.4: Optics

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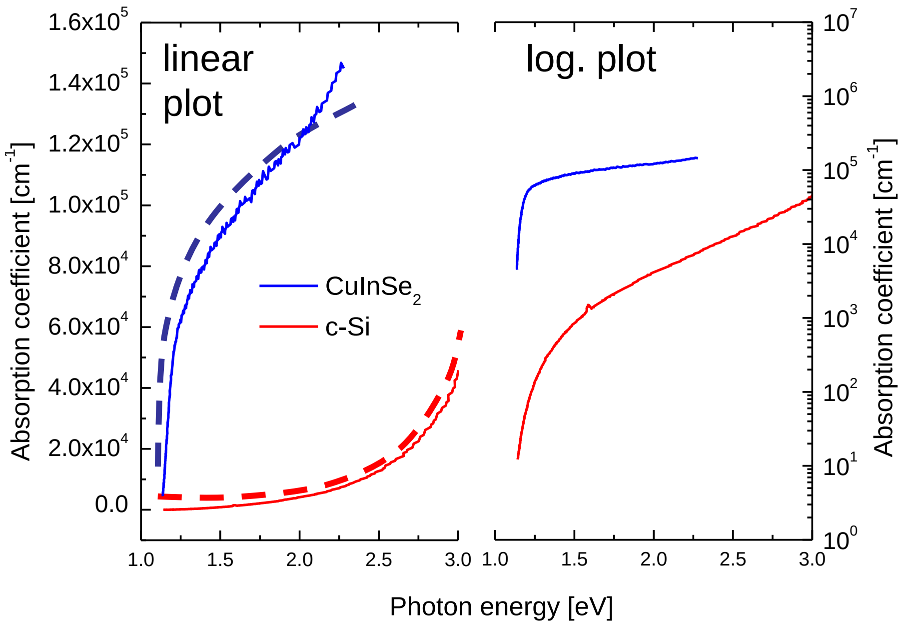
PV-Lab

Absorption coefficient

Direct vs. indirect band gap



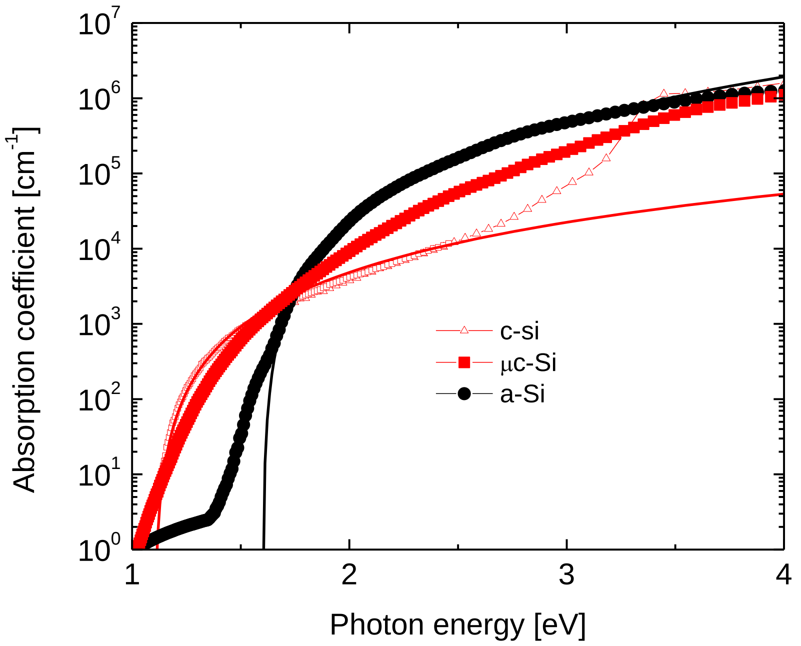
Direct gap (GaAs, $CuInSe_2$):

$$\alpha \sim (E - E_g)^{1/2}$$

Indirect gap (c-Si):

$$\alpha \sim (E - E_g)^2$$

Indirect gaps in all types of silicon



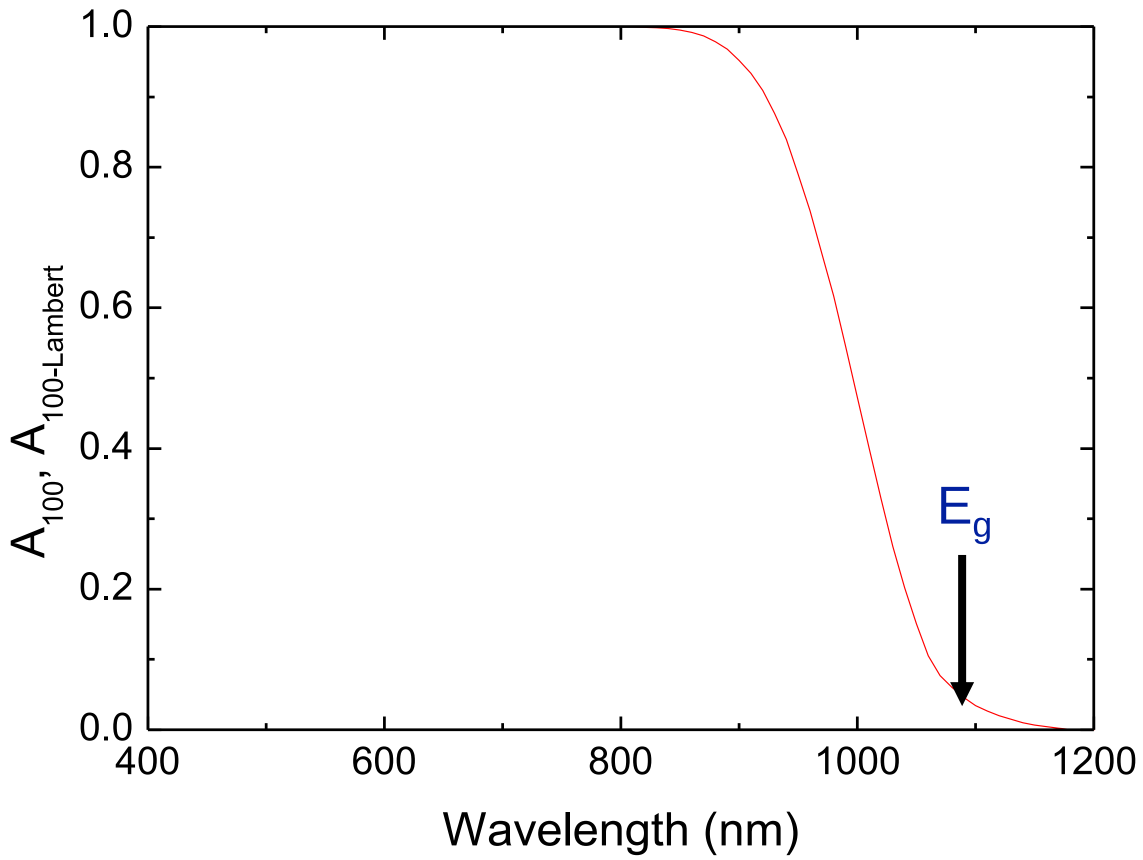
a-Si:H: ~1.75 eV

μc-Si:H:~1.1 eV (like c-Si)

weak IR absorption (<10^4 cm^{-1})

Green, Sol. En. Mat. 2008

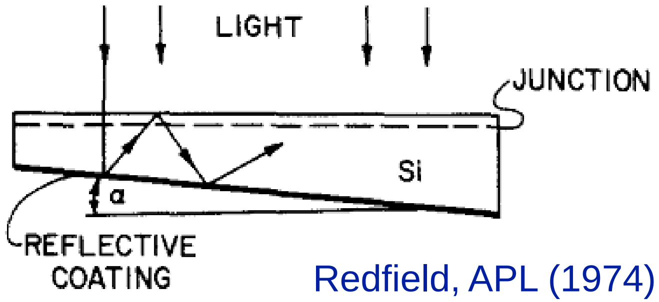
Absorption in silicon



100 µm thick wafer
(may become standard)

$$A = 1 - \exp\{-\alpha d\}$$

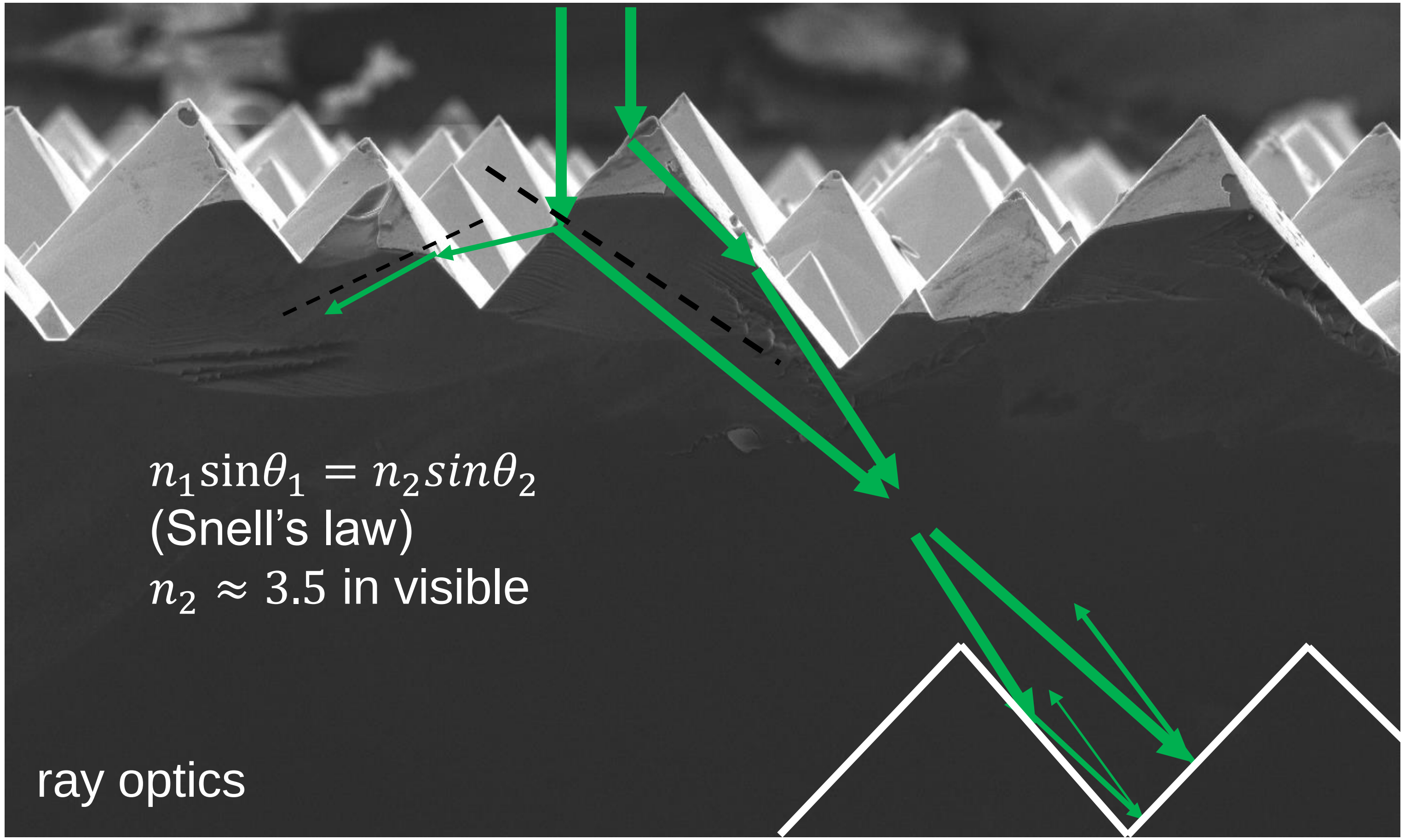
assumes ideal front
anti-reflection,
ideal back reflector



Redfield, APL (1974)

Workaround: path enhancement by texture

Natural texture: 111 facets of 100 surface



Ideal facet angle: 54.7°

Reduced reflection by surface texture

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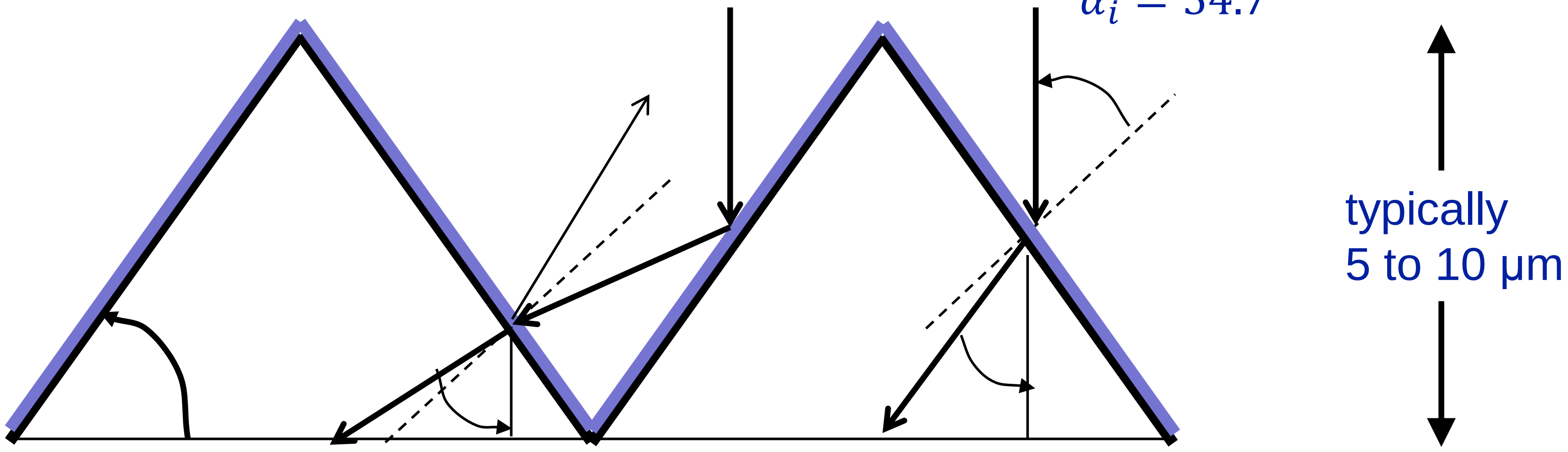


$\alpha_i = 54.7°$

$\alpha_{111} = 54.7°$

$\alpha_2 = 59°$

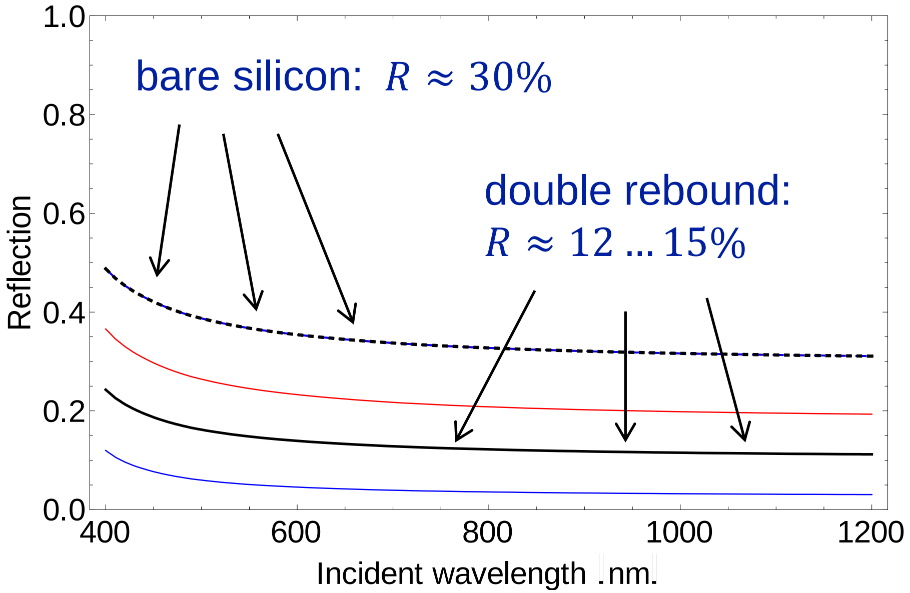
$$\alpha_1 = \alpha_i - \arcsin\frac{\sin\alpha_i}{n_{Si}} \approx 54° - 13° = 42°$$

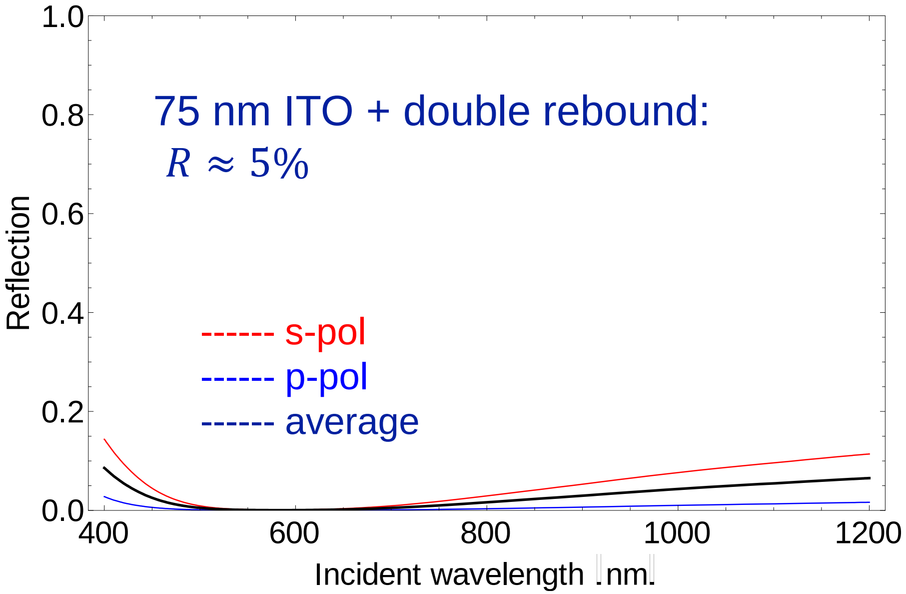
If facet angle >45°: forward scattering with second hit (double rebound)

AR properties

AR coating: depending on technology

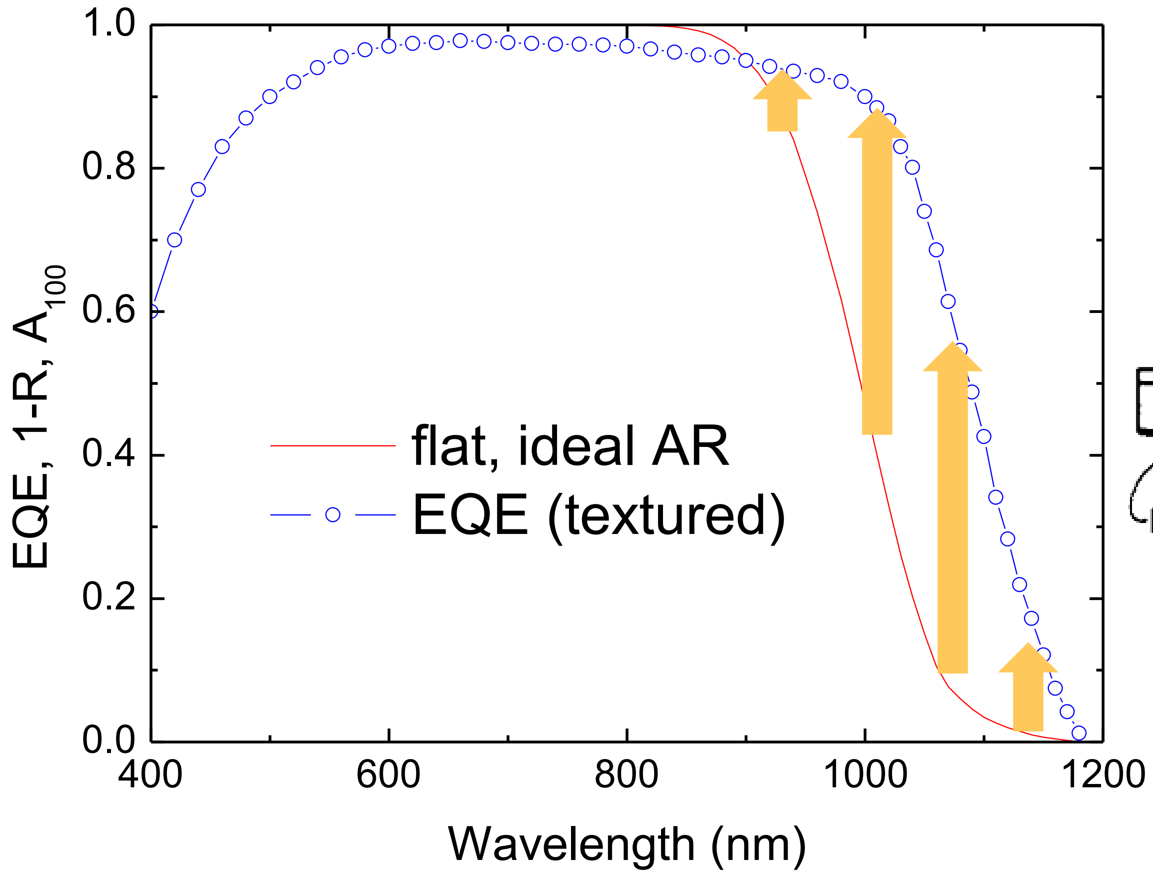
- SiO_2/Si_3N_4: passivation for diffused p-n junction cells
- ITO: electric contact in heterojunction cells

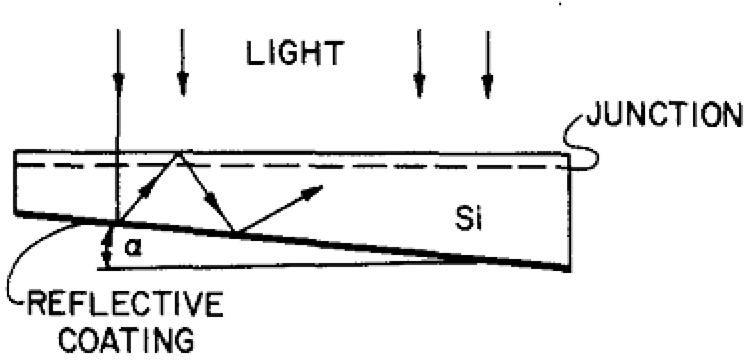




Texture and passivation/contact are mandatory => AR is “free”
Any additional feature incurs cost (e.g. double AR coating, etc.)

Enhanced absorption by surface texture





concept:: Redfield, APL (1974)
data: e.g. Holman, JAP (2013)

Light trapping in (thick) c-Si cells

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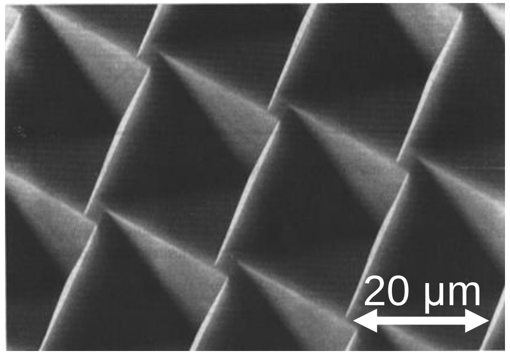
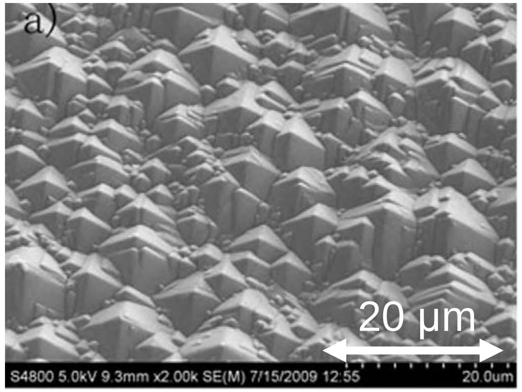
c-Si high eff. cells:
inverted pyramids
(lithography: costly)



Apply geometric ray tracing to one square

from Goetzberger, Sonnenenergie (1997)

mc-Si low cost option:
random etch



Need to describe random scattering

from Xiao, Appl. Surf. Sci. 257, p472, (2010)

State of the art texture on mono-Si(100)

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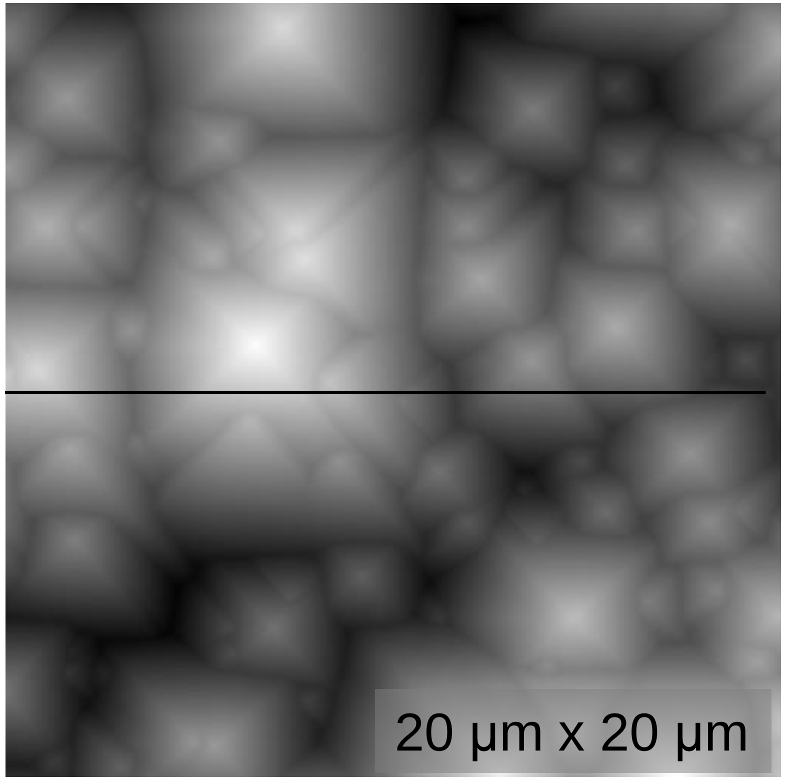
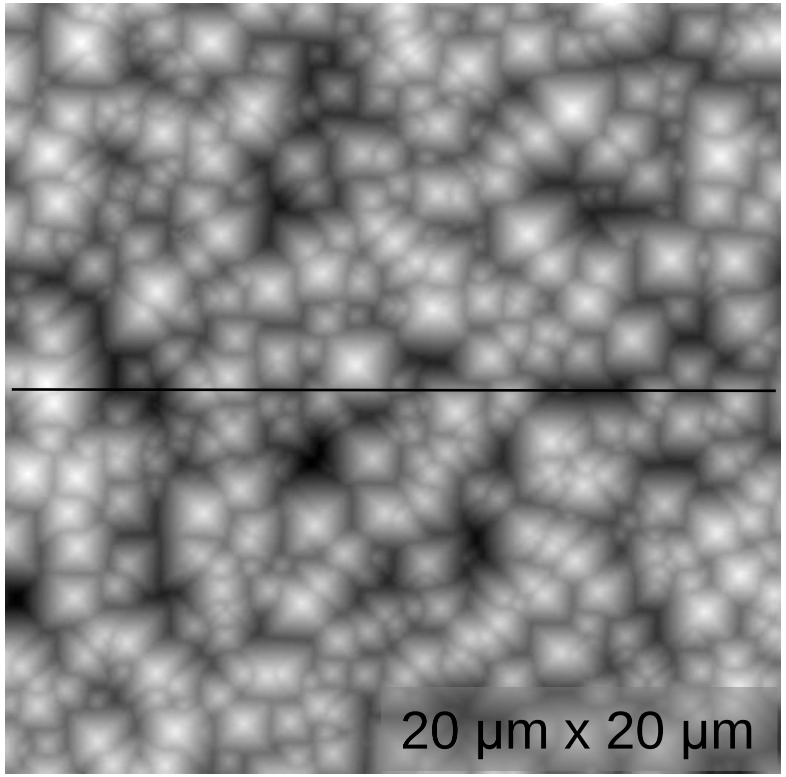


typical texture for HIT solar cells



test structure w. small features

smaller feature size interesting for thin wafers (<100 µm) or exfoliated epi-layers

Haug, Opt. Express (2017)

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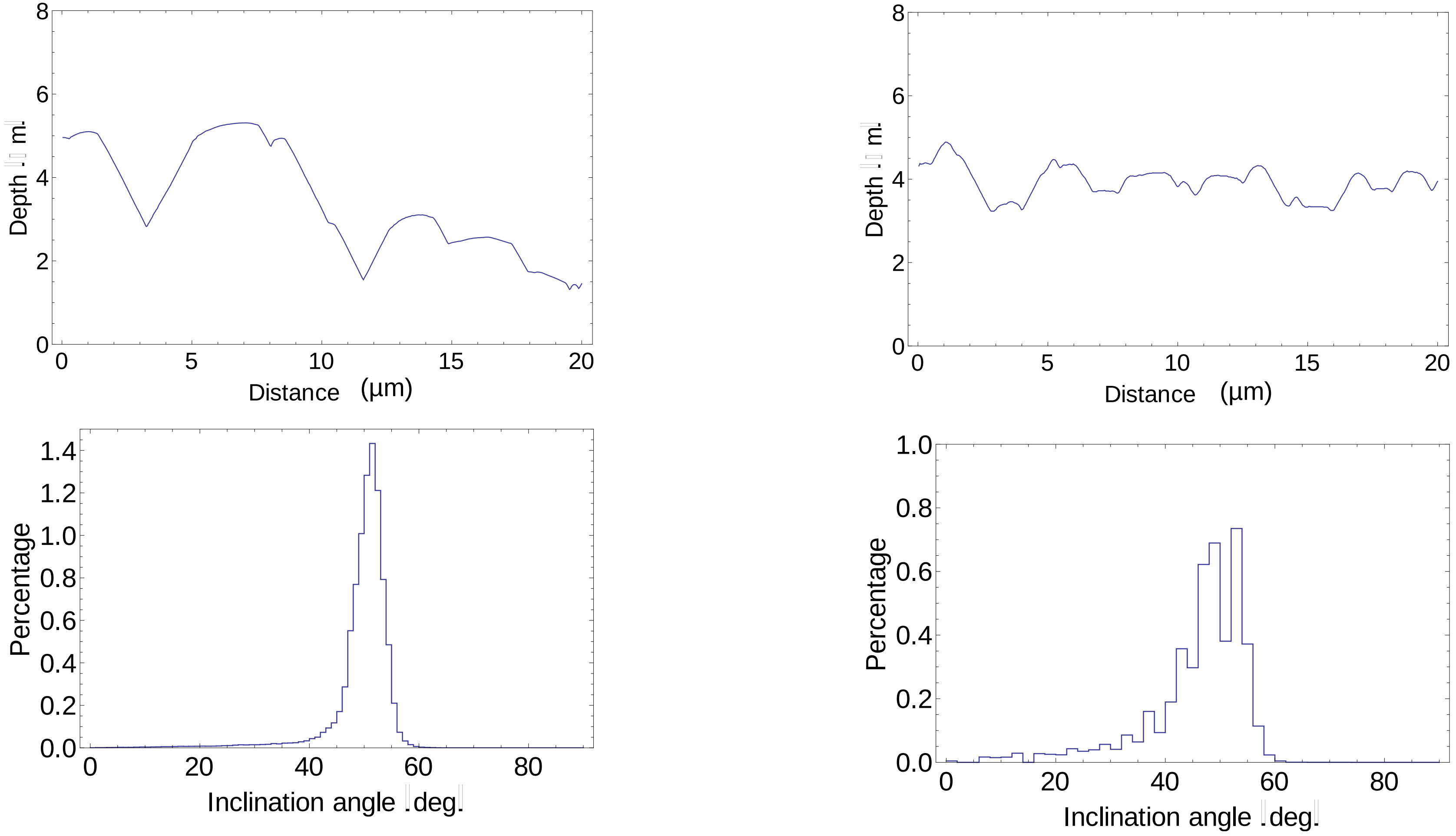
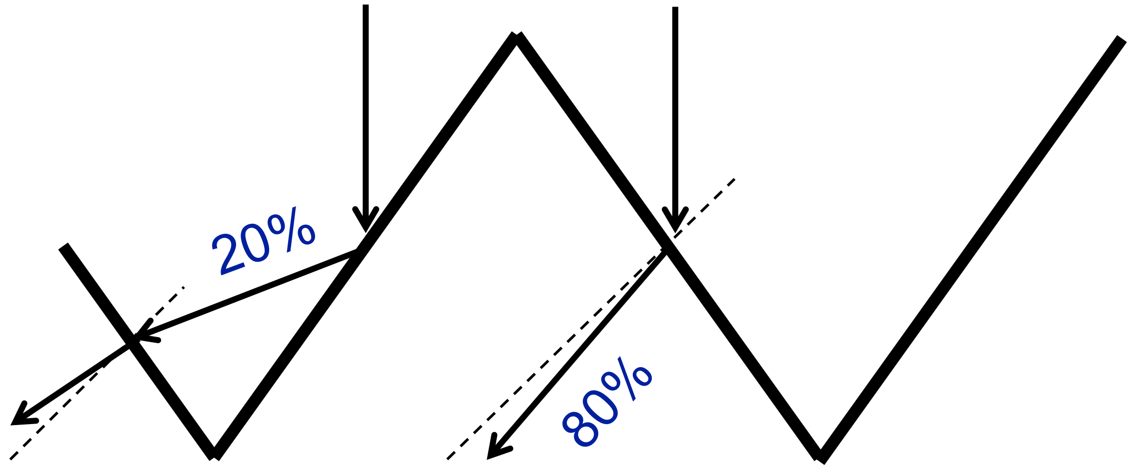
State of the art texture on mono-Si(100)



close to theoretical facet angle (54.7°)

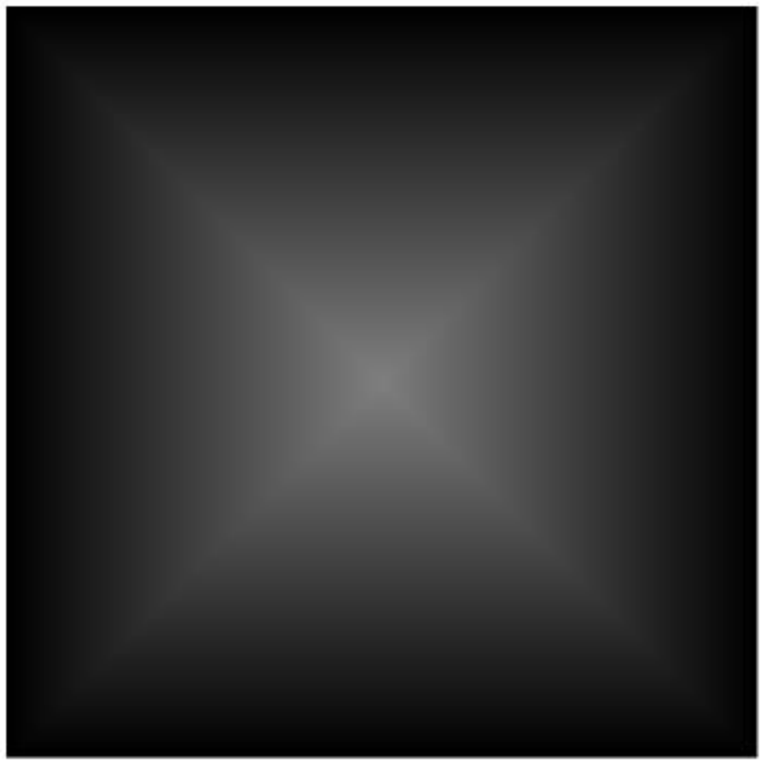
Ray tracing

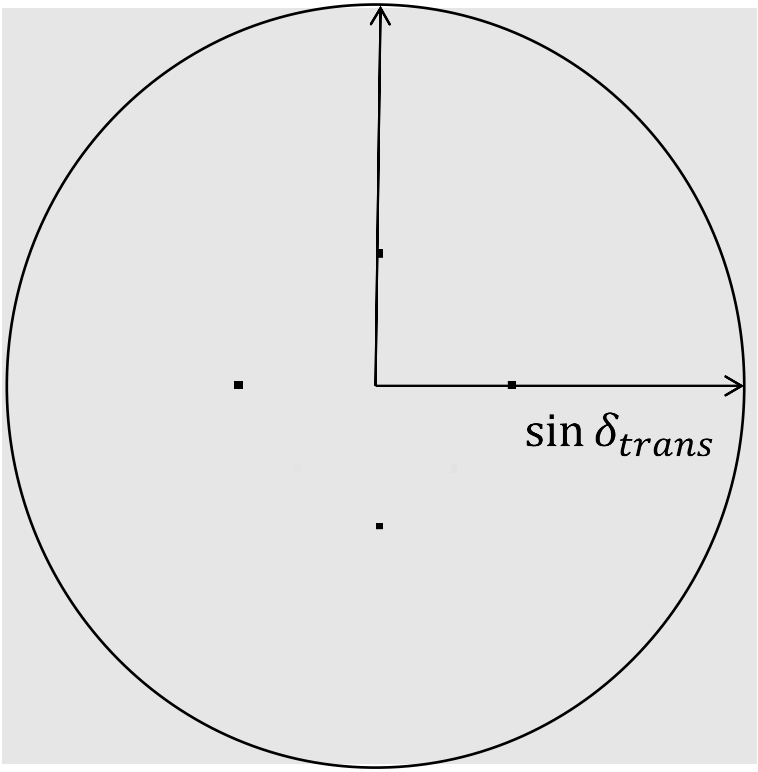


large pyramids (> 5 µm):
adequately treated by ray tracing

$$\vec{t} = \frac{n_1}{n_2}\vec{\imath} + \left(\frac{n_1}{n_2}\cos\theta_i - \sqrt{1 - \left(\frac{n_1}{n_2}\right)^2 (1 - \cos^2\theta_i)}\right)\vec{n}$$

Ray tracing

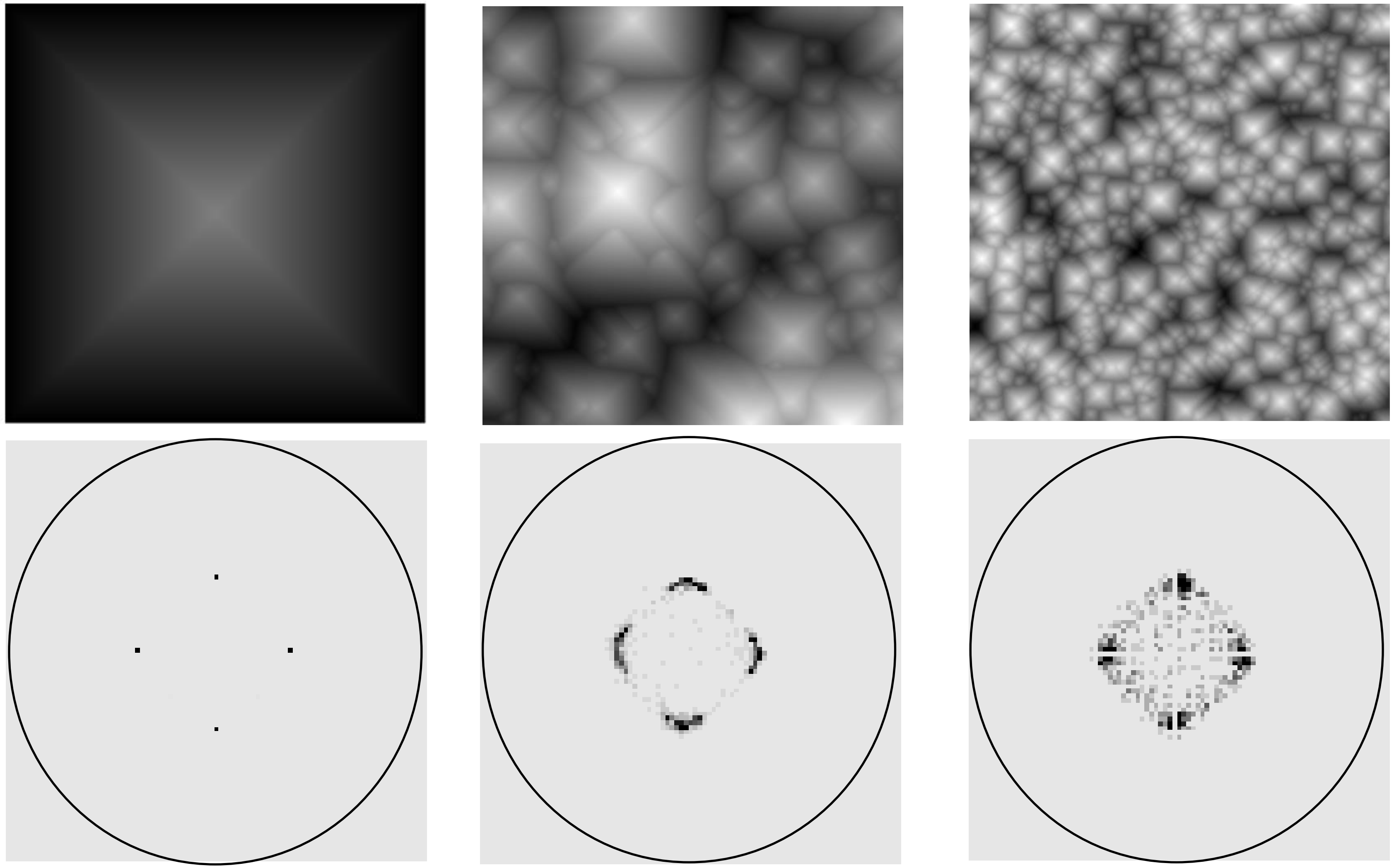




Example: 1000 rays, reflective boundaries, $n_{543\ nm}$ =1.5 (typical polymers)

Circle of direction cosine separates propagating from evanescent modes (for later use)

Ray tracing



Isotropic scattering (Lambertian)

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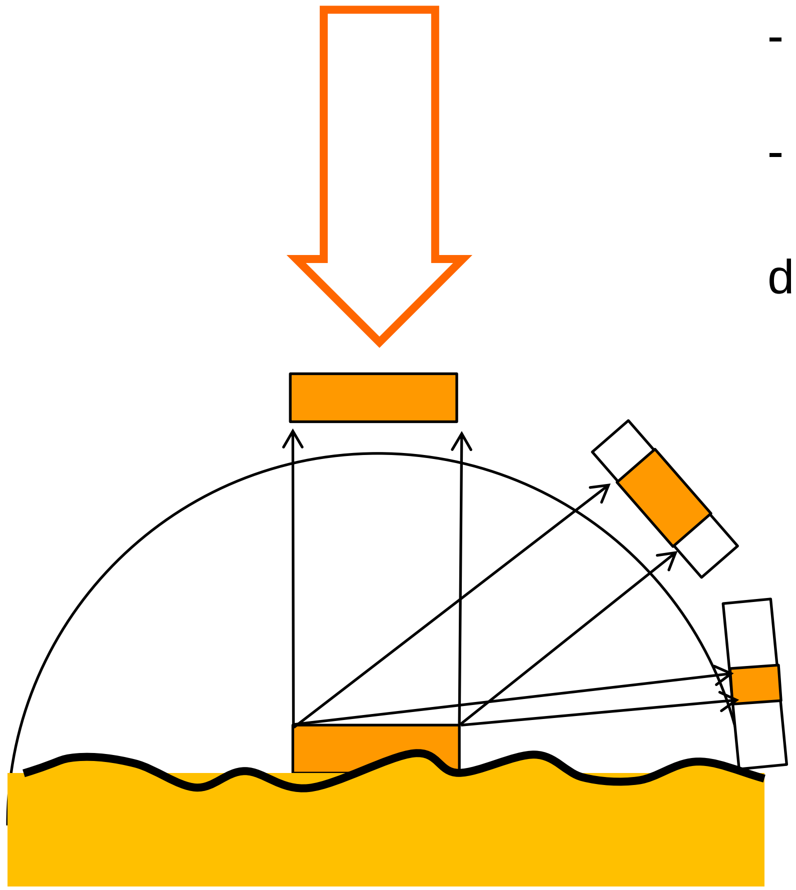

Concept:
- surface scatters equally in all directions
  (e.g. white paper, projection screen, etc.)
- angular dependence because of projection

described by: $ARS_{Lambert} = \frac{1}{\pi}\cos\theta$

Lambert, Photometria (1760)

Lambertian path prolongation

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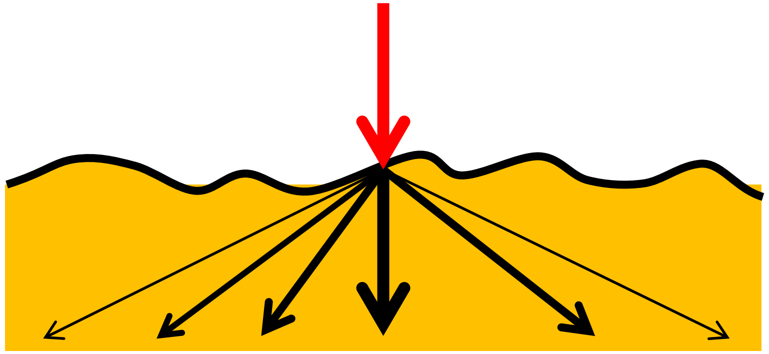
Prolongation of an oblique path

$$d' = d/\cos\theta$$



Average prolongation

$$d_{av} = \int d' \cdot ARS_{Lambert} d\Omega$$

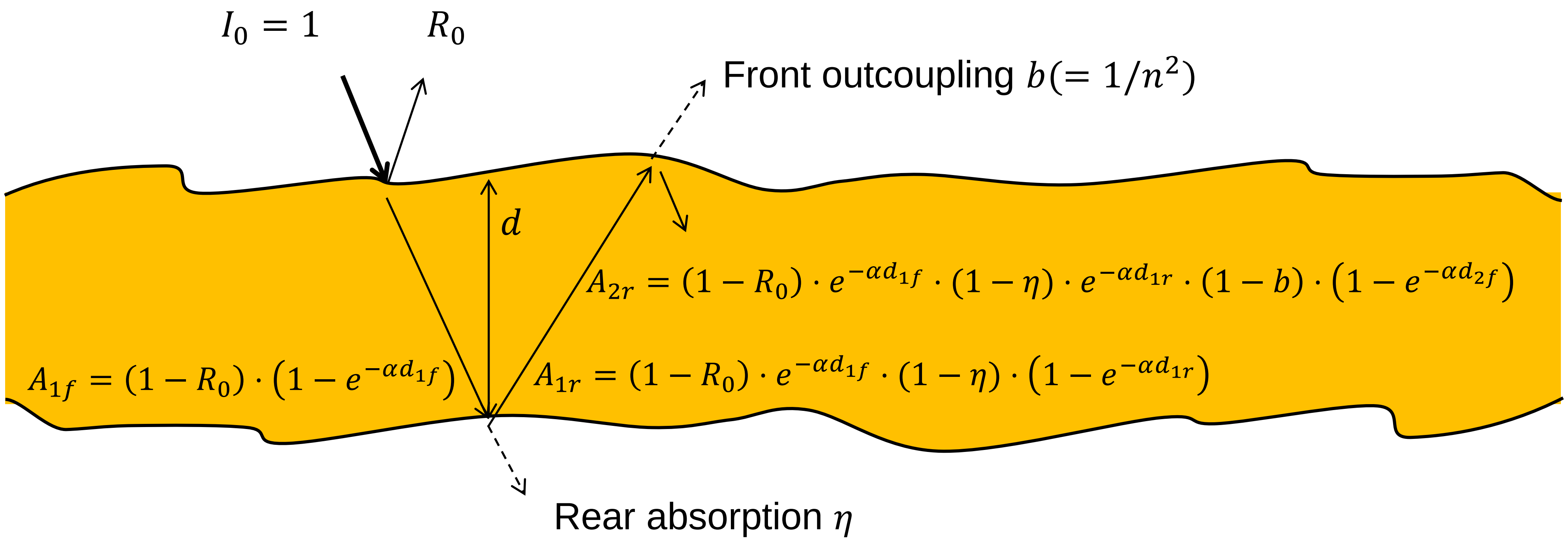
$$= 2\pi \cdot \int \frac{d}{\cos\theta} \cdot \frac{\cos\theta}{\pi} \cdot \sin\theta \, d\theta = 2 \cdot d$$

weighting factor, probability to find angle btw. θ and $\theta + d\theta$

length of oblique path

A very simple (but illustrative) analytic model

Sum up absorption upon bouncing forth and back

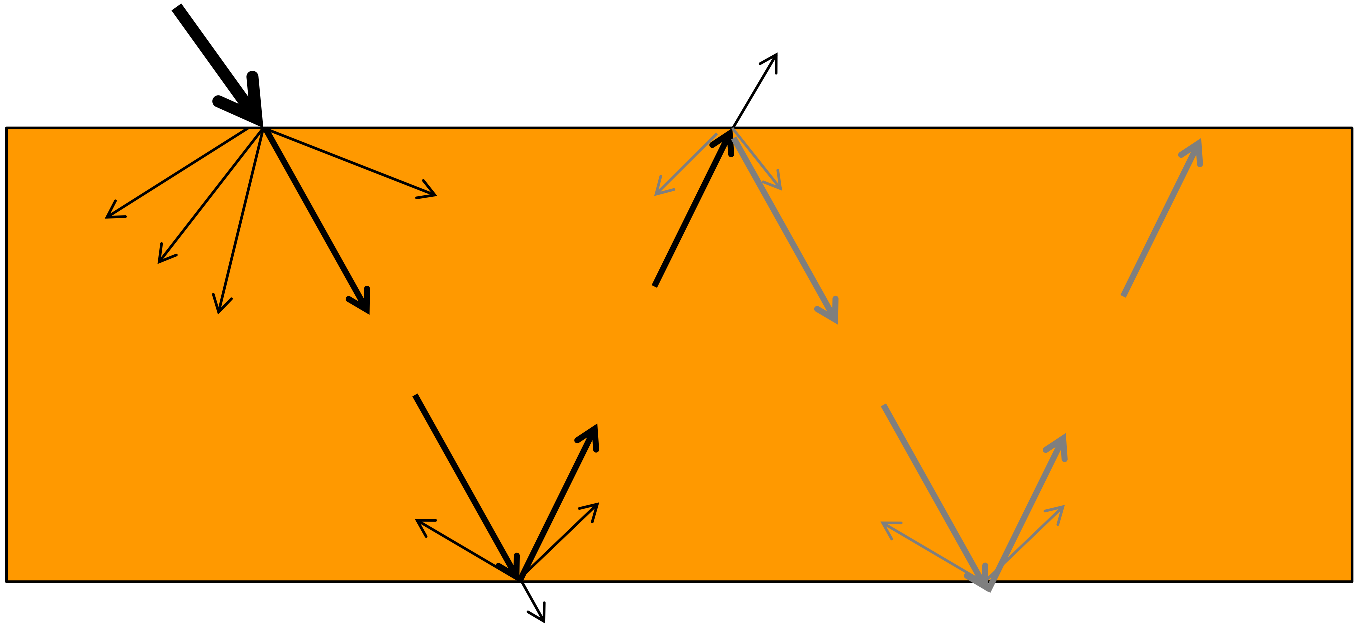


d_{1f}: average length after 1st scattering event

d_{1r}: average length after scattering at rear

Deckman, APL (1982)
Boccard, APL (2012)

Geometric series with scattering



Add absorption after each rebound (Lambertian path length, x2)

$$A = \sum_{k=0}^{\infty} \underbrace{\left[(1-e^{-2\alpha l}) + e^{-2\alpha l}(1-\eta)(1-e^{-2\alpha l})\right]}_{A_{\text{double pass}}} \cdot \underbrace{\left[e^{-4\alpha l}(1-\eta)(1-1/n^2)\right]^k}_{\text{Attenuation}}$$

$$= \frac{1-\eta e^{-2\alpha l} - (1-\eta)e^{-4\alpha l}}{1-(1-\eta)e^{-4\alpha l} + [(1-\eta)/n^2]e^{-4\alpha l}}.$$

$\approx \; 4n^2\alpha l$ if: $\eta = 0, \alpha l \ll 1$

Deckman, APL (1983)
Boccard, APL (2012)
Yablonovitch, TED (1982)

Upper limit of light trapping

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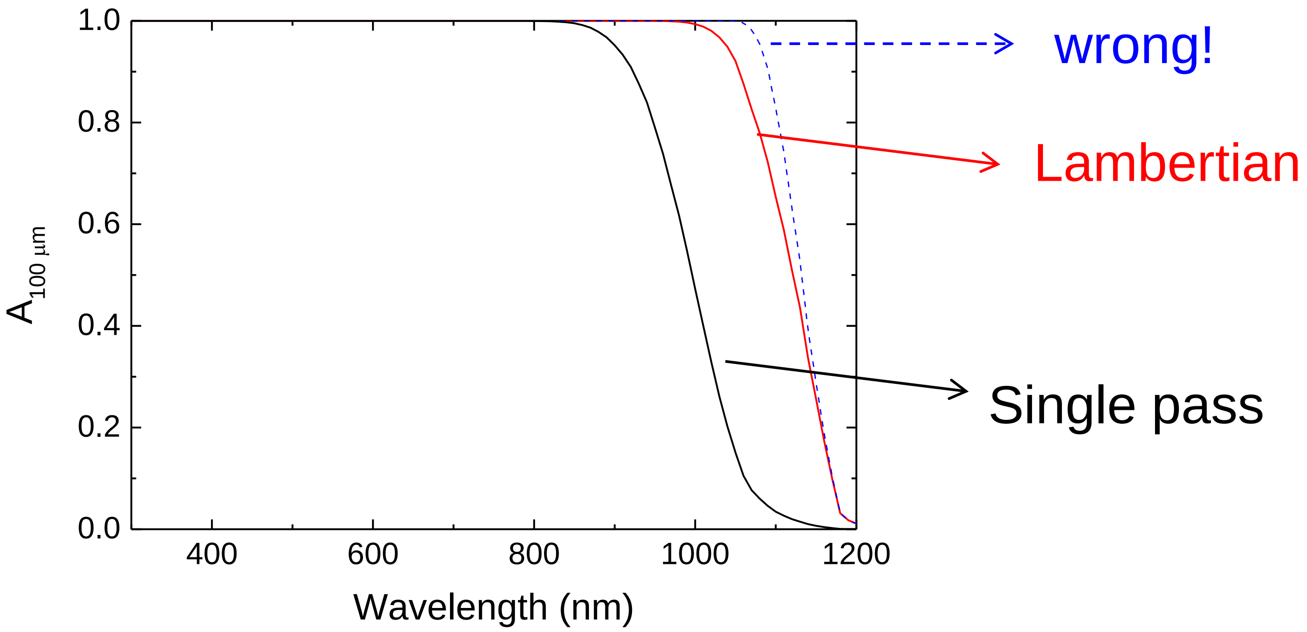
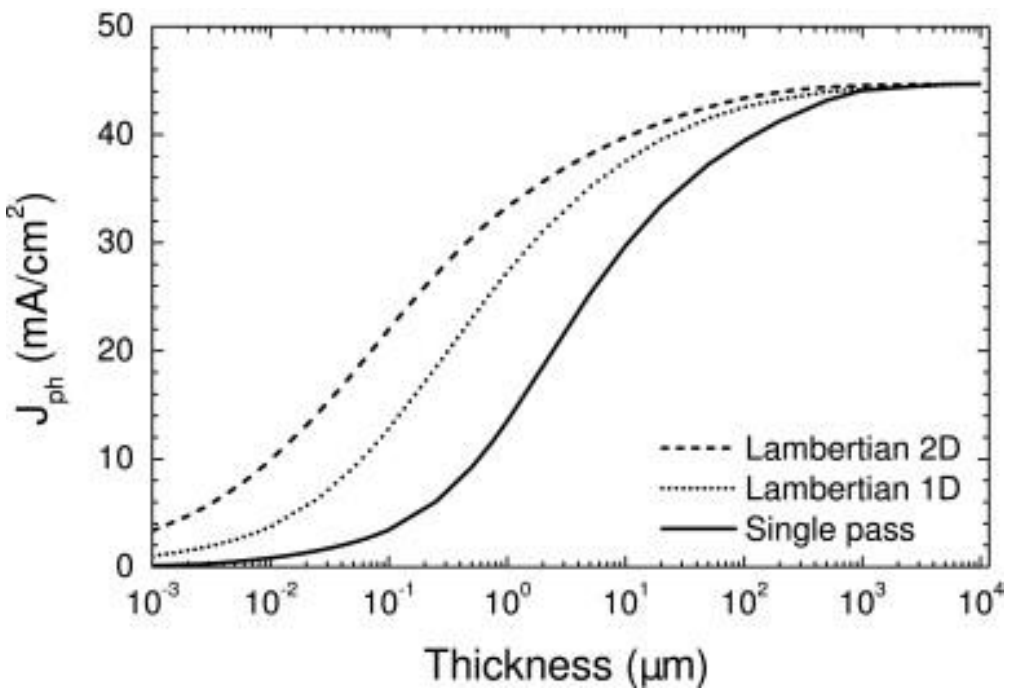


Single pass (100 µm): $A = 1 - e^{-\alpha l}$

Lambertian enhancement: $$A = \frac{1 - e^{-4\alpha l}}{1 - e^{-4\alpha l} + 1/n^2 \cdot e^{-4\alpha l}}$$

Attention, Yablonovitch's formula is often used wrongly: $A = 1 - e^{-\alpha \cdot 4n^2 l}$

Maximum photocurrent



70 to 100 µm sufficient for almost-ideal absorption

Issue: most surfaces don't scatter Lambertian
maybe for some, but not for all wavelengths

Andreani, SolMat (2015)

Wavelength dependence: recall radar science

Incoherent scattering intensity, parameterize via rms roughness

$$R_{spec} = R_0 \cdot \exp\left\{-\left(4\pi \cdot \sigma_{\mathrm{rms}} / \lambda\right)^2\right\}$$

$$R_{diff} = R_0 - R_{spec}$$

Davis, Proc. Inst. Electr. Eng. 101, p209, (1951)
Rice, Commun. Pure. Appl. Math. 4, p351 (1954)
Bennett, J. Opt. Soc. Am. 51, p123, (1961)

Haze:

$$H_R = R_{\mathrm{diff}} / R_{\mathrm{tot}}$$

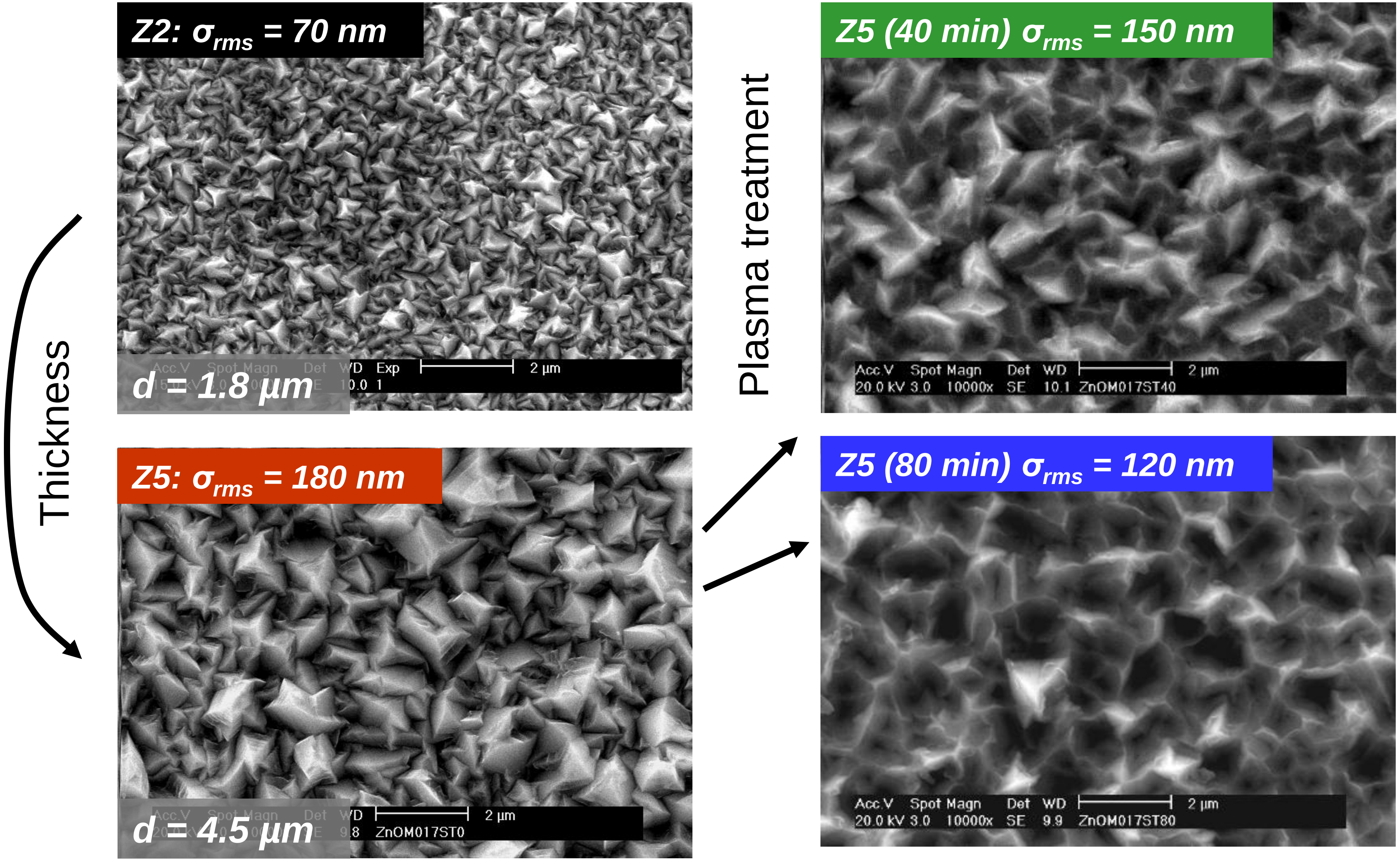
$$H_T = T_{\mathrm{diff}} / T_{\mathrm{tot}} = 1 - \exp\left\{-\left(2\pi / \lambda \cdot \sigma_{\mathrm{rms}} \cdot \left|n_1 \cos\theta_i - n_2 \cos\theta_t\right|\right)^2\right\}$$

Needs: assumption or surface profile data for σ_{rms}

Carniglia, Opt. Eng.18, p104, (1979)

Empiric modifications:
effective roughness σ_{eff}, usually less than AFM roughness σ_{rms}
replace exponent 2 by δ, e.g. 3 or 3.5

Examples: texture of LPCVD-ZnO



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Description of haze: scalar theory

$$H_T = T_{\text{diff}} / T_{\text{tot}} = 1 - \exp\left\{ -\left(2\pi / \lambda \cdot \sigma_{\text{rms}} \cdot \left| n_1 \cos\theta_i - n_2 \cos\theta_t \right| \right)^{\delta} \right\}$$

Exponent δ:

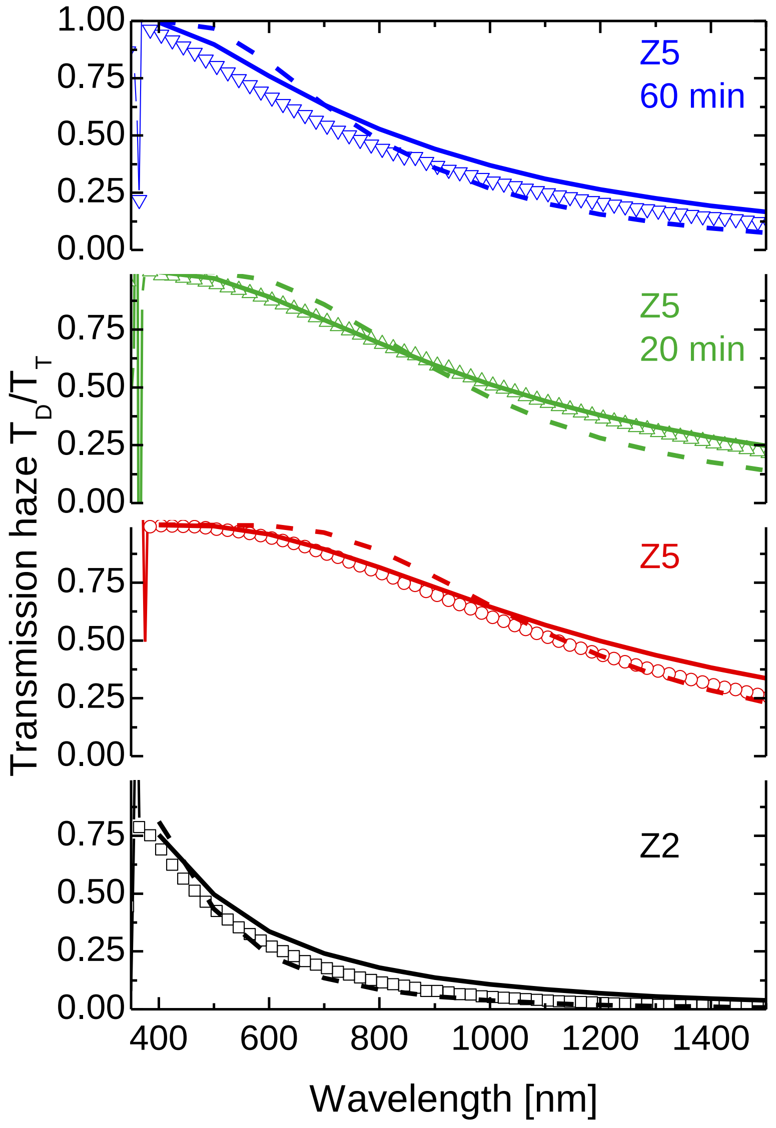
- scattering theory: $\delta = 2$ →
- literature (empiric): $\delta = 3$ - - →

Roughness σ:

- shown: $\sigma_{rms} = \sigma_{AFM}$
- literature (empiric): $\sigma_{rms} < \sigma_{AFM}$

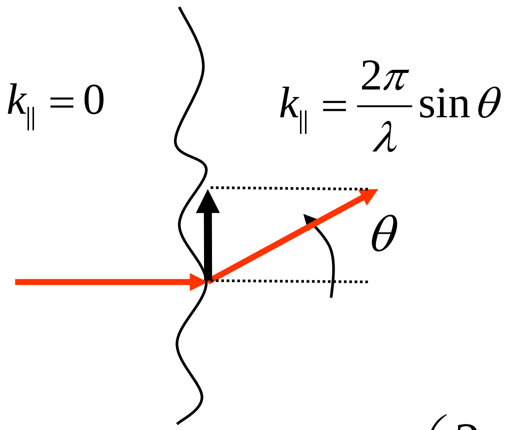
Not applicable to wide spectral range

Changes of δ and σ_{rms} remain empiric



Angular intensity distribution (ARS)

- Assumed (e.g. Lambertian, $ARS_L = 1/\pi \cdot \cos\theta$)
- Measure ARS, project to other interfaces and wavelengths
- Estimate momentum change via power spectral density $g(k)$



$$ARS(\theta) \sim g(k_x)\cdot\cos\theta = g\left(\frac{2\pi}{\lambda}\sin\theta\right)\cdot\cos\theta$$

Needs: assumption or surface profile data for $g(k)$

Angular distribution

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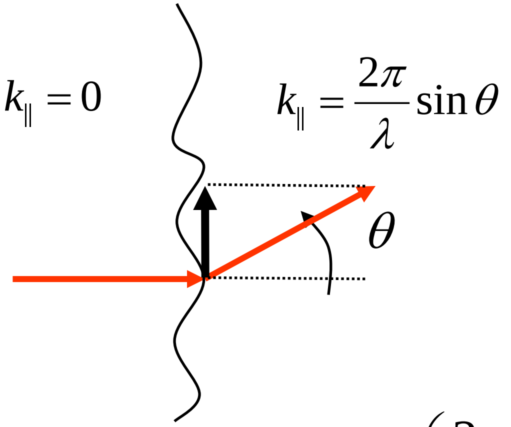
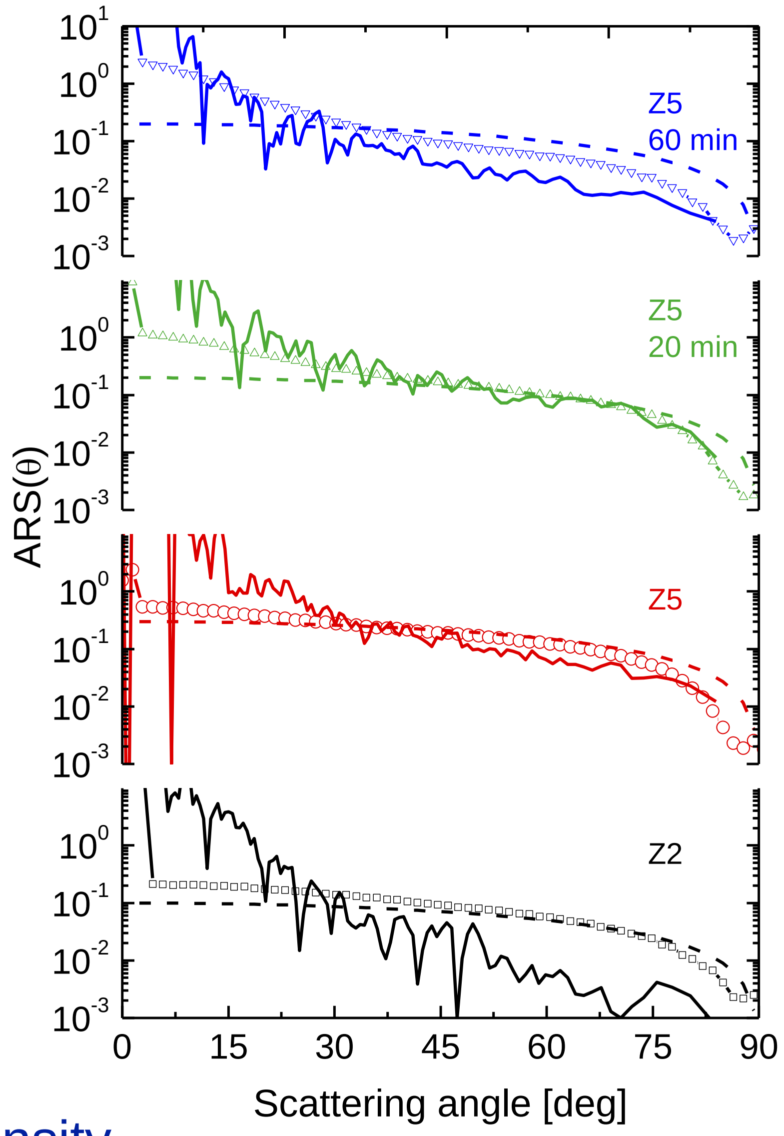
- Measured (symbols: 543 nm)
- Assumed (e.g. Lambertian)
- Estimate momentum change via power spectral density *g(k)*

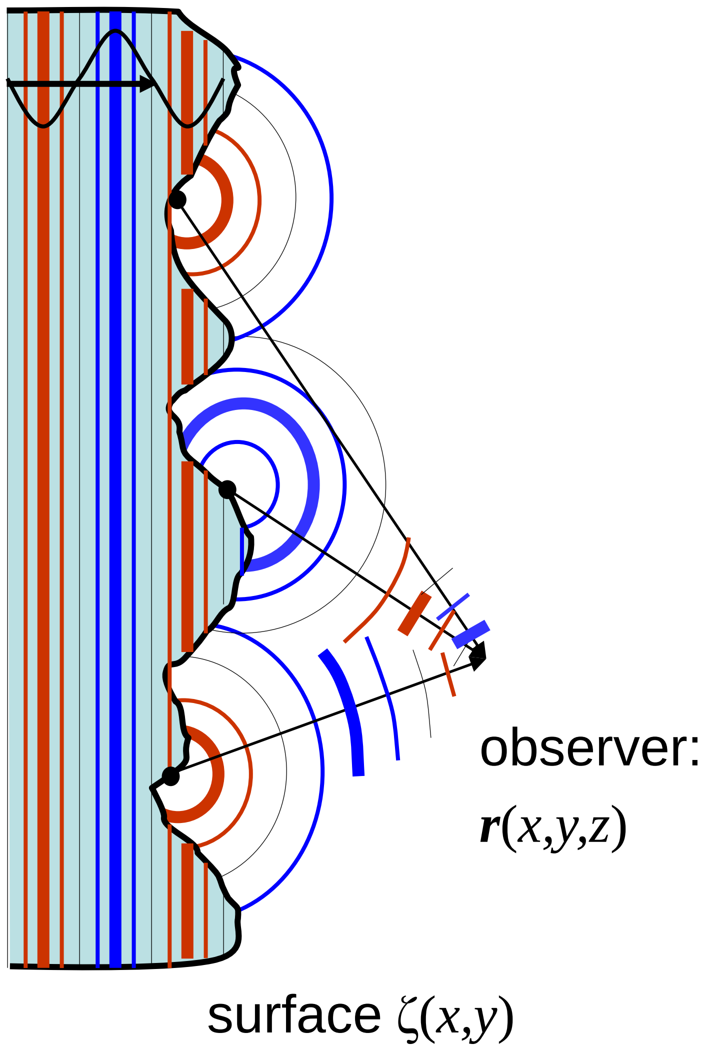


$$ARS(\theta) \sim g(k_x)\cdot\cos\theta = g\left(\frac{2\pi}{\lambda}\sin\theta\right)\cdot\cos\theta$$



- Lambertian too high for high angles
- PSD too high for low angles
- Both: no prediction of specular beam intensity

Alternate approach: Fourier theory



Huygens principle:

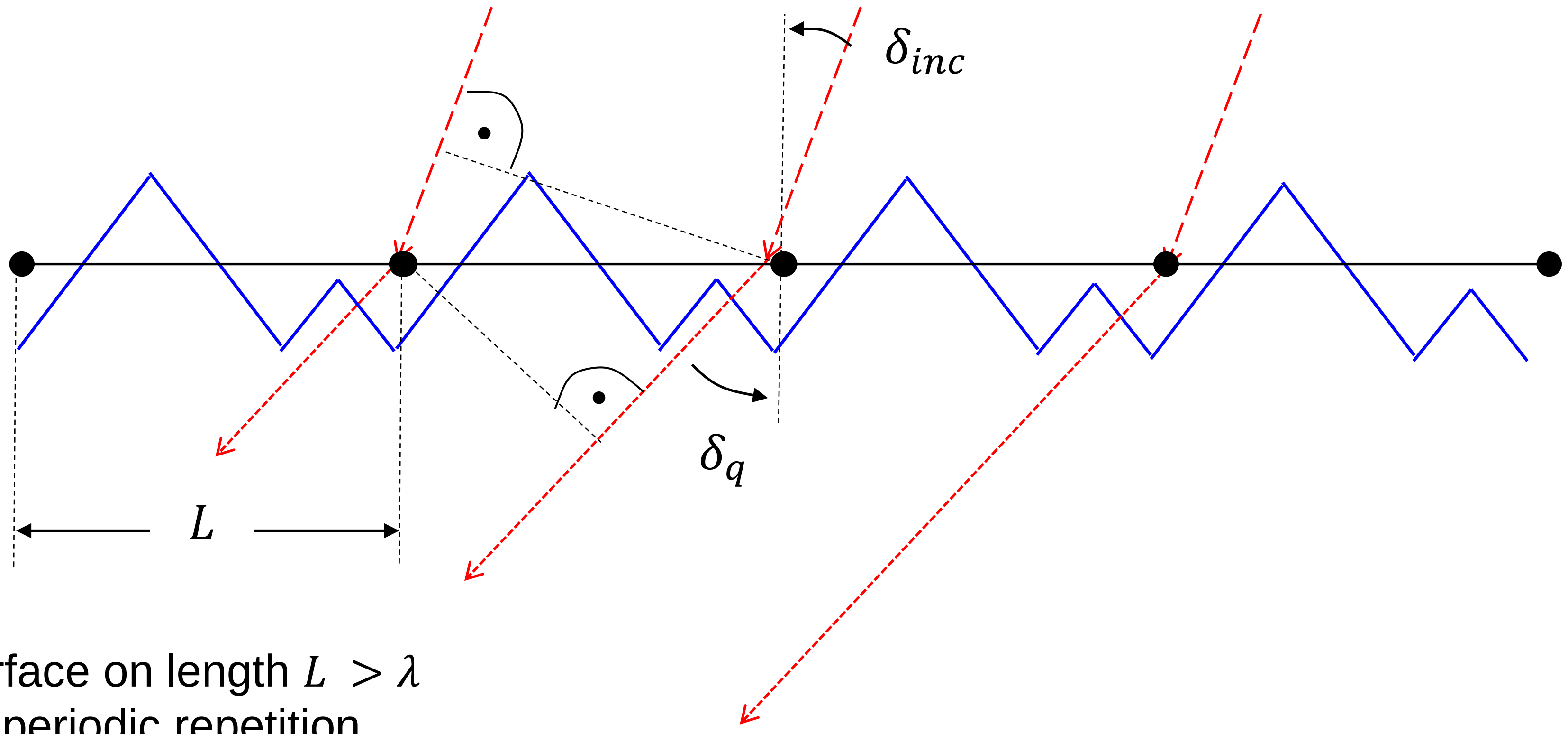
consider field at $\mathbf{r}(x,y,z)$ as superposition of spherical waves emitted from each point $\zeta(x,y)$ with local phase

Two choices of aperture function $U_0(x,y)$:

- **Amplitude modulation**
  for apertures or grey-levels, reproduces PSD (not applicable, ZnO is transparent)
- **Phase modulation**
  more likely, but how to define?

e.g. Goodman, Fourier Optics

Fourier scattering model

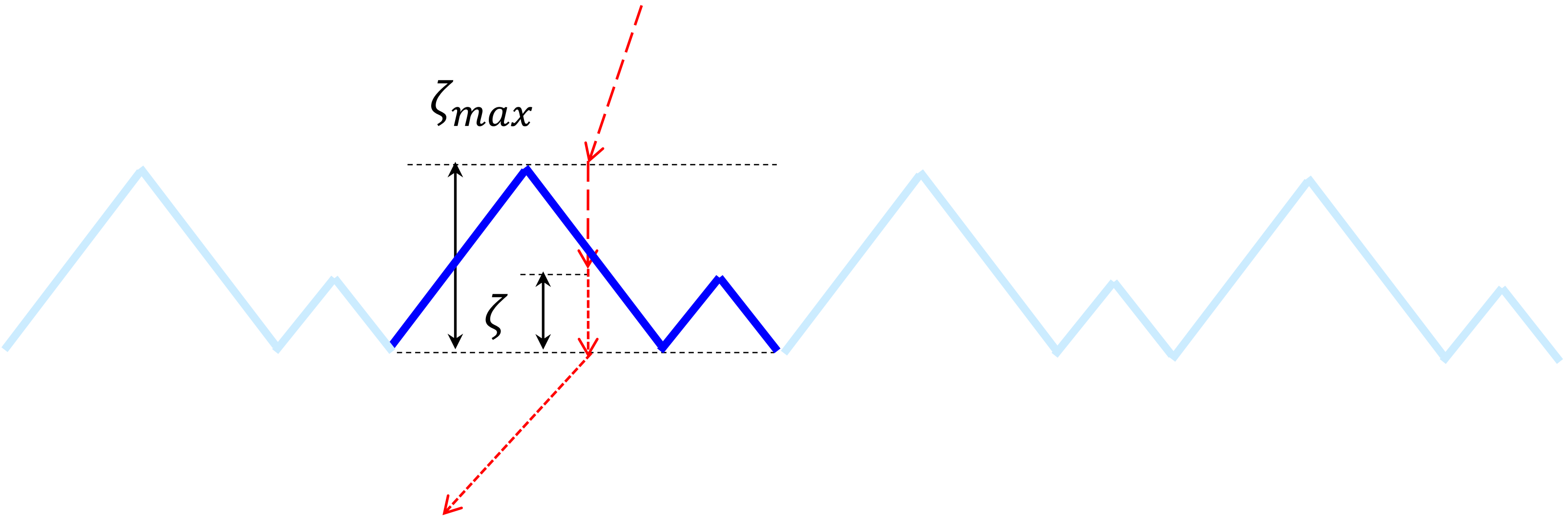


Scan surface on length $L > \lambda$
Assume periodic repetition
Periodicity L diffracts into orders q
Angles given by grating equation

$$n_1 \cdot \sin \delta_{inc} - n_2 \cdot \sin \delta_q = q \cdot \lambda / L$$

Goodman, Fourier Optics

Diffraction intensity



Fourier transform (for discrete 1D-data): $f_q = \frac{1}{\sqrt{N}} \sum_{p=1}^{N} U_t \cdot e^{-2\pi i \cdot p \cdot q / N}$

$U_t(\zeta(p/L))$: phase changing pupil function $U_0 \cdot e^{ik_0[\zeta \cdot n_1 + (\zeta_{max} - \zeta) \cdot n_2]}$

Intensity going into q-th order: $\sim f_q f_q^*$ (more precisely: radiance)

Needs: AFM profile and n_1, n_2; no empiric parameters!

Harvey, Appl. Opt. (1999)
Dominè, JAP (2010)

Propagating and evanescent modes

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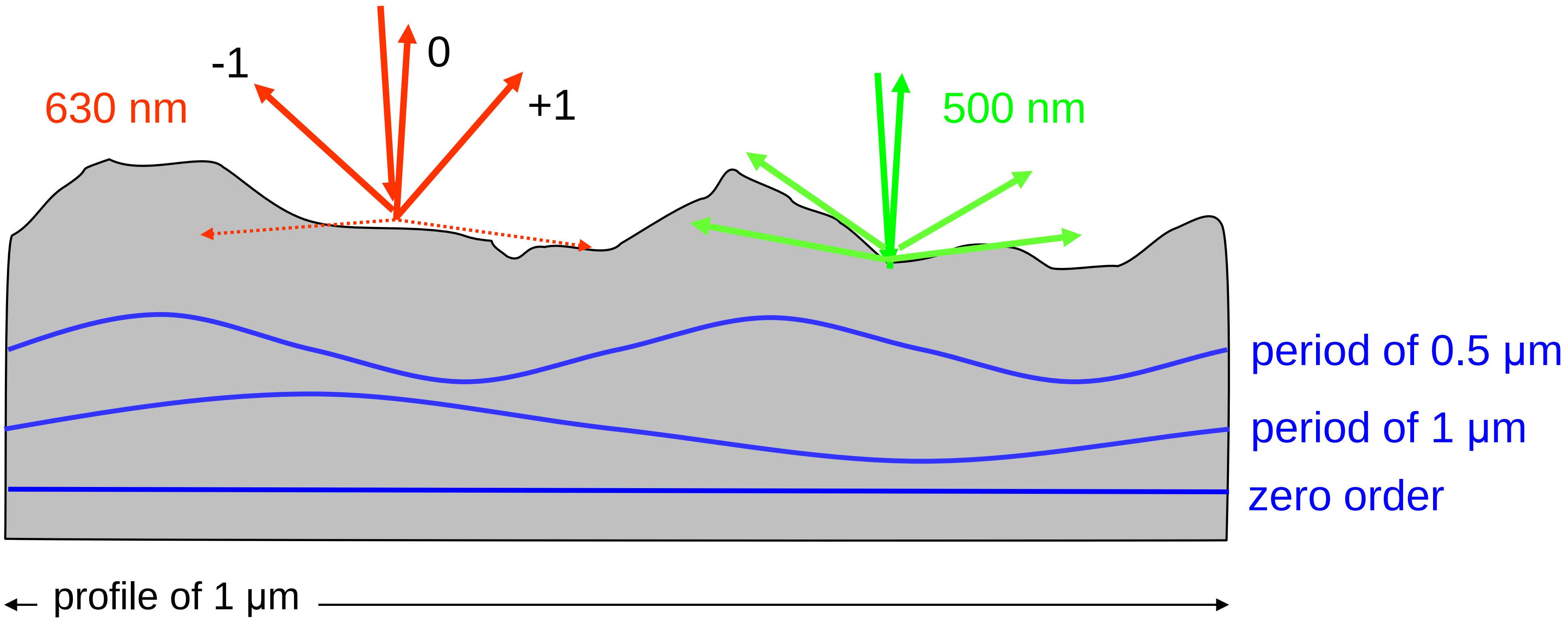
Fourier theory predicts mode amplitudes,
including zero order (specular beam) and evanescent modes

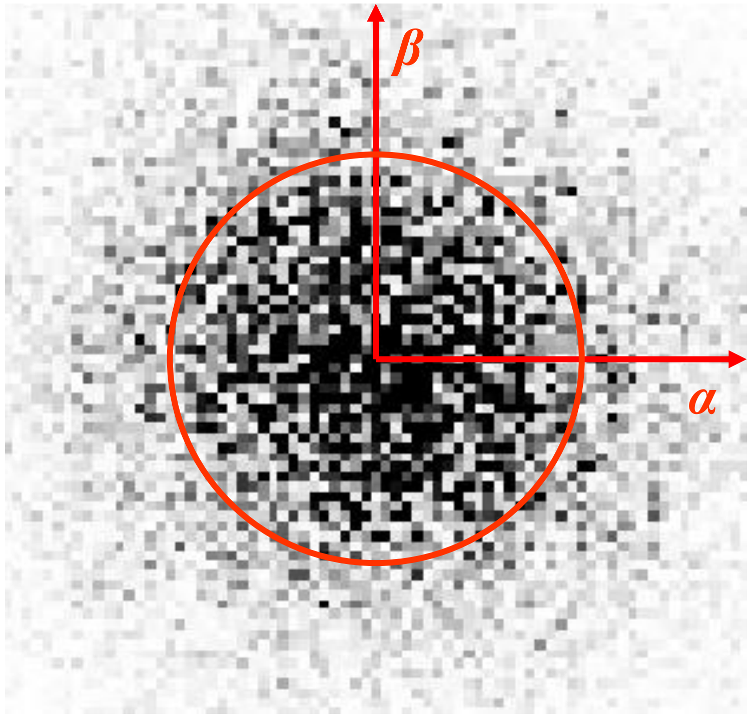
Grating analogy: λ > period: specular reflection, no diffraction



Normalization procedure

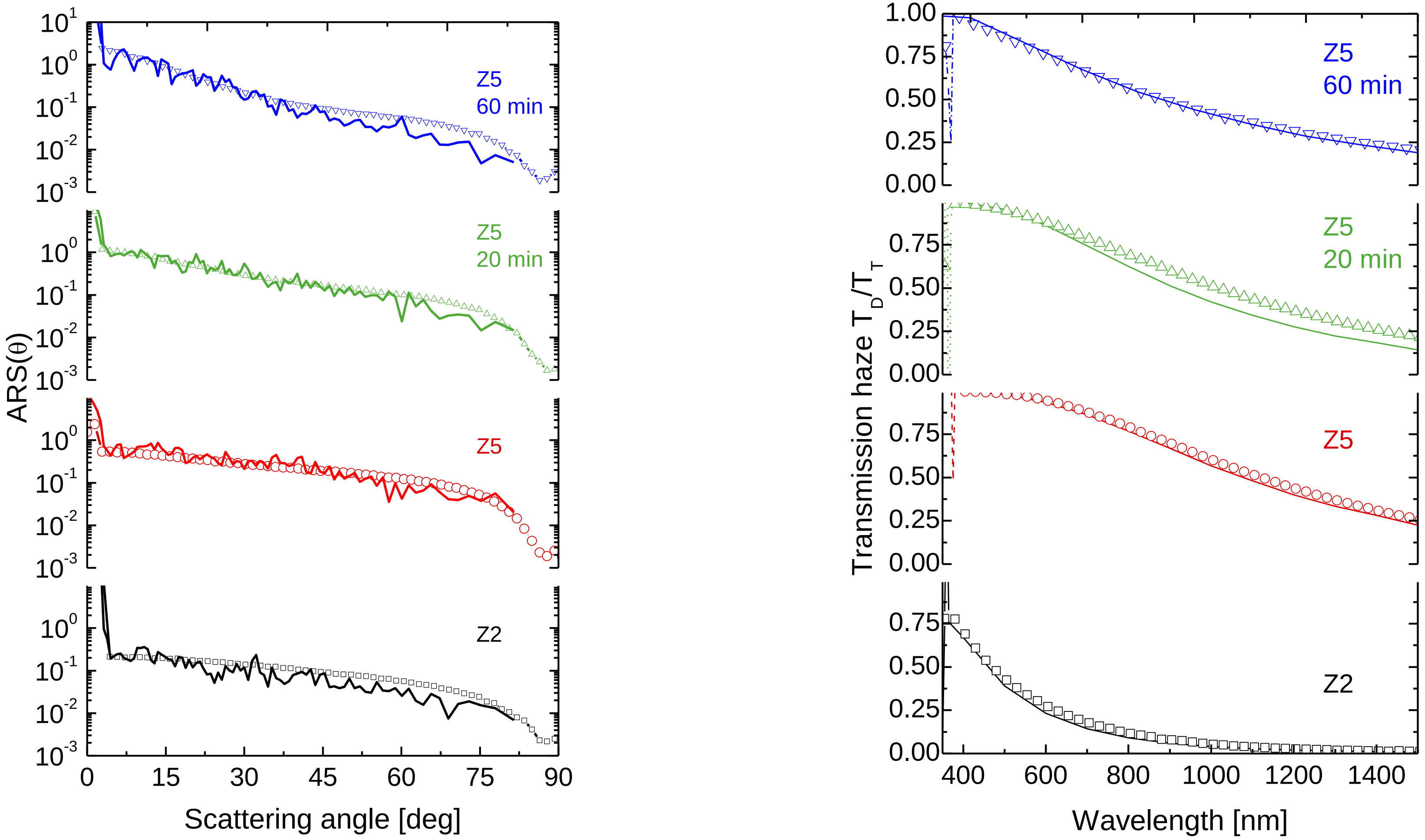
- Find diffraction angles >90°
  convenient index scaling of FFT:
  direction cosine space
- distribute intensity between
  propagating modes only

- ARS: cut along axis, possibly
  polar average
- Haze: ratio of value at origin to
  everything within unit circle



Harvey, Proc. SPIE (1989)
Domine, JAP (2009)

Comparison to experiment

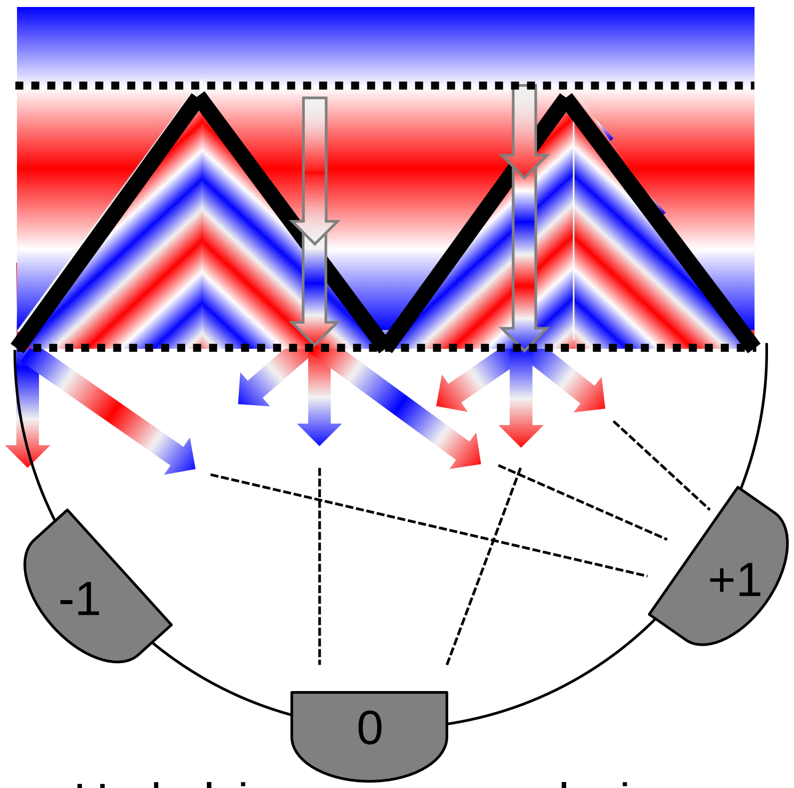


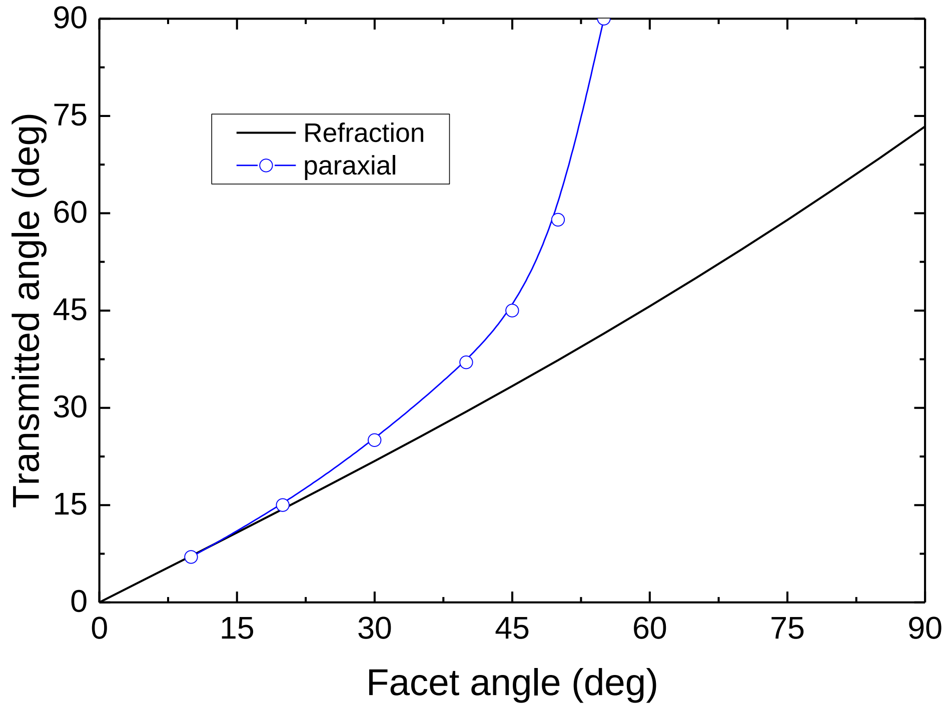
Excellent agreement for ARS at 514 nm and for spectral haze, no empiric parameters

Domine, JAP (2009)

Caveat: paraxial error for large angles

Test: apply to large wedge
($> 10 \times \lambda$, avoid scattering)

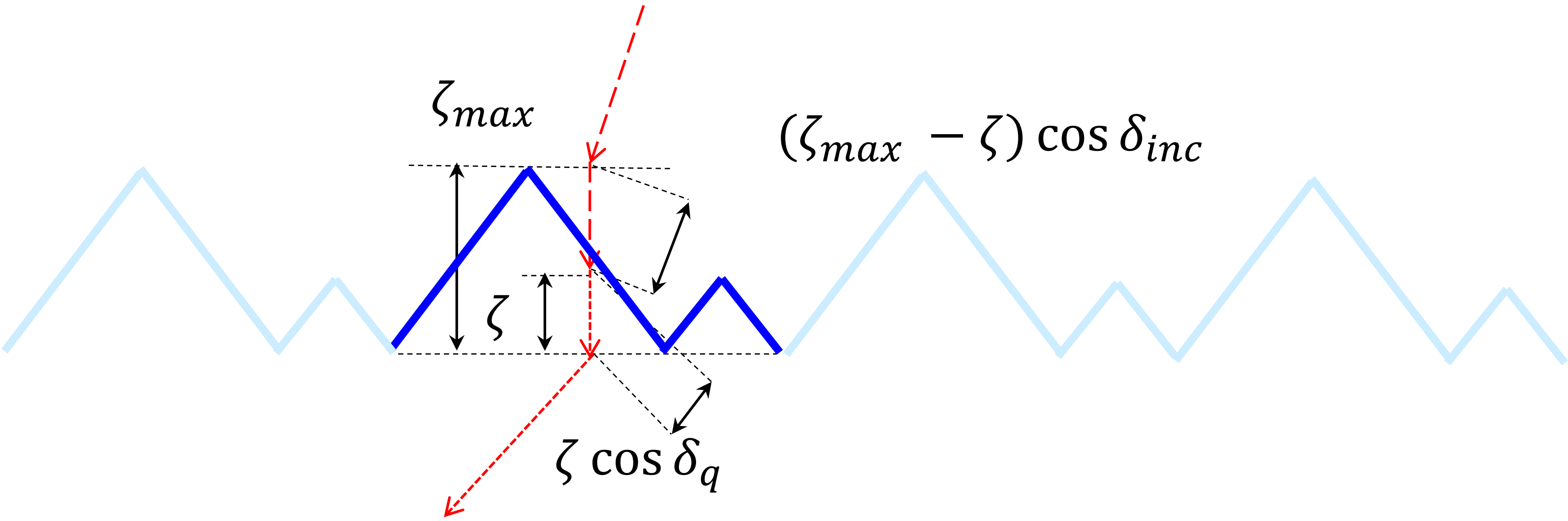




Underlying reason: replacing roughness zone with flat phase screen ignores interference within roughness

D. Dominè, PhD thesis (2009)

Removal of paraxial error

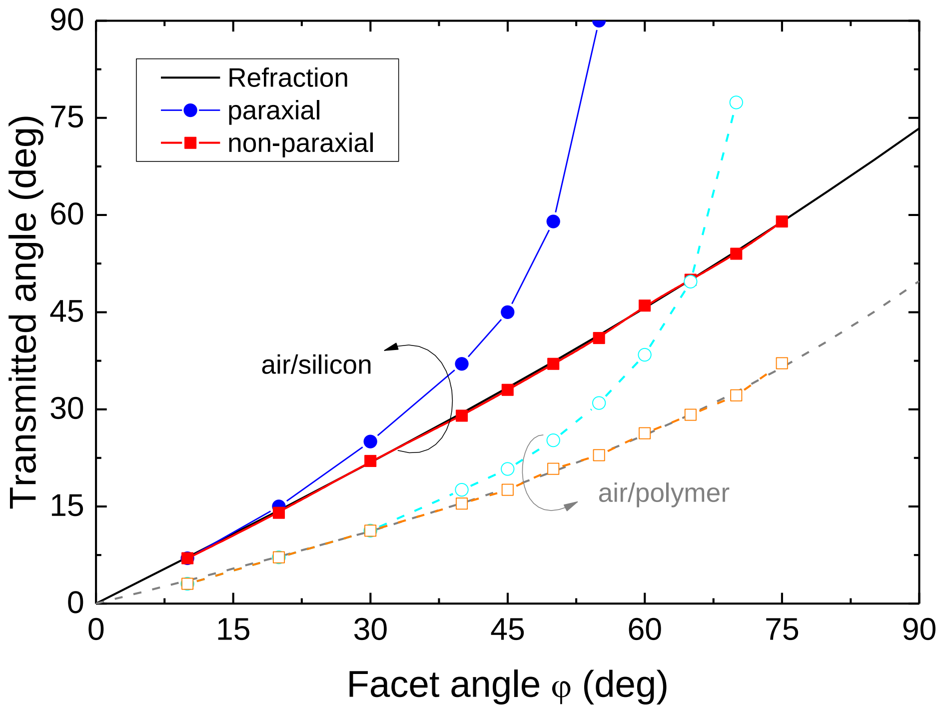


Use projections of surface profile along incoming and outgoing beams

$$\Delta\phi = k_0\left(n_1\cos\delta_{inc} + n_2\cos\delta_q\right)\cdot z(x,y)$$

Harvey, JOSAA (2006)
(defined for reflection)

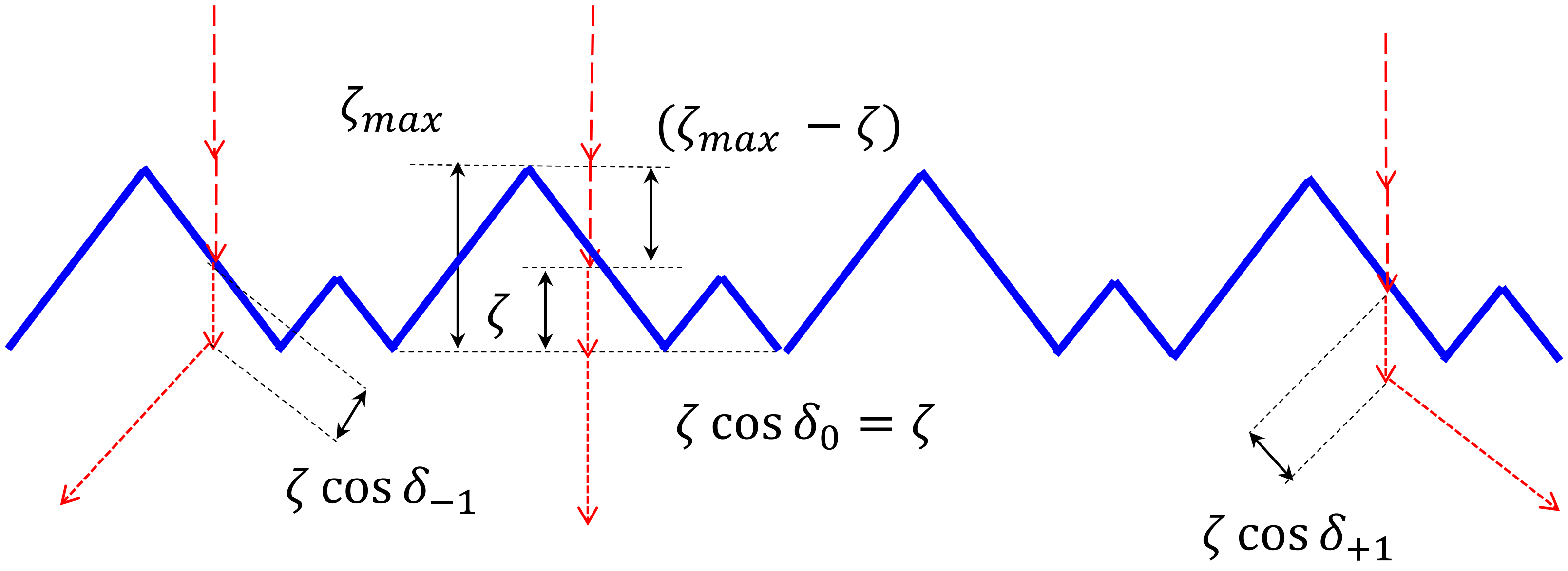
Removal of paraxial error



Corrected Fourier model reproduces Snell's law

Issue: δ_q varies with q = diffraction order
fine for discrete definition, just slow, especially for 2D
BUT: FFT no longer applicable

Workaround



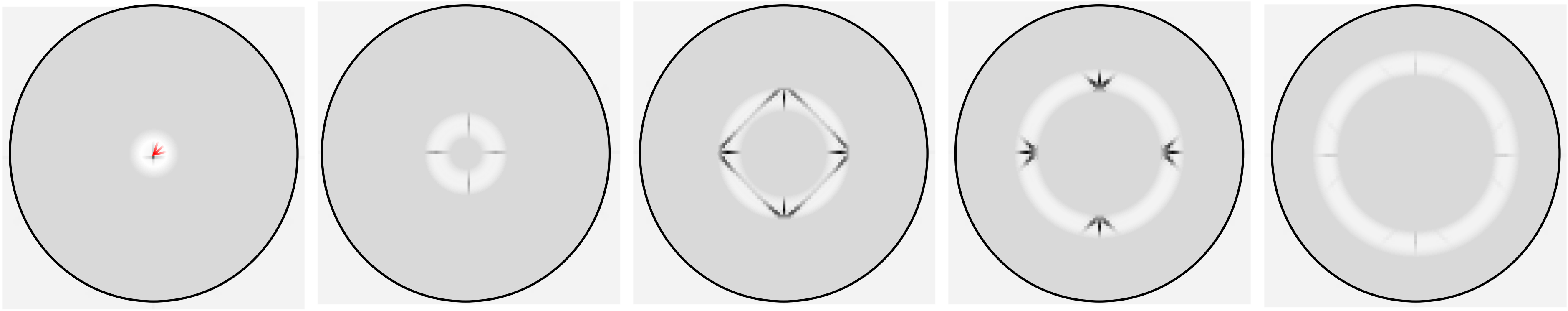
Consider perpendicular incidence
Define U_t for $q = 0$, calculate FFT_0 (fast)
Define U_t for $q = +1$, calculate FFT_1 (fast)
etc.

FFT_1 is also applicable for $|q| = 1$ (great for 2D data!)

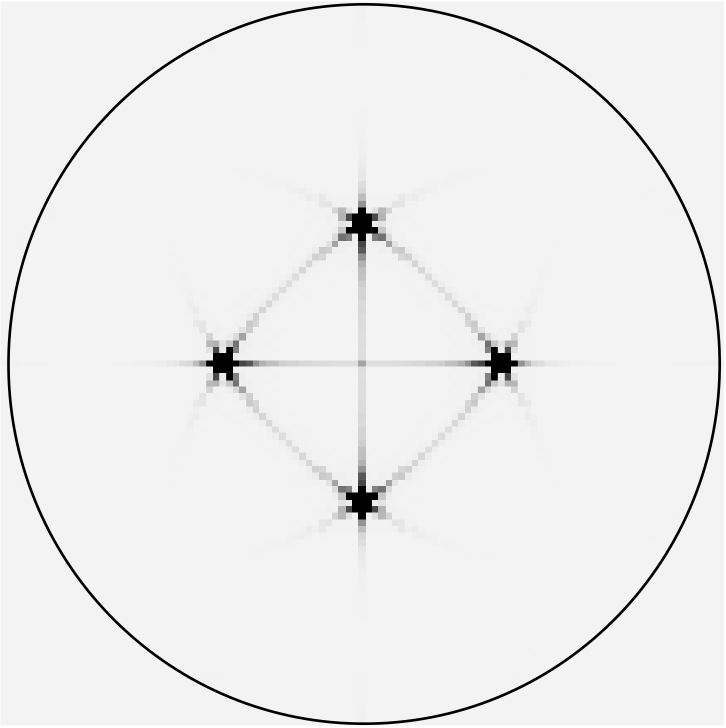
Application

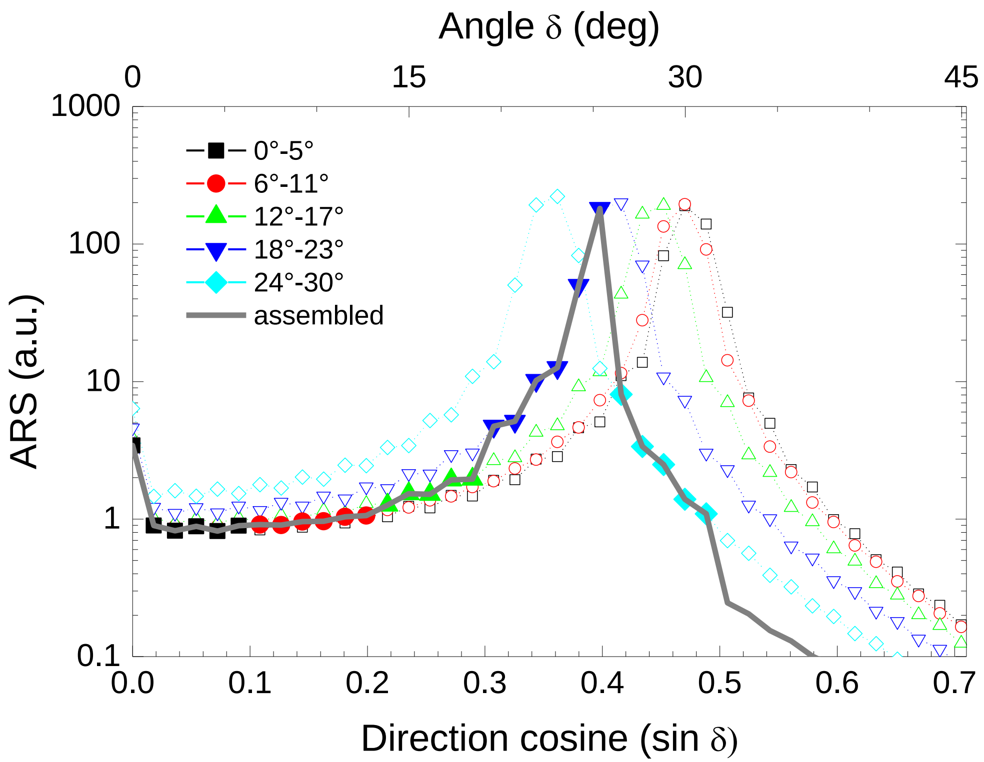
Example: calculate 10 patterns
Perfect pyramid (n =1.5 => Snell refraction into 22.9°)
Perpendicular illumination => rotationally symmetric 2D diffraction patterns

#1: 0…6° #2: 6…11° #3: 12…17° #4: 18…23° #5: 24…30°



Assembly of full characteristic

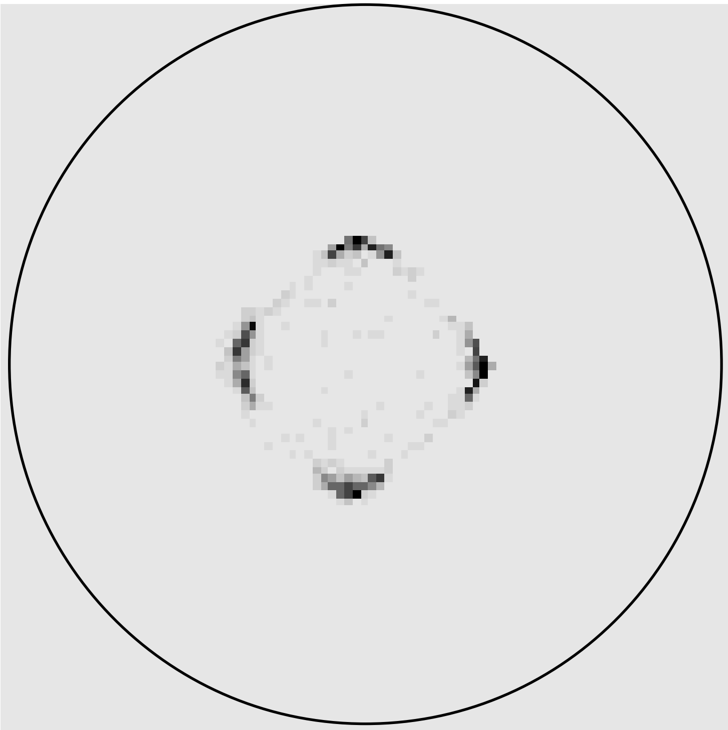




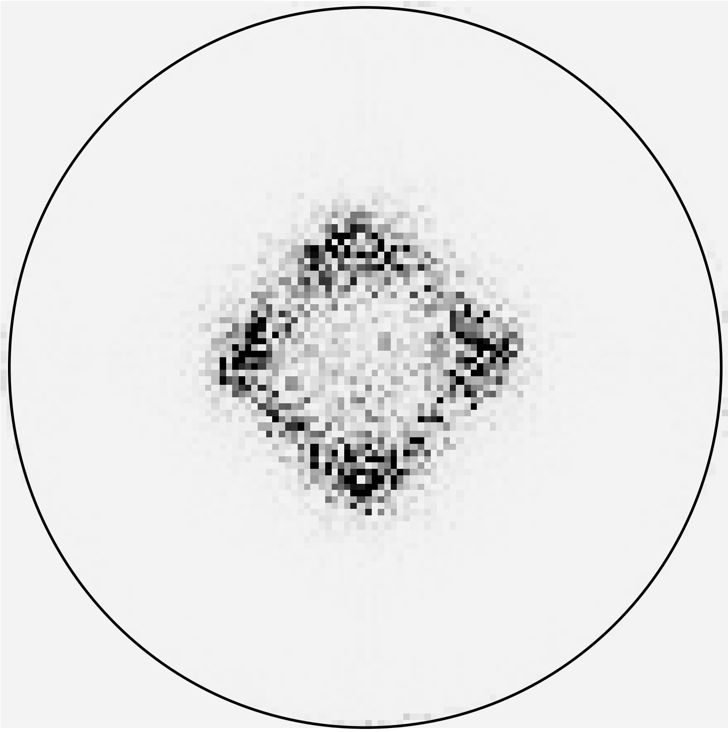
10 FFTs of 512x512 array; 12 sec with Mathematica on my laptop

Ray tracing or Fourier model?

Compare predictions for AFM profile of large pyramids

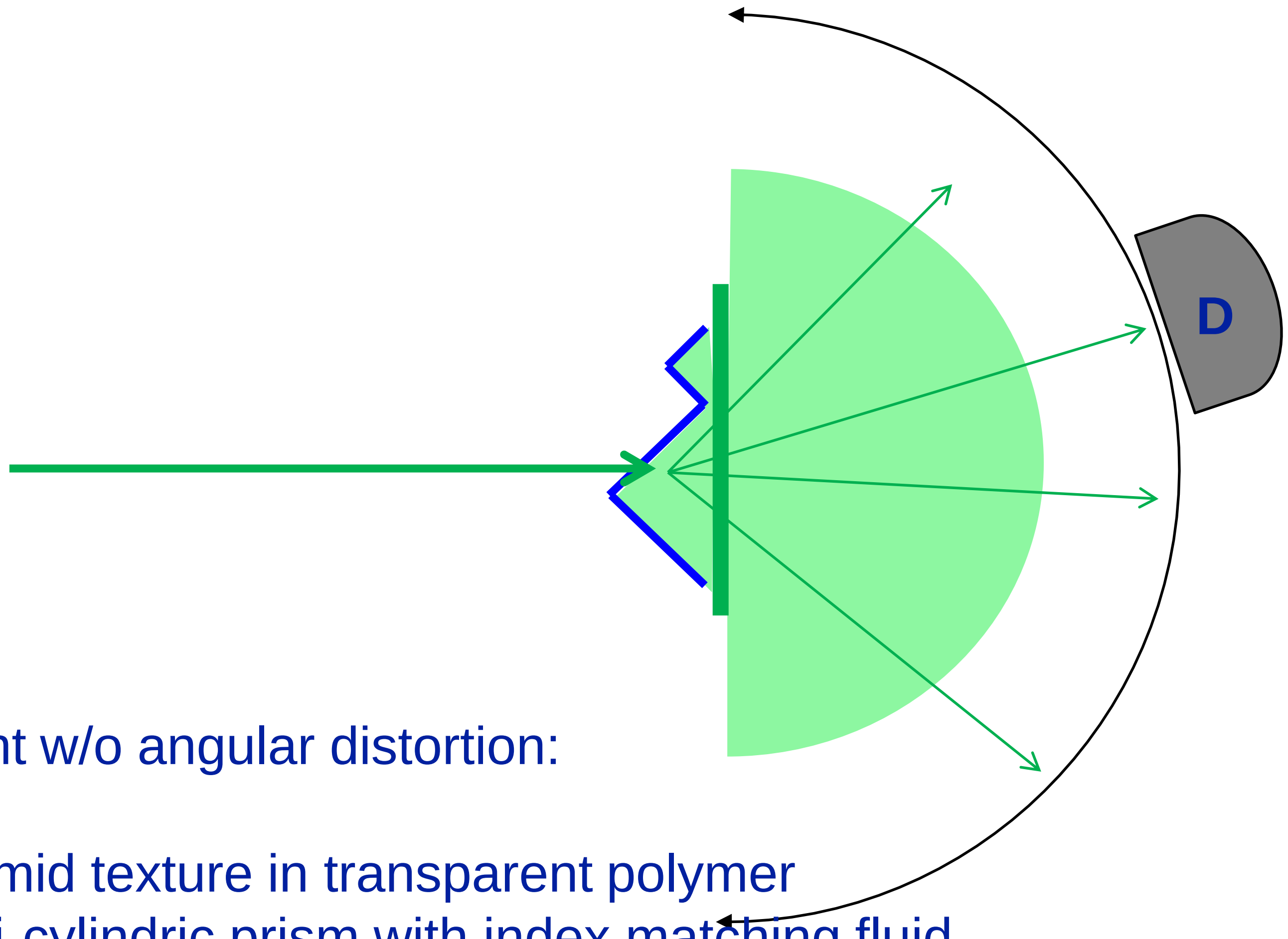


Ray tracing: four clear peaks



Fourier: broader peaks w. connection

Comparison with measurement (n =1.5)

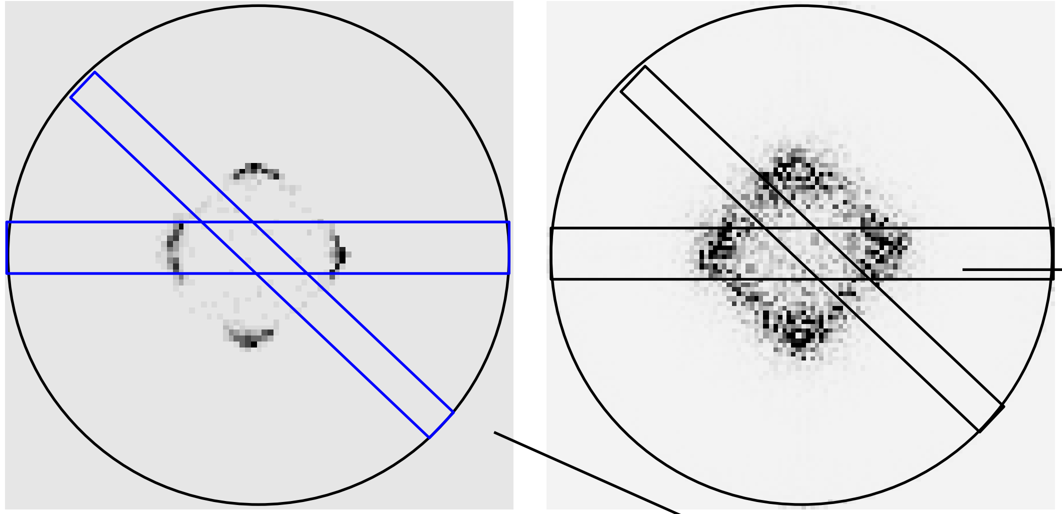


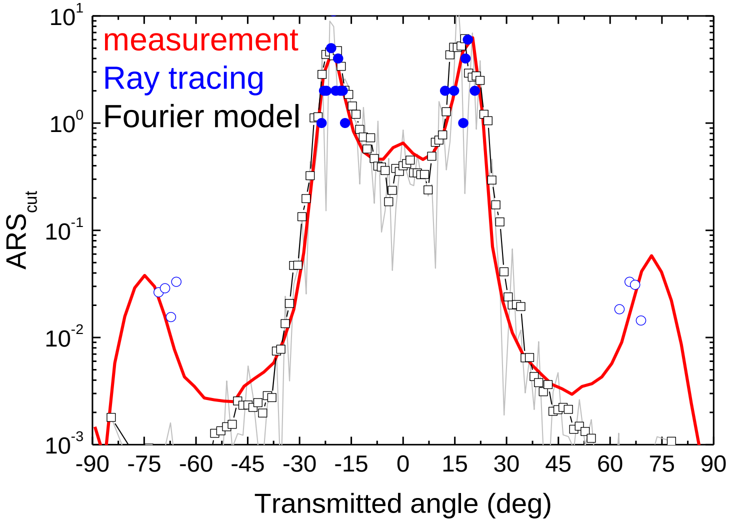
measuremeant w/o angular distortion:

replicate pyramid texture in transparent polymer
attach to hemi-cylindric prism with index matching fluid

Replica:
Escarre, SolMat (2012)

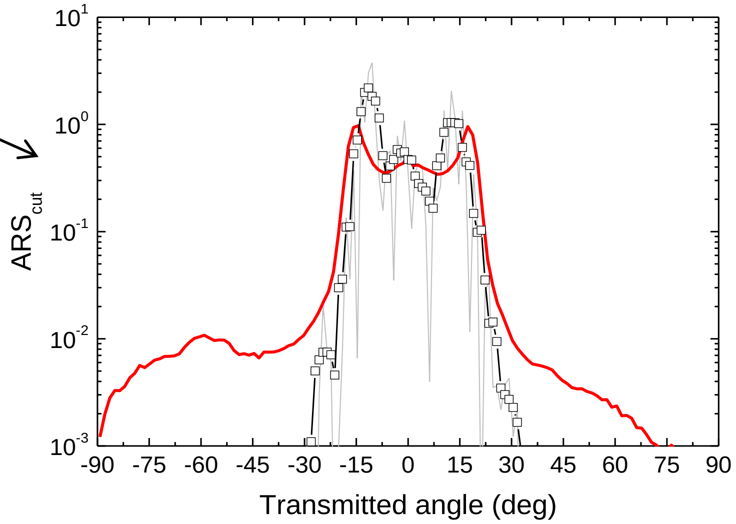
Comparison with measurement



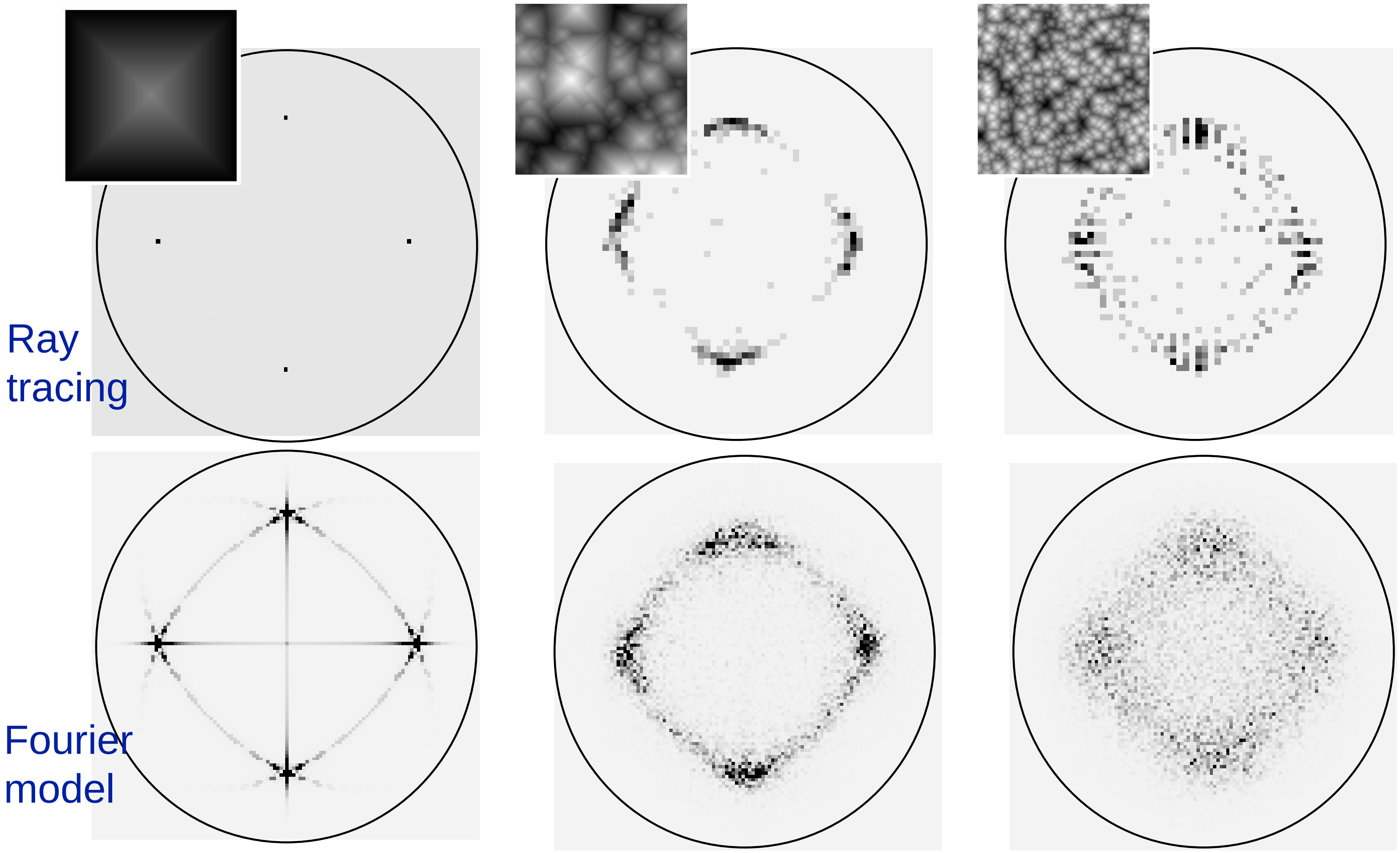


Ray tracing:
- peak positions reproduced
- 2^{nd} rebound at high angles
- little or no signal along diagonal

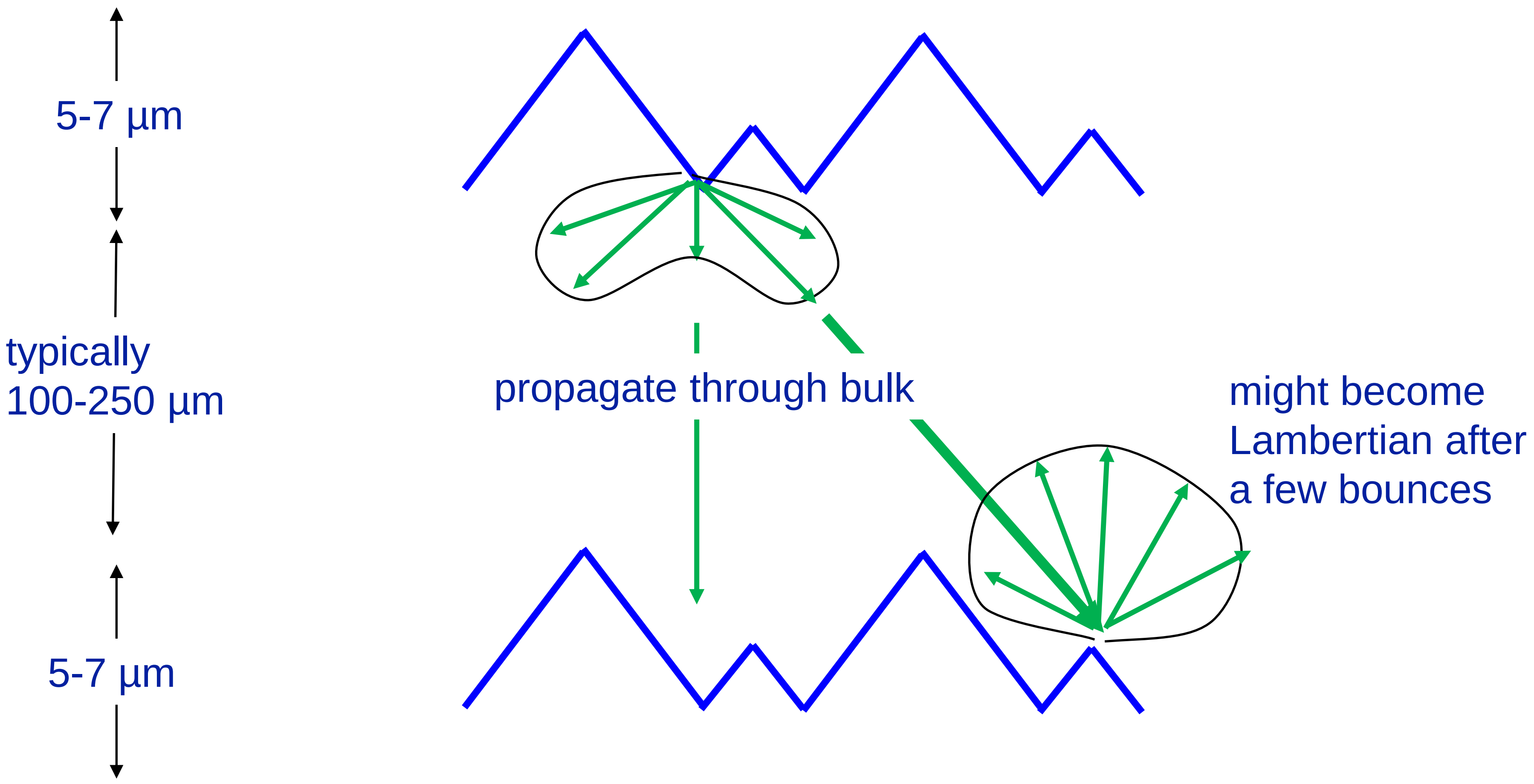
Fourier model
- Main peaks reproduced over 4 orders
- Diagonal over 3 orders
- But: no 2^{nd} rebound



Refraction vs. diffraction into silicon (n =3.5)



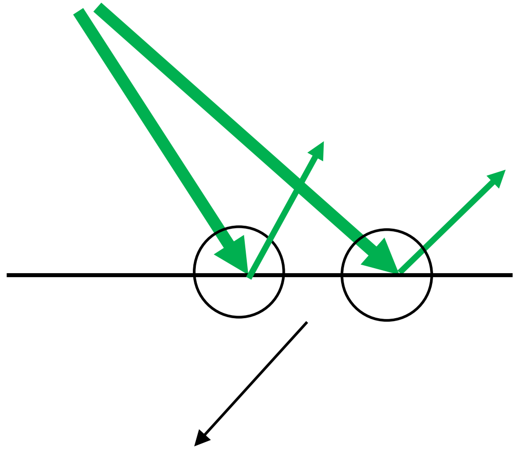
Use in a combined modelling approach



Back reflector

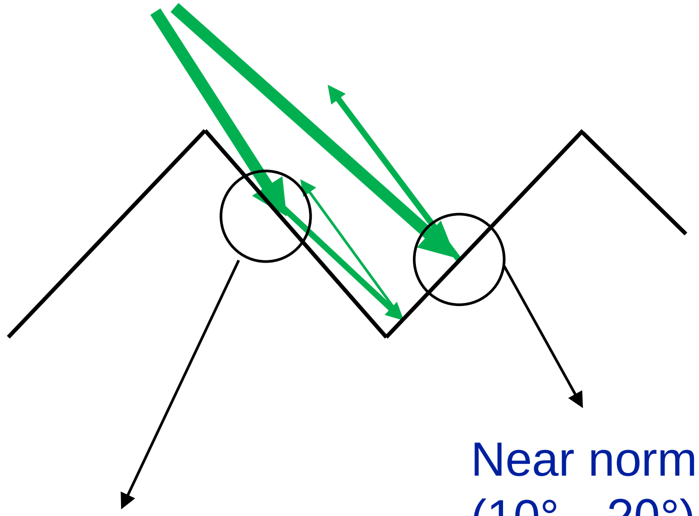
F.-J. Haug

Flat



Incidence btw. 40° and 60°

Textured



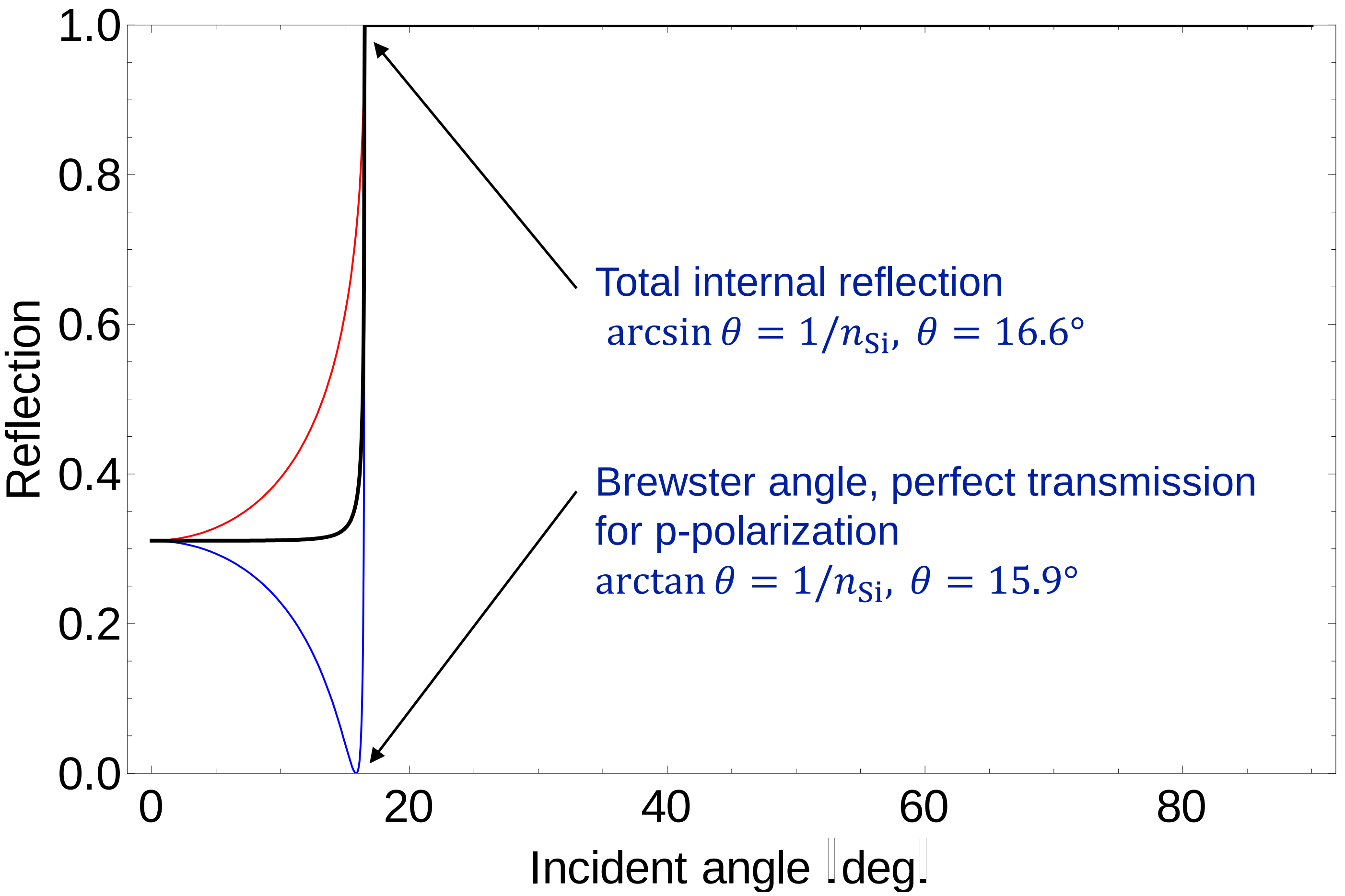
Grazing incidence
(70°…80°)

Near normal incidence
(10°…20°)

need to study angular properties
important only at long wavelengths, e.g. at 1100 or 1200 nm

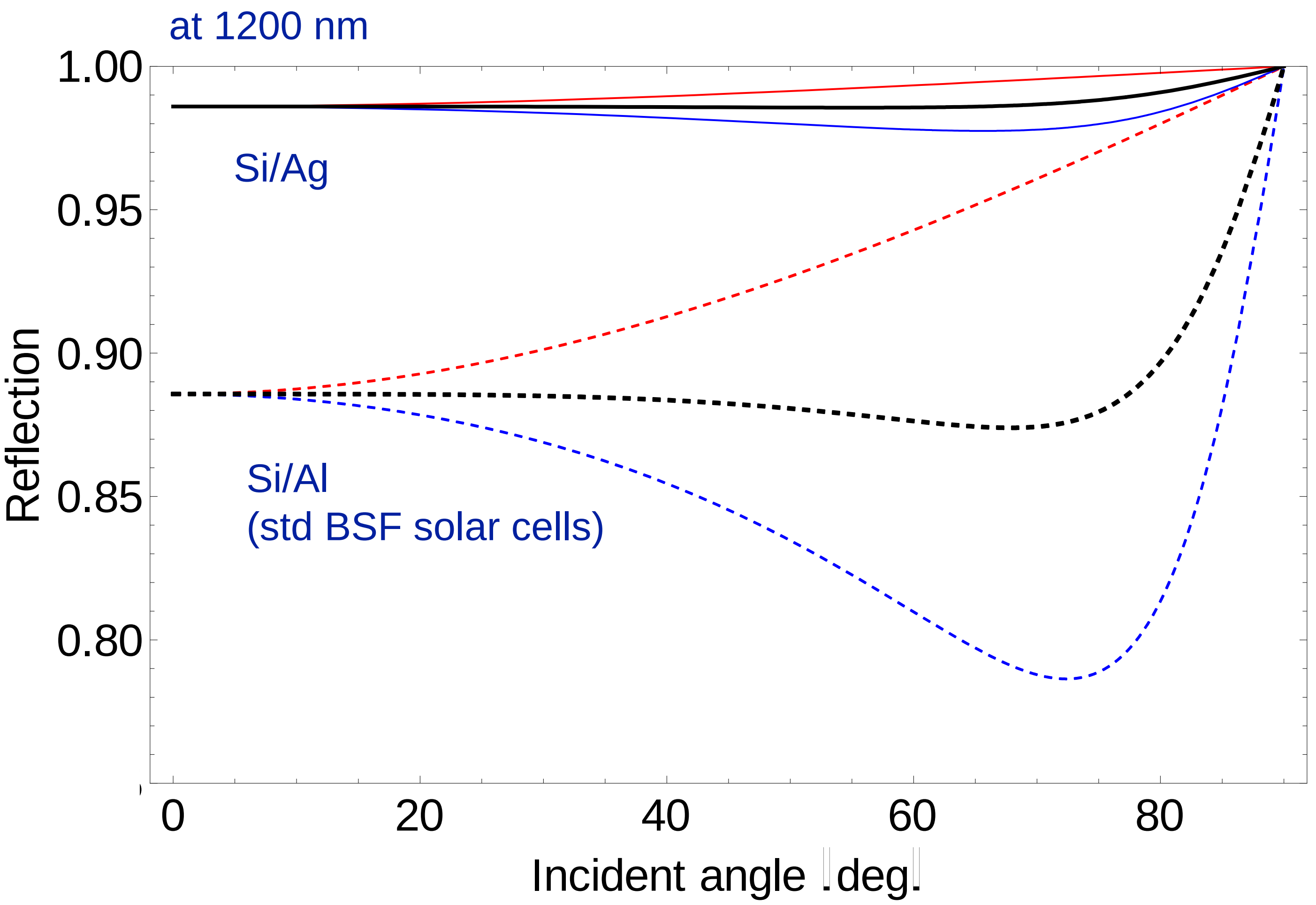
Angular reflection from wafer into air

at 1200 nm



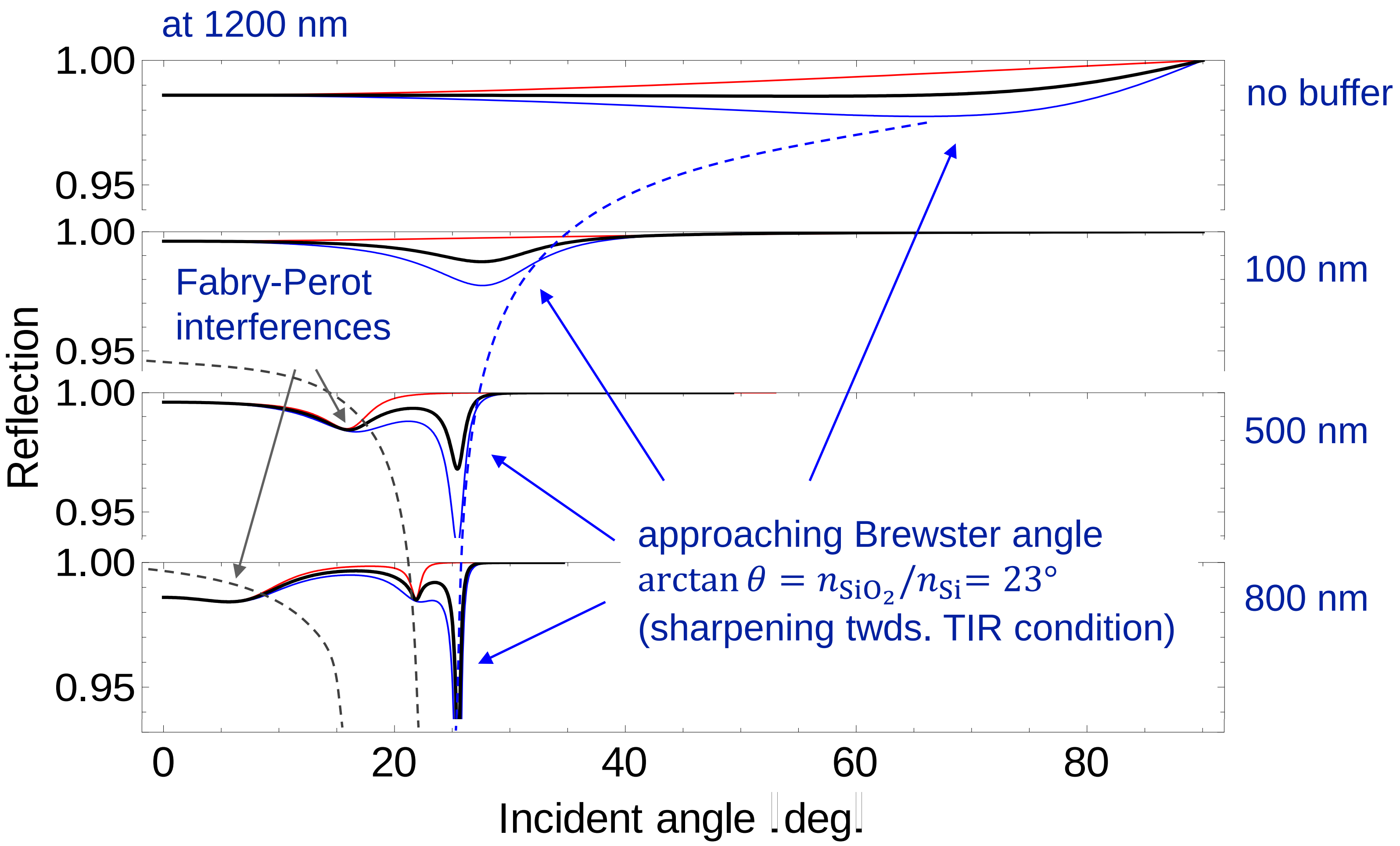
more information: Holman, JAP (2013)

Back surface with metal contact



better for low angles (even with Al), much worse for high angles (no TIR any more)
Technological constraint: massive recombination at semiconductor/metal interfaces

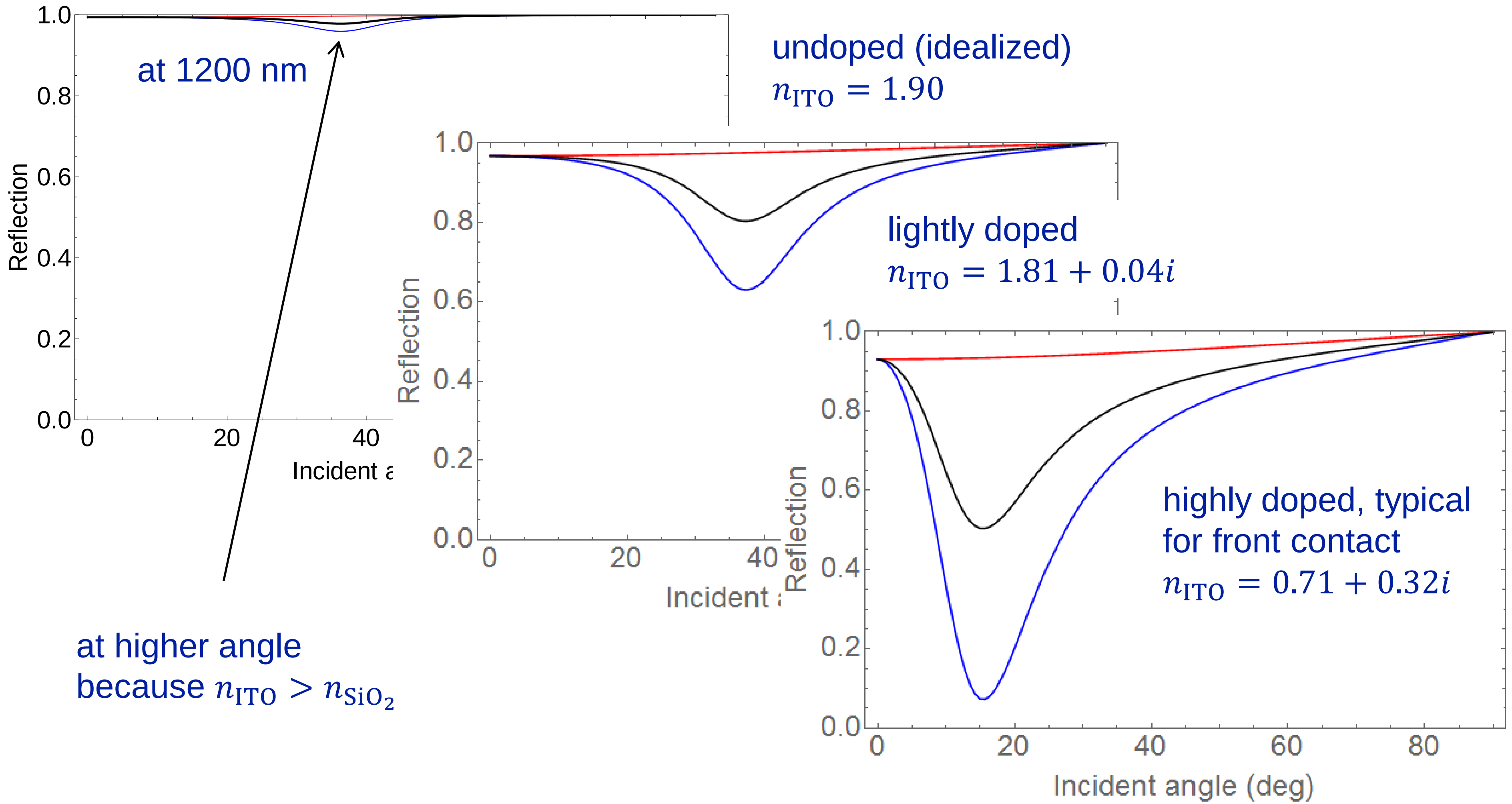
Ag back surface with SiO_2 buffer layer



Used in high-efficiency PERC and PERL cells, but needs contact openings in SiO_2

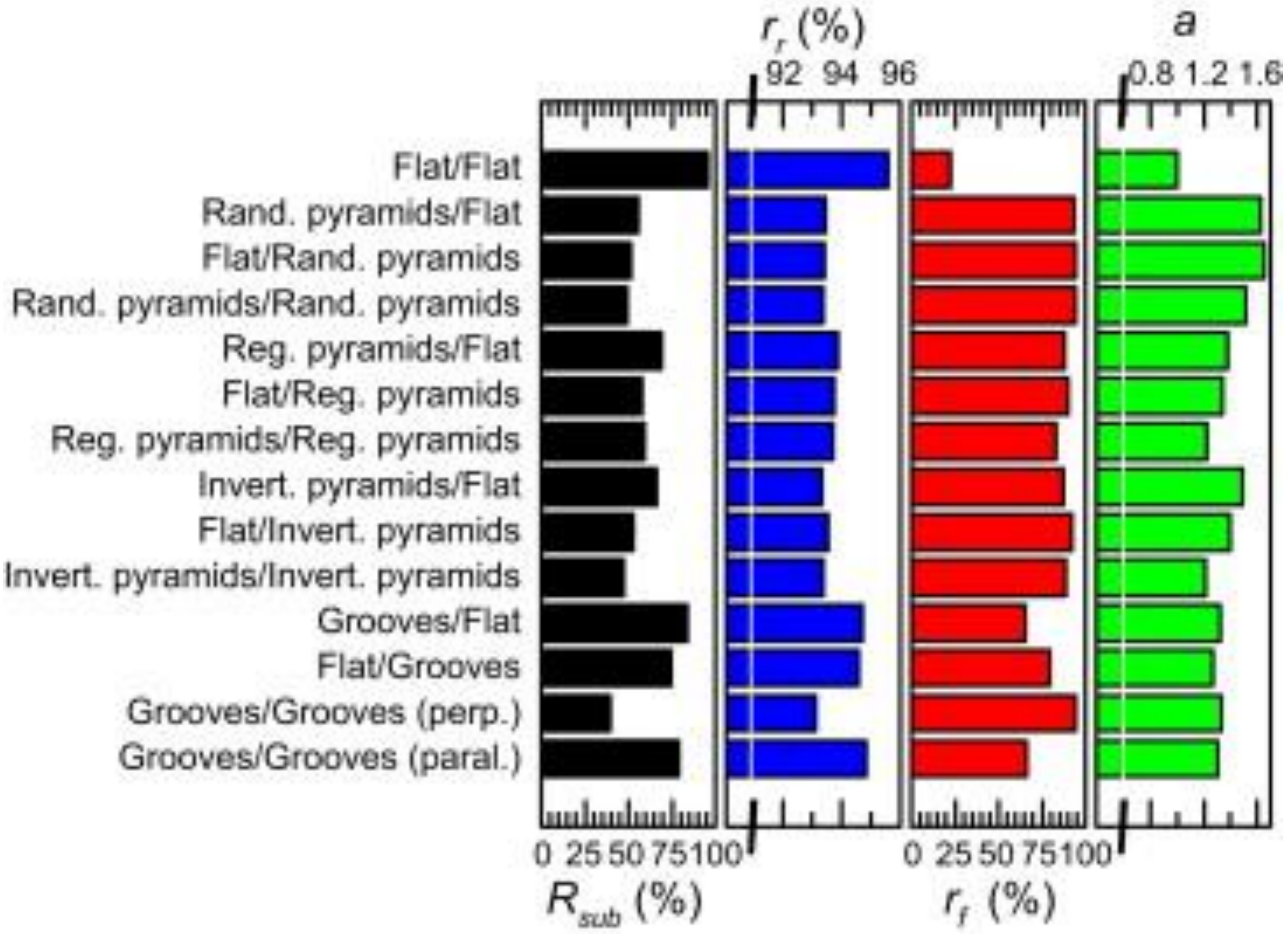
Ag-back contact with ITO buffer (HIT cell)

F.-J. Haug



Use lightly doped material (needs only transverse conductivity for 100 nm)

Combine ray tracing of front and back



path length enhancement

Holman, SolMat (2014)

Conclusions

- Excellent light trapping in silicon with pyramids
  - AR-effect by double rebound
  - path length enhancement (theoretically up to $4n^2$-fold for very weak absorption)

- Boost by single layer AR coating
  => needed anyway
  - passivation (100 nm SiO_2 or 70 nm Si_3N_4)
  - contact (70 nm ITO)

- Thinner wafers (near future) may require smaller texture