Modern PV-Technologies
3.4: Optics

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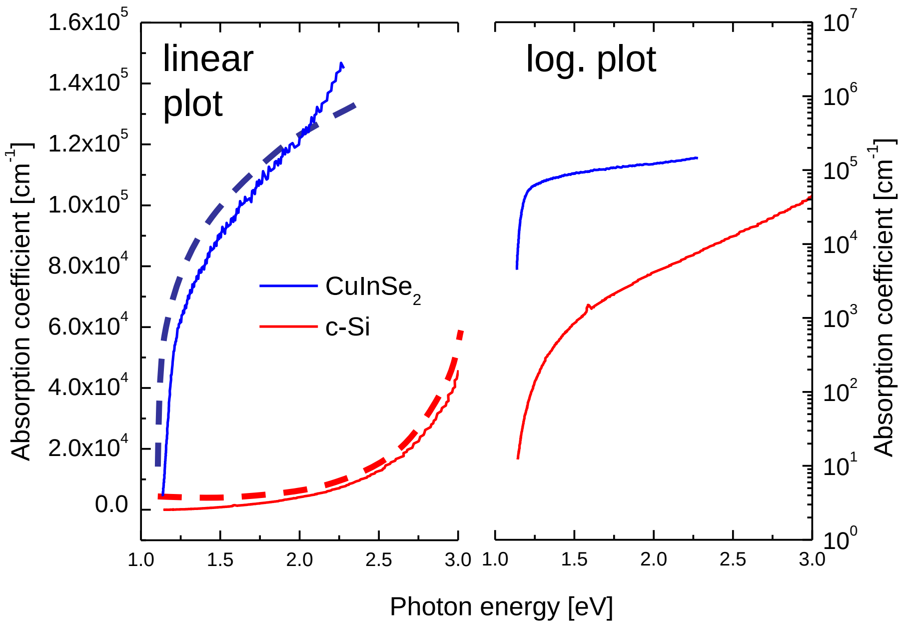
Absorption coefficient

Direct vs. indirect band gap



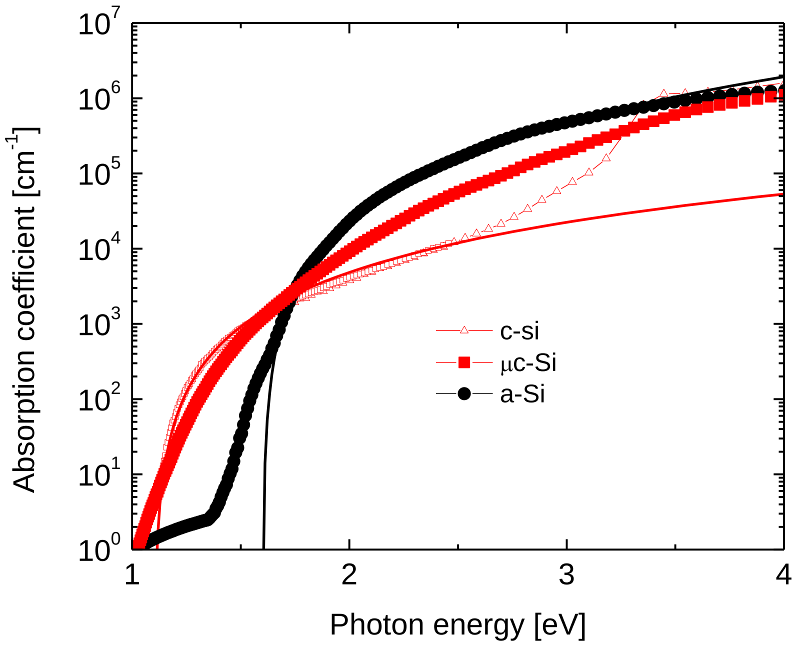
Direct gap (GaAs, $CuInSe_2$):

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

Indirect gap (c-Si):

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

Indirect gaps in all types of silicon



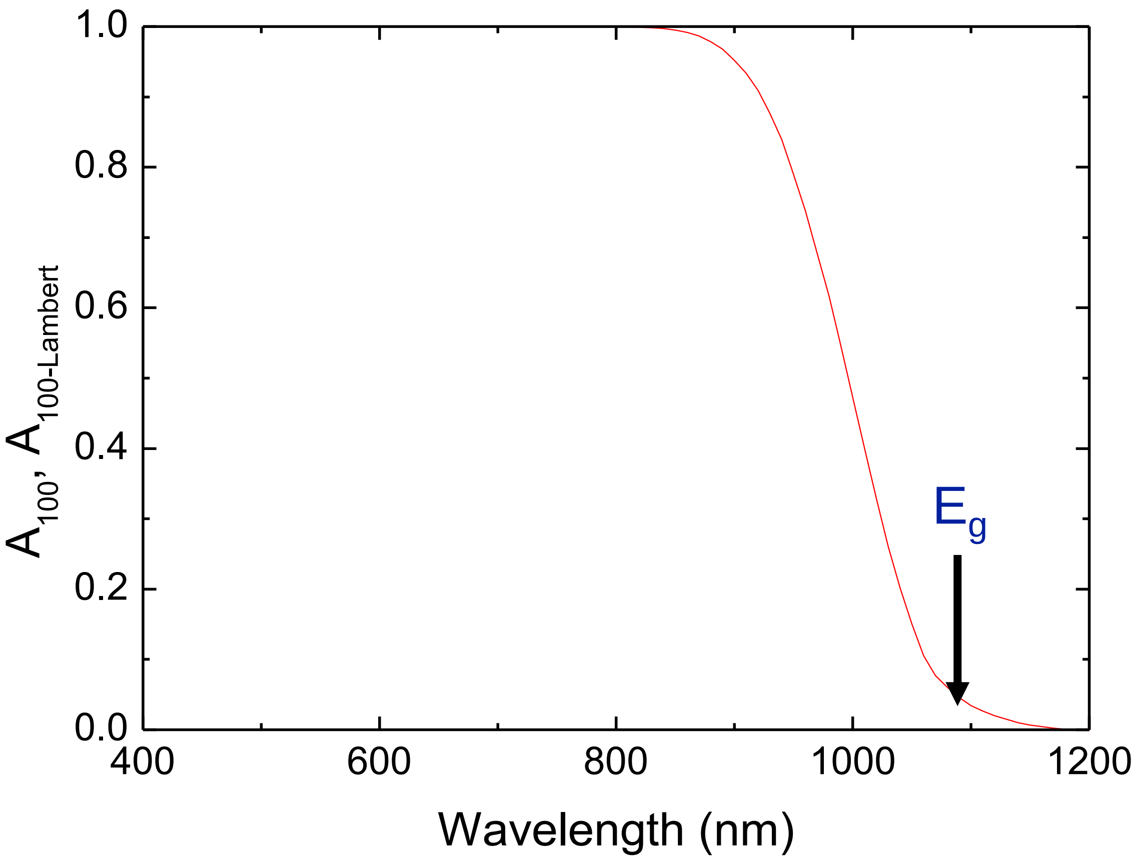
a-Si:H: ~1.75 eV

μc-Si:H:~1.1 eV (like c-Si)

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

Green, Sol. En. Mat. 2008

Absorption in silicon

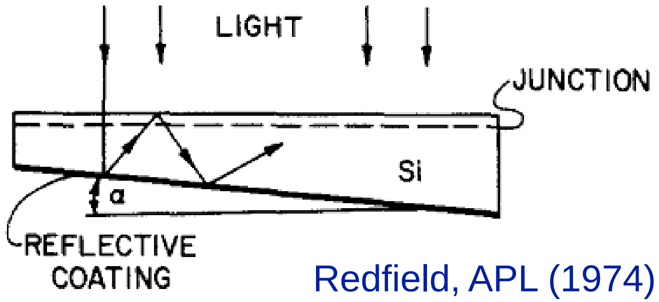


100 µm thick wafer
(may become standard)

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

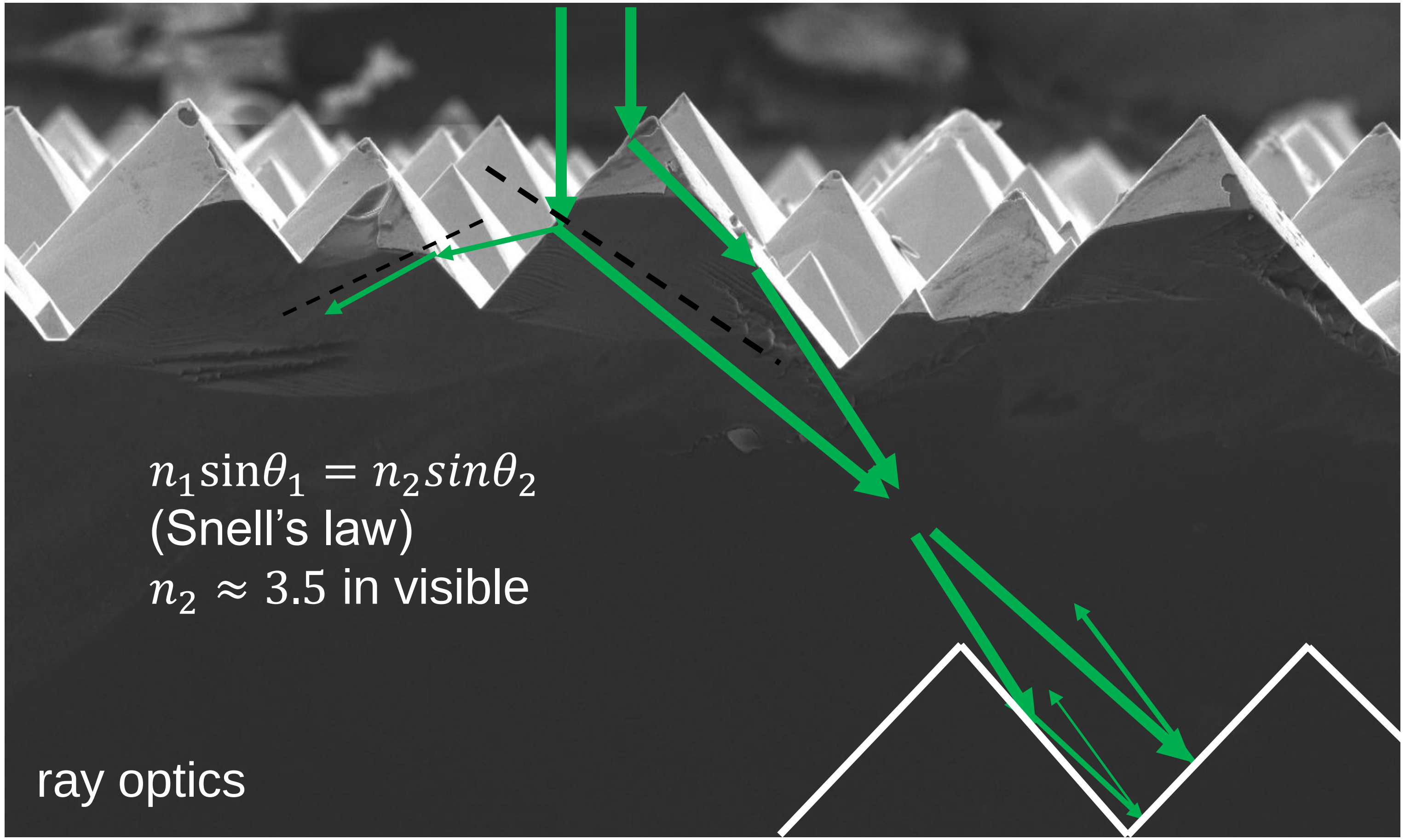
assumes ideal front
anti-reflection,
ideal back reflector

Workaround: path enhancement by texture



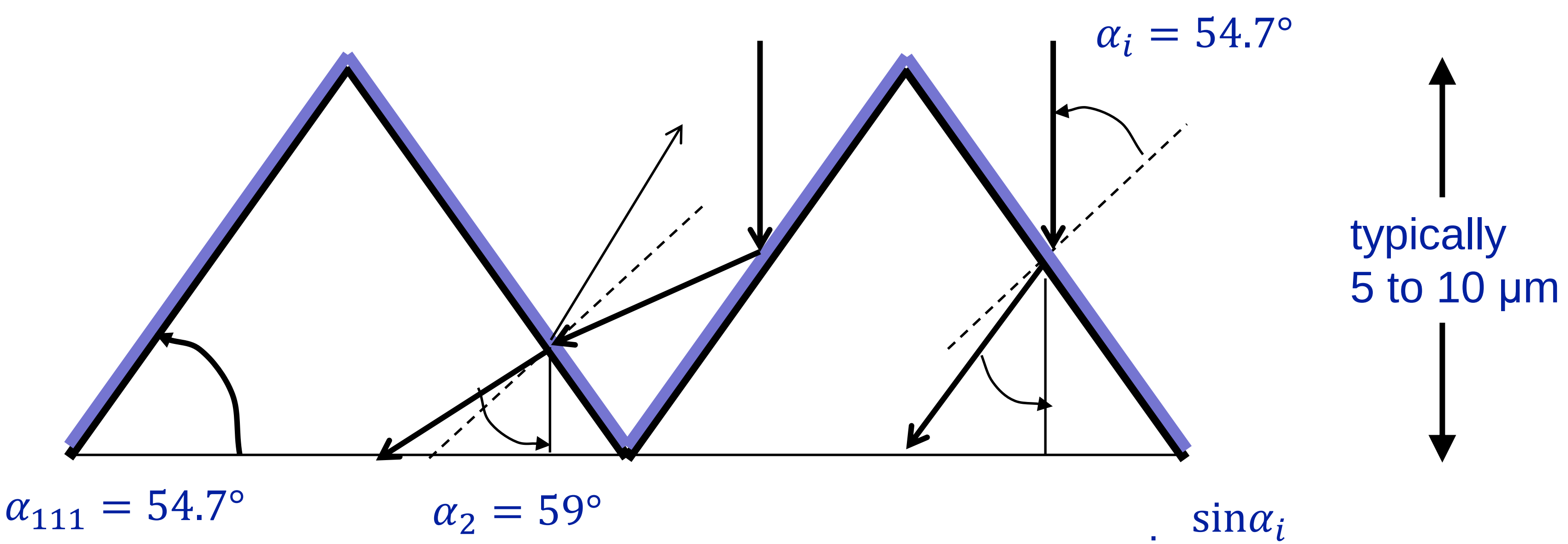
Redfield, APL (1974)

Natural texture: 111 facets of 100 surface



Ideal facet angle: 54.7°

Reduced reflection by surface texture



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

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

AR properties

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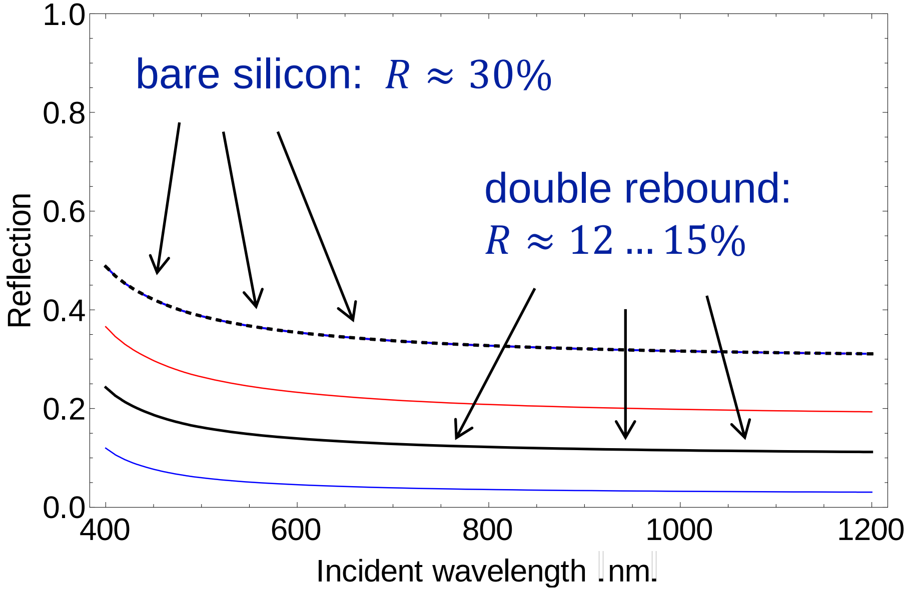
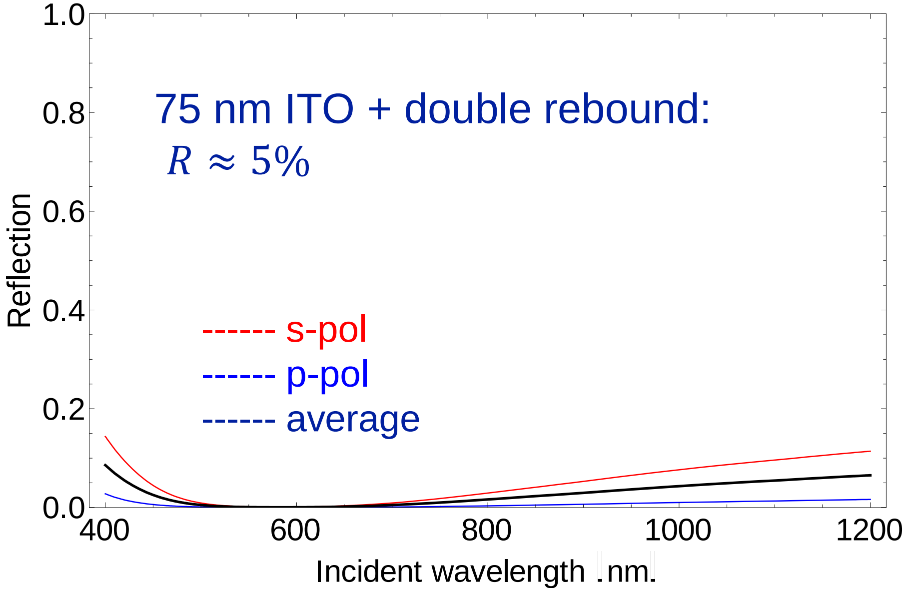
AR coating: depending on technology

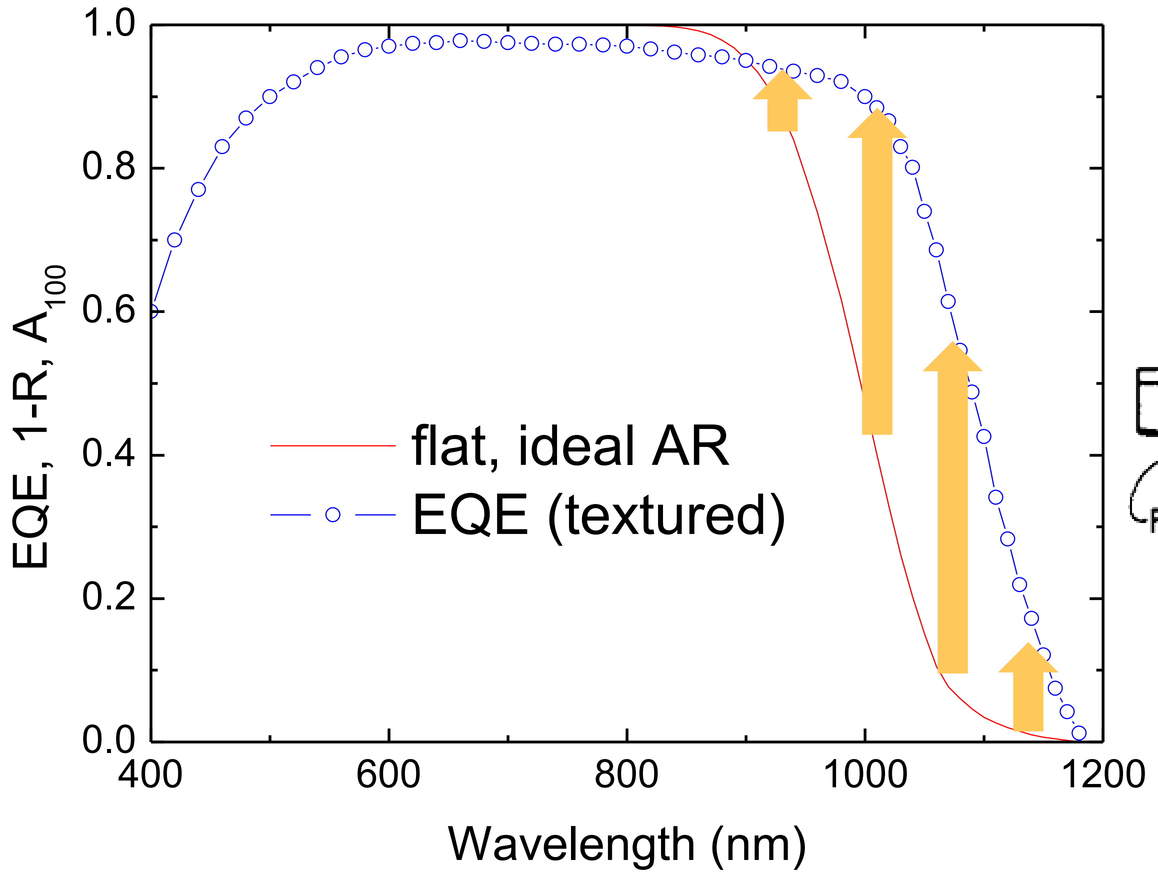
- SiO_2/Si_3N_4: passivation for diffused p-n junction cells
- ITO: electric contact in heterojunction cells

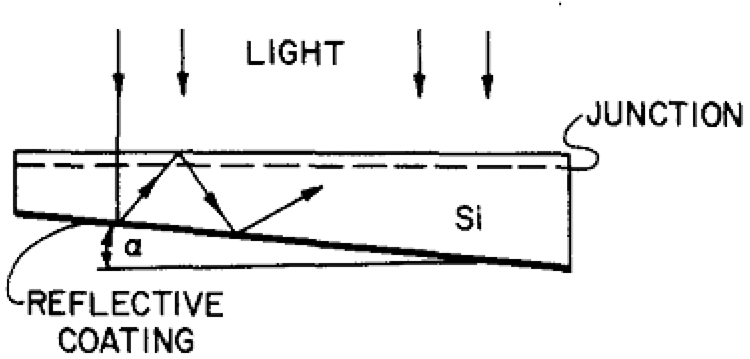




Texture and passivation/contact are mandatory => AR is “free”
Any additional feature incurs cost (e.g. double AR coating, etc.)

Enhanced absorption by surface texture

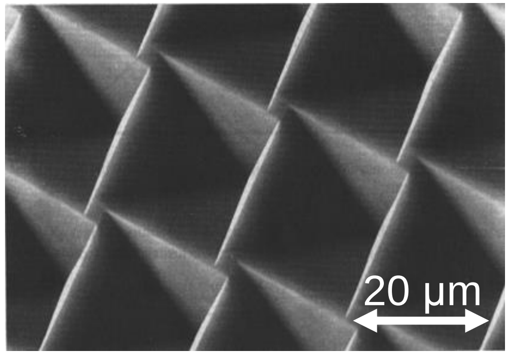




concept:: Redfield, APL (1974)
data: e.g. Holman, JAP (2013)

Light trapping in (thick) c-Si cells

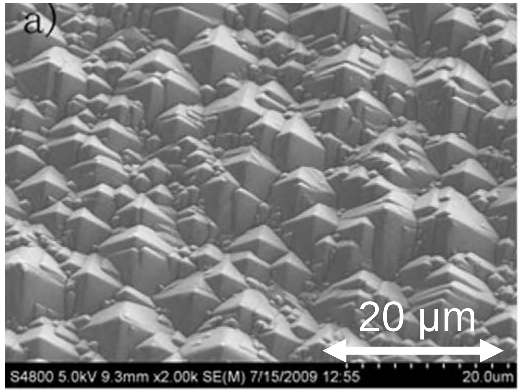
c-Si high eff. cells:
inverted pyramids
(lithography: costly)



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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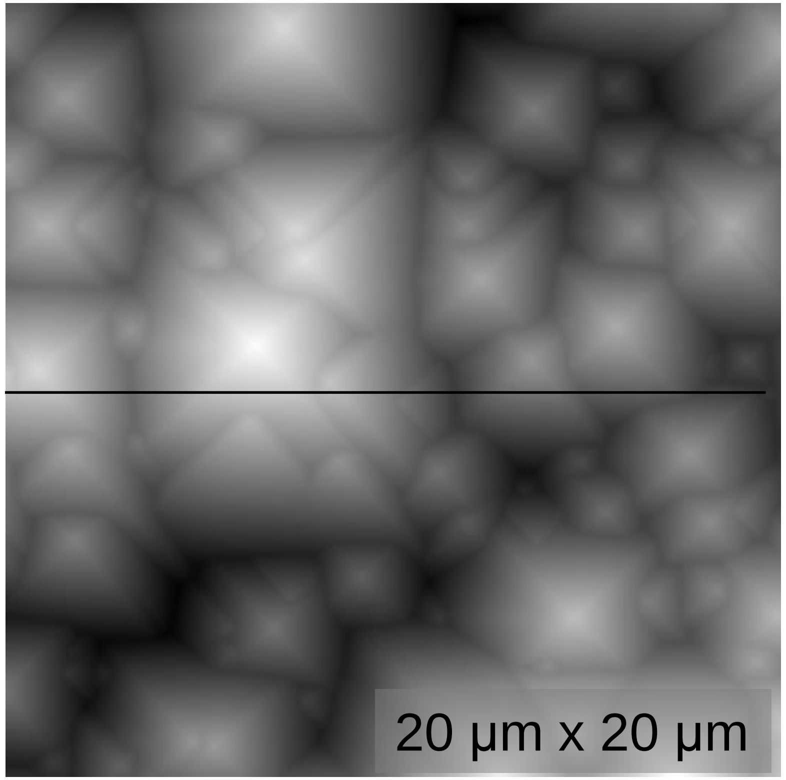
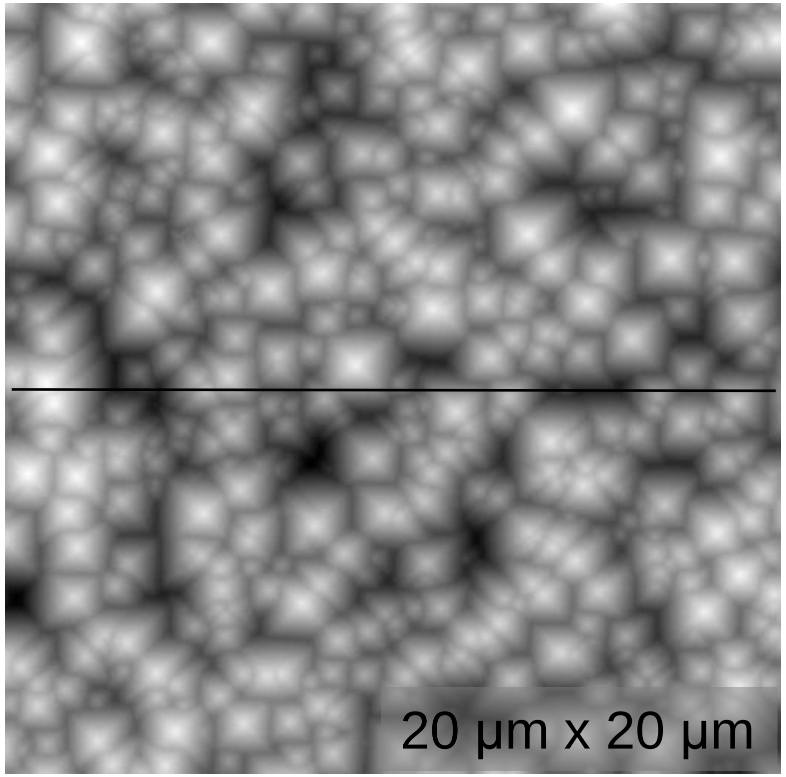


typical texture for HIT solar cells

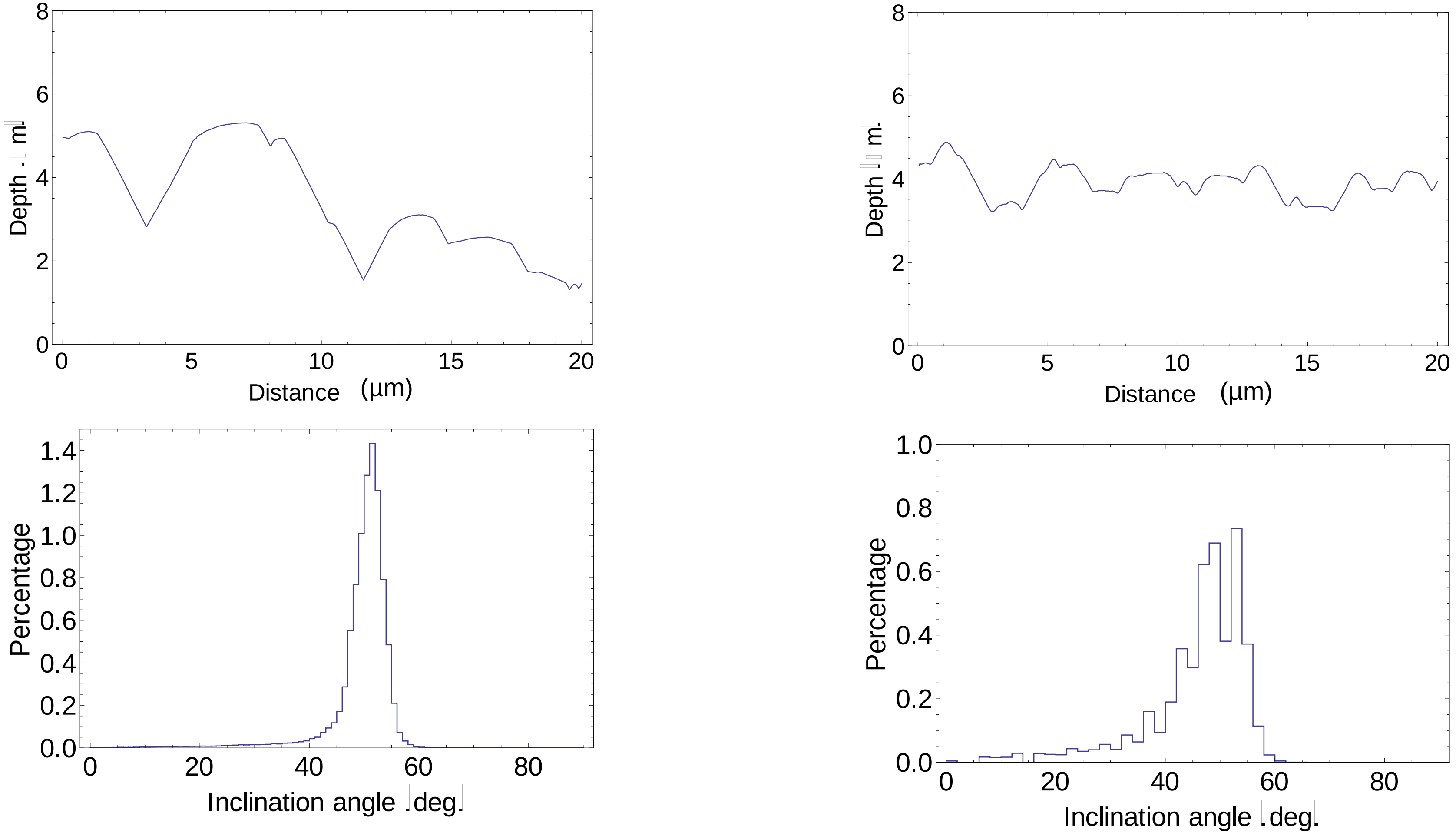


test structure w. small features

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

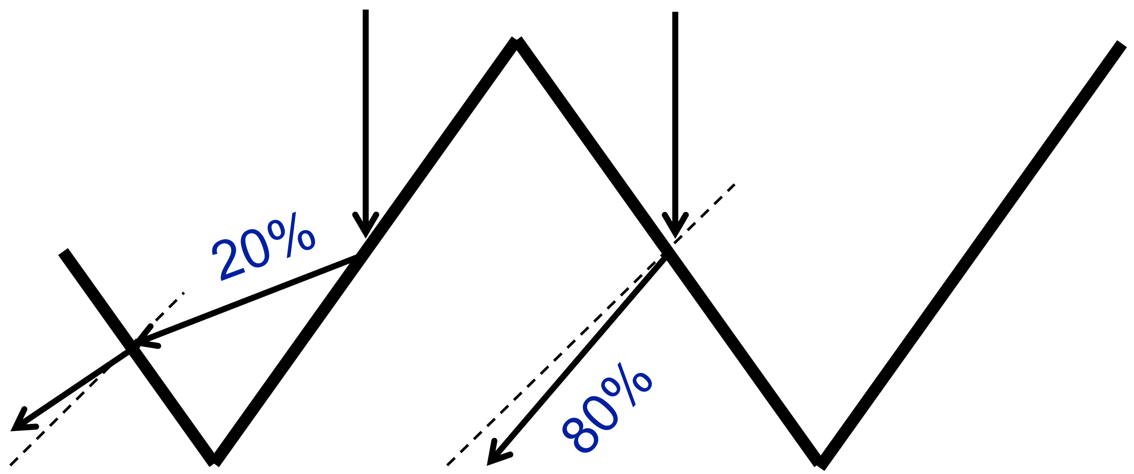
Haug, Opt. Express (2017)

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



close to theoretical facet angle (54.7°)

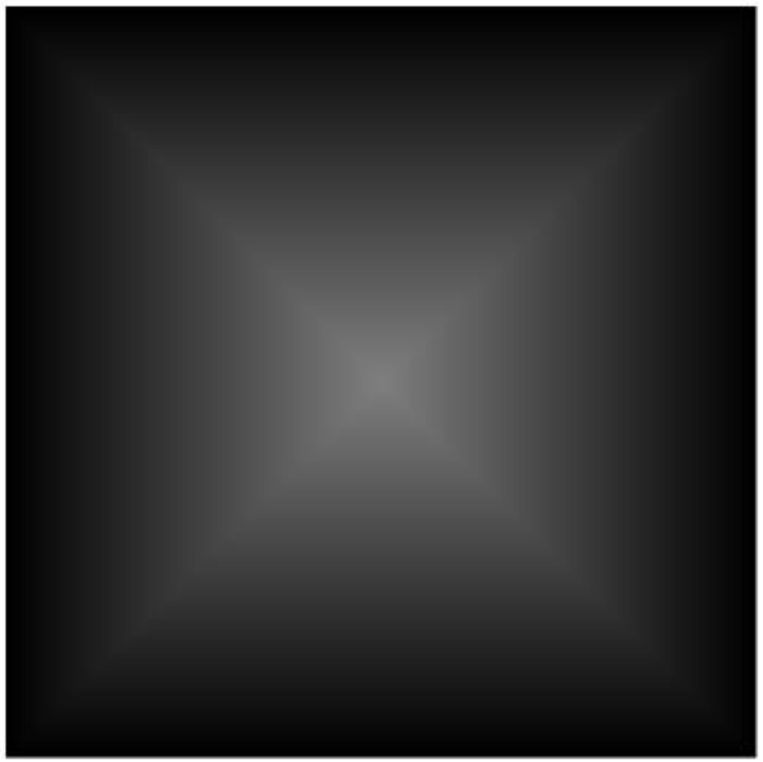
Ray tracing

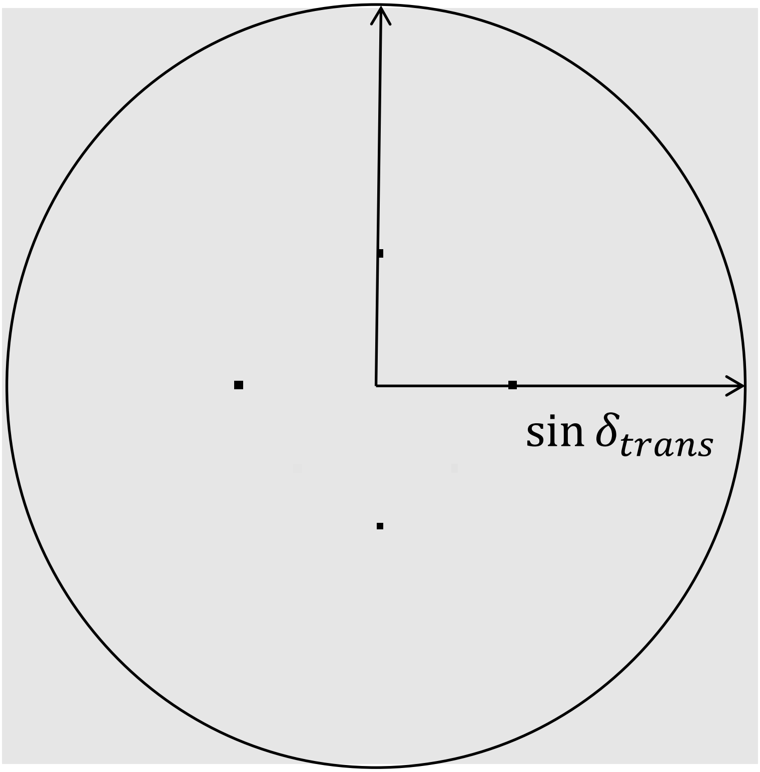


large pyramids (> 5 µm):
adequately treated by ray tracing

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

Ray tracing

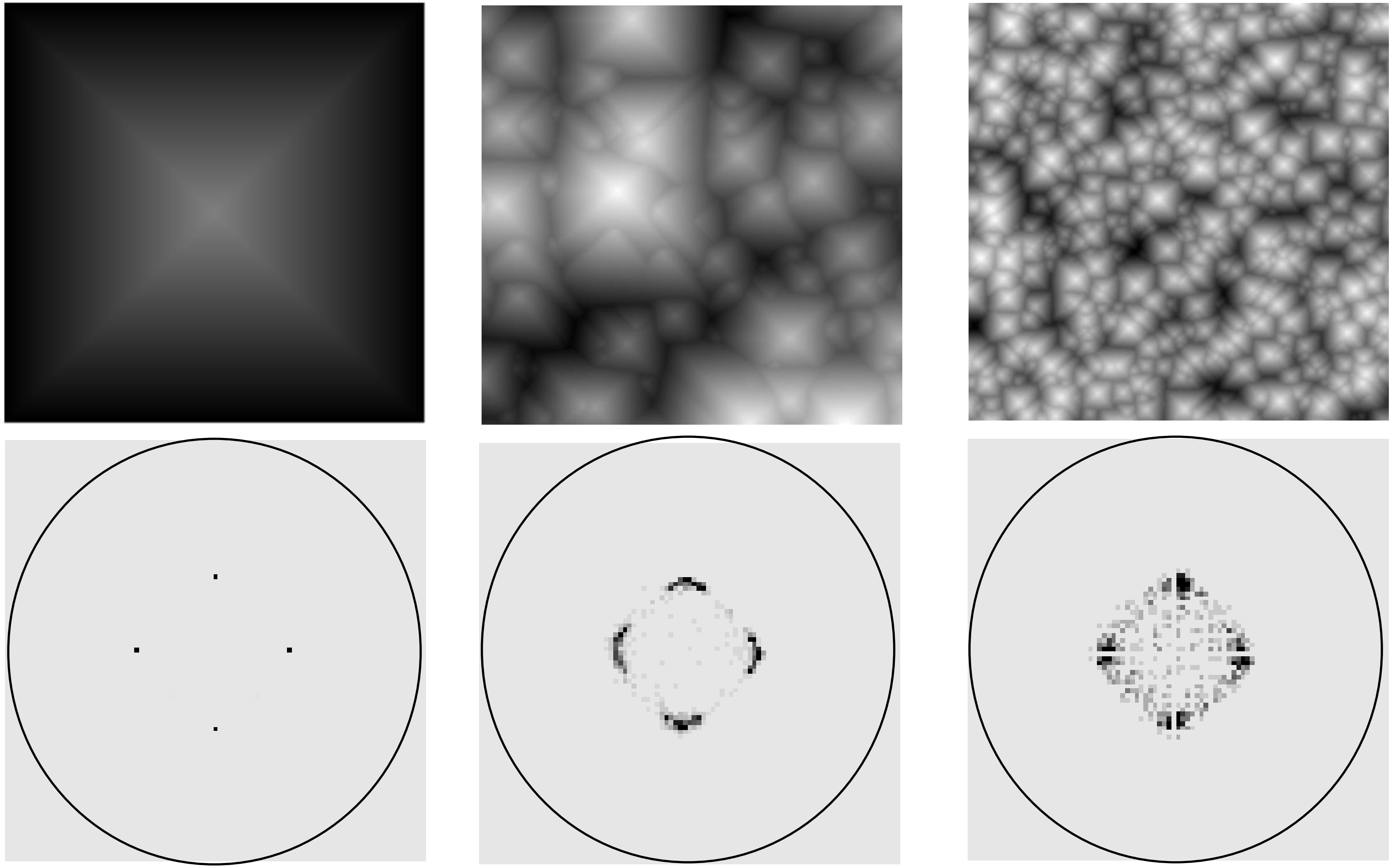




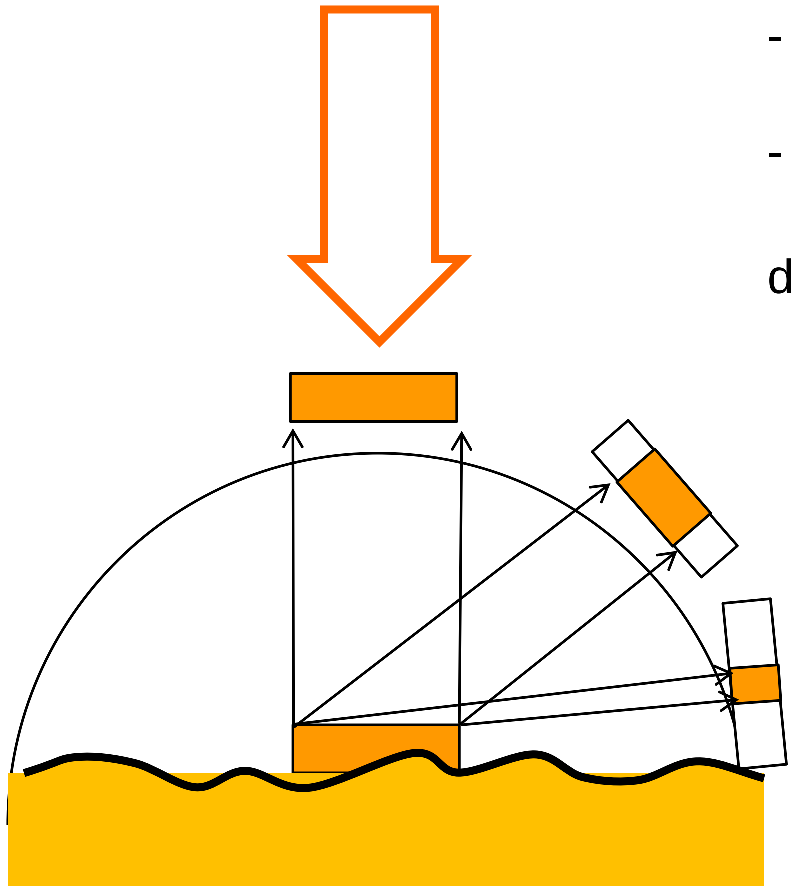
Example: 1000 rays, reflective boundaries, $n_{543\ nm}$ =1.5 (typical polymers)

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

Ray tracing



Isotropic scattering (Lambertian)



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

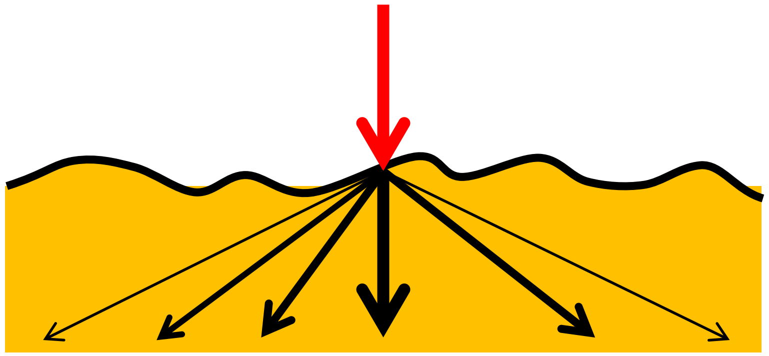
described by: $ARS_{Lambert} = \frac{1}{\pi}\cos\theta$

Lambert, Photometria (1760)

Lambertian path prolongation

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

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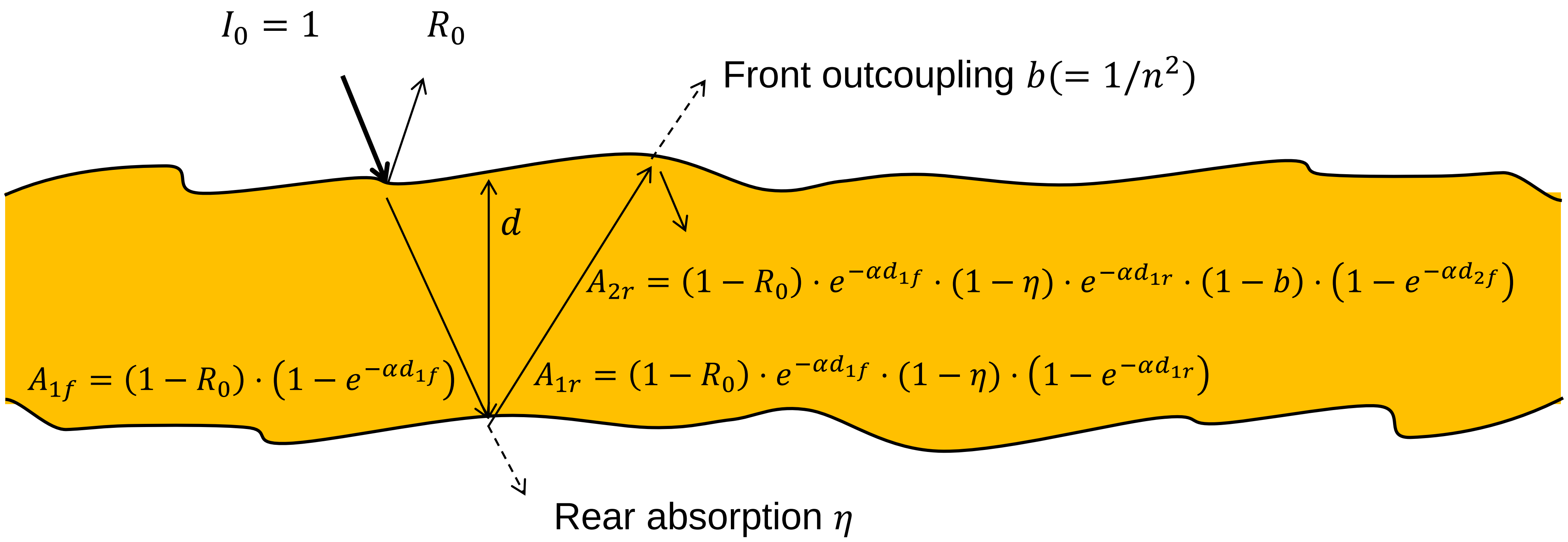
A very simple (but illustrative) analytic model

Sum up absorption upon bouncing forth and back

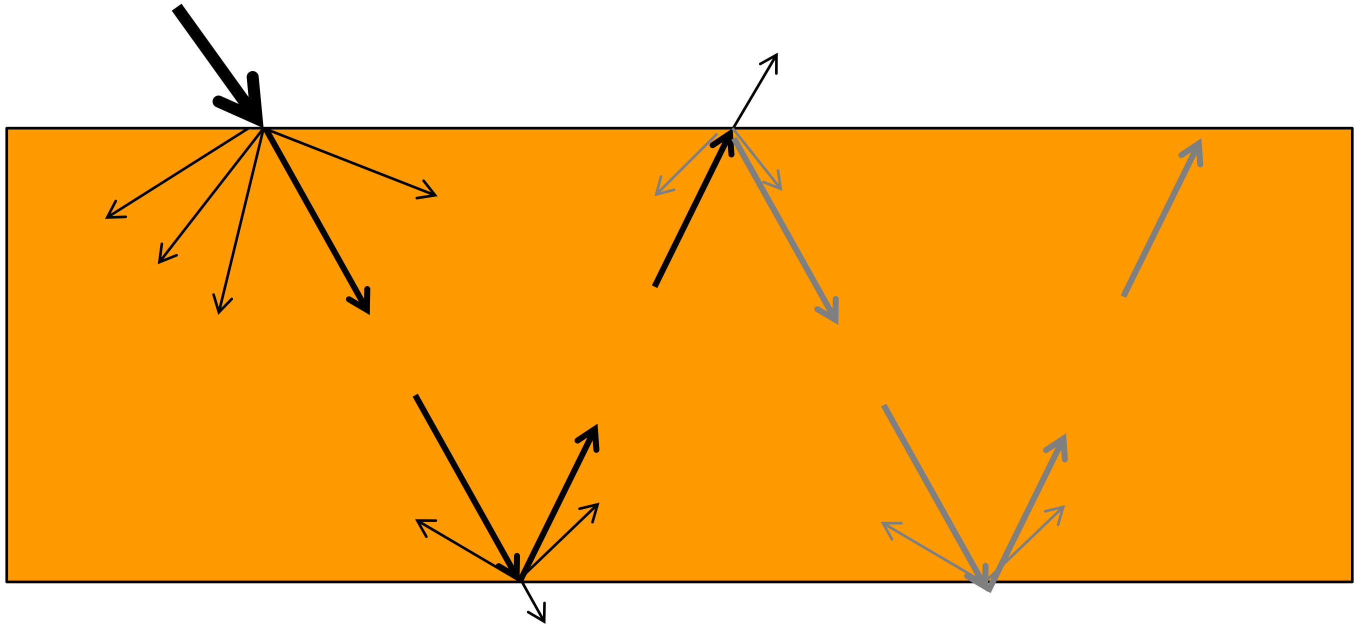


d_{1f}: average length after 1st scattering event

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)

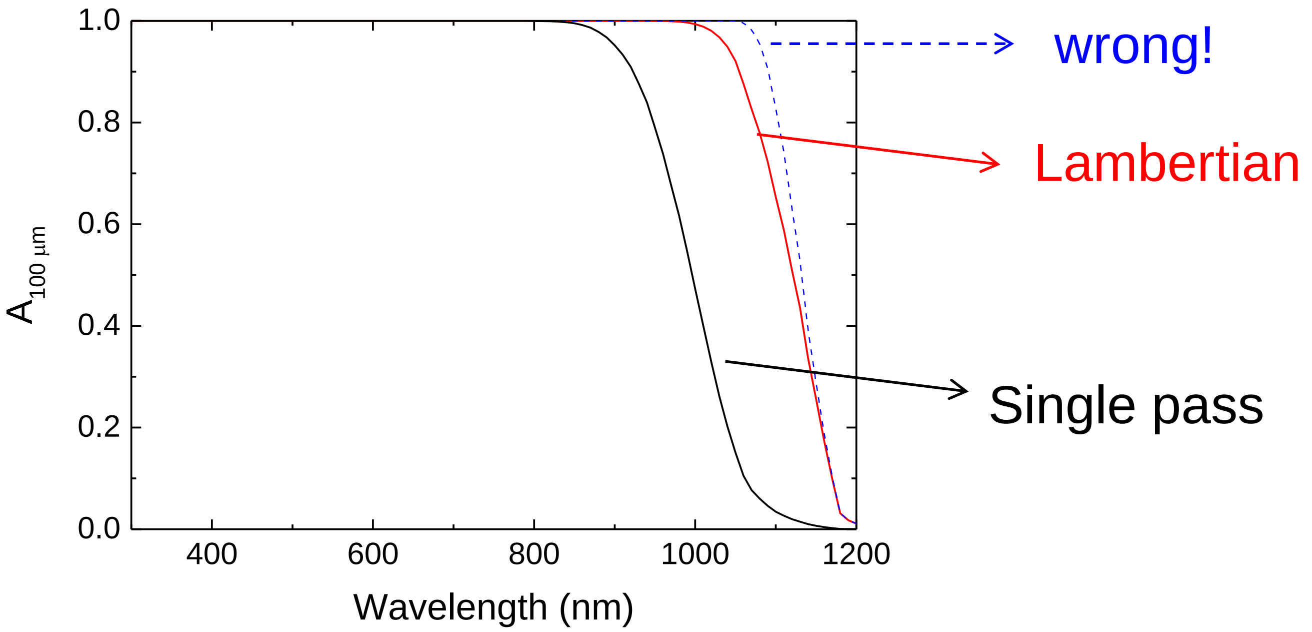
$$A = \sum_{k=0}^{\infty} \underbrace{[(1-e^{-2\alpha l}) + e^{-2\alpha l}(1-\eta)(1-e^{-2\alpha l})]}_{A_{\text{double pass}}} \cdot \underbrace{[e^{-4\alpha l}(1-\eta)(1-1/n^2)]^k}_{\text{Attenuation}}$$

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

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

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

Upper limit of light trapping

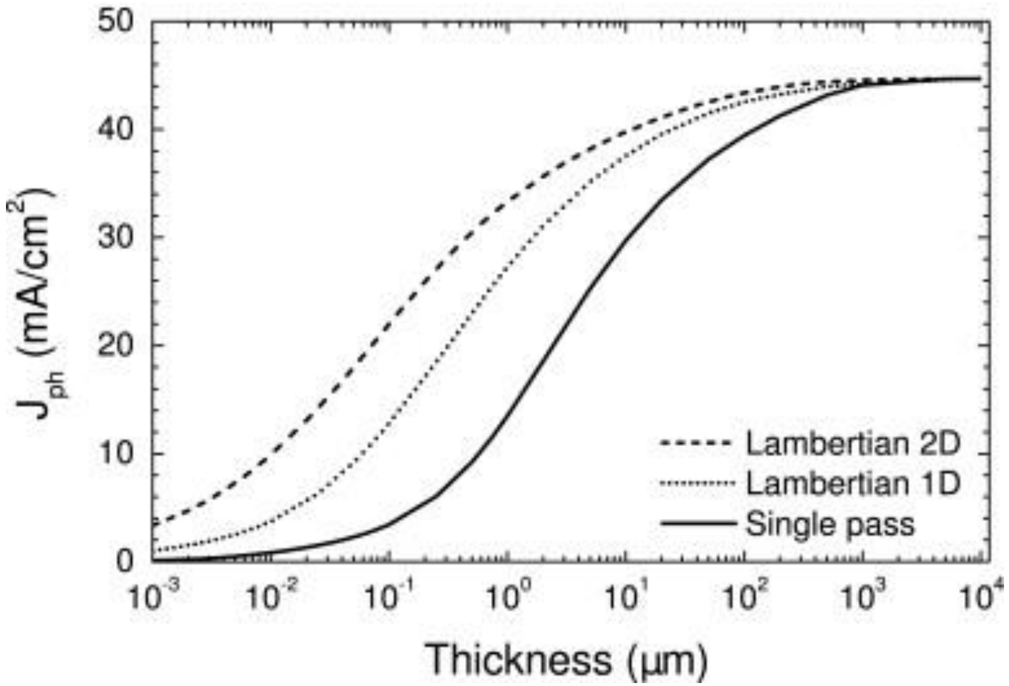


Single pass (100 µm): $A = 1 - e^{-\alpha l}$

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

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

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

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:

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

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

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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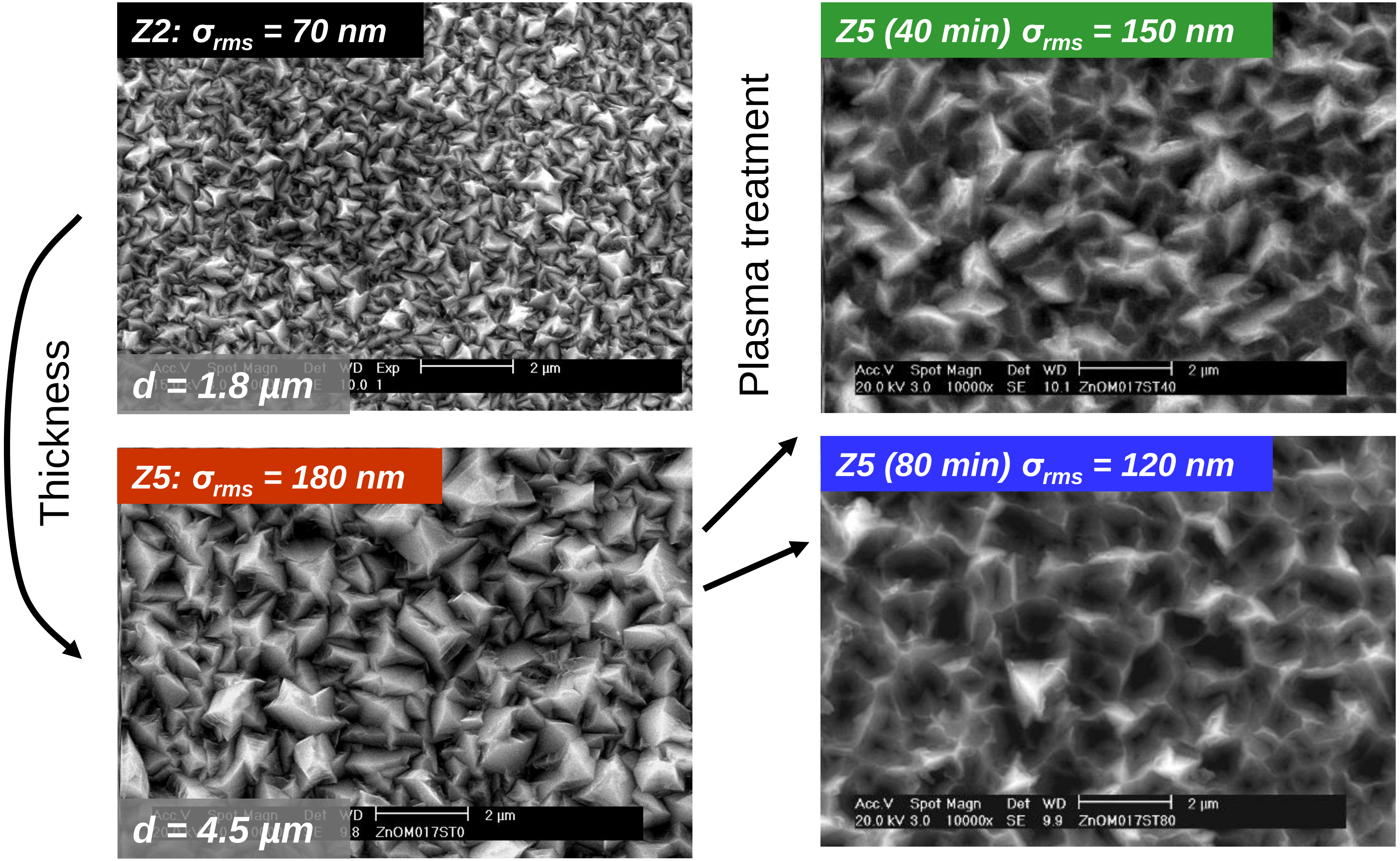


Description of haze: scalar theory

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

Exponent δ:

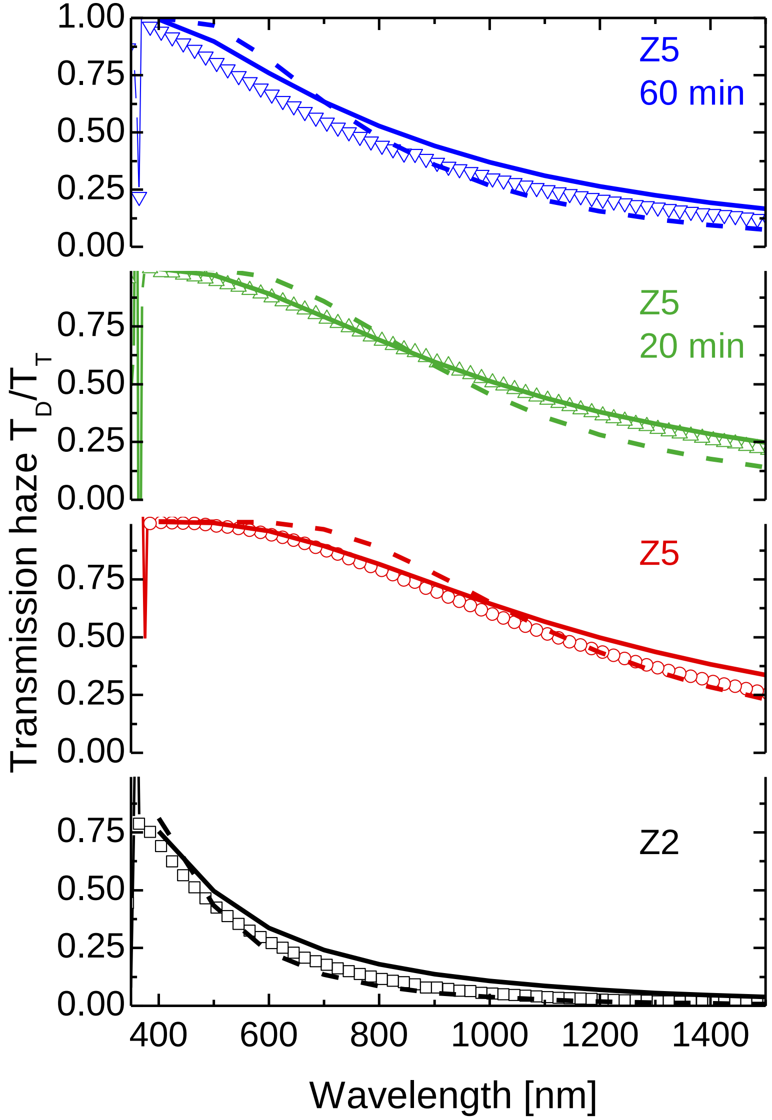
- scattering theory: $\delta = 2$ ⟶ (solid line)
- literature (empiric): $\delta = 3$ ⟶ (dashed line)

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)

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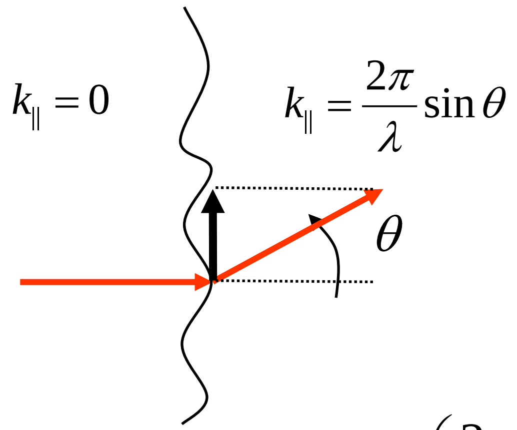
- Assumed (e.g. Lambertian, $ARS_L = 1/\pi \cdot \cos\theta$)
- Measure ARS, project to other interfaces and wavelengths
- Estimate momentum change via power spectral density $g(k)$

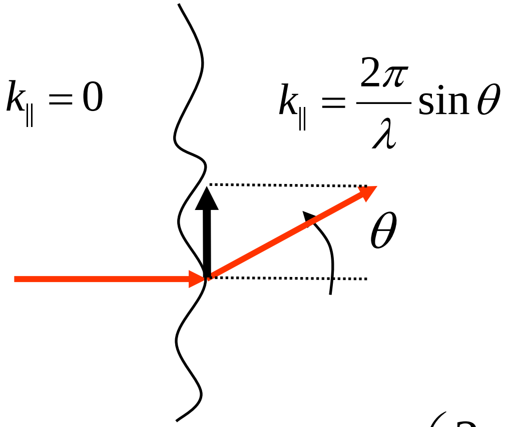


$$ARS(\theta) \sim g(k_x)\cdot\cos\theta = g\left(\frac{2\pi}{\lambda}\sin\theta\right)\cdot\cos\theta$$

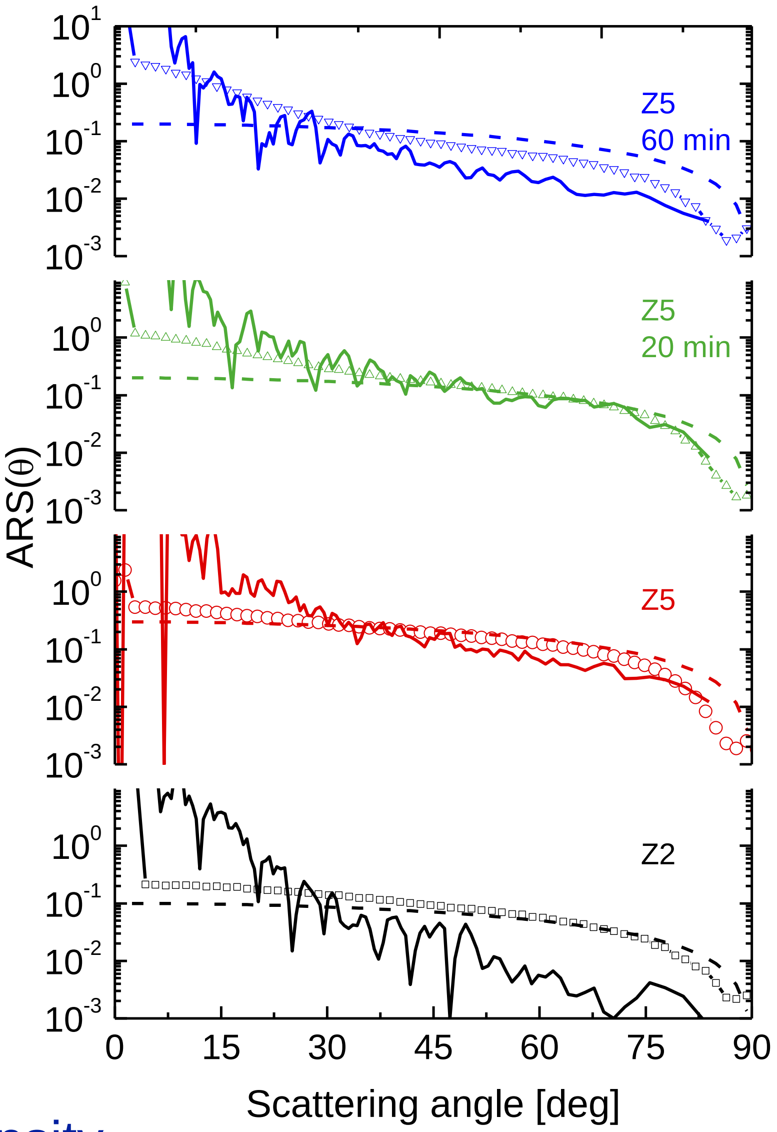
Needs: assumption or surface profile data for $g(k)$

Angular distribution

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

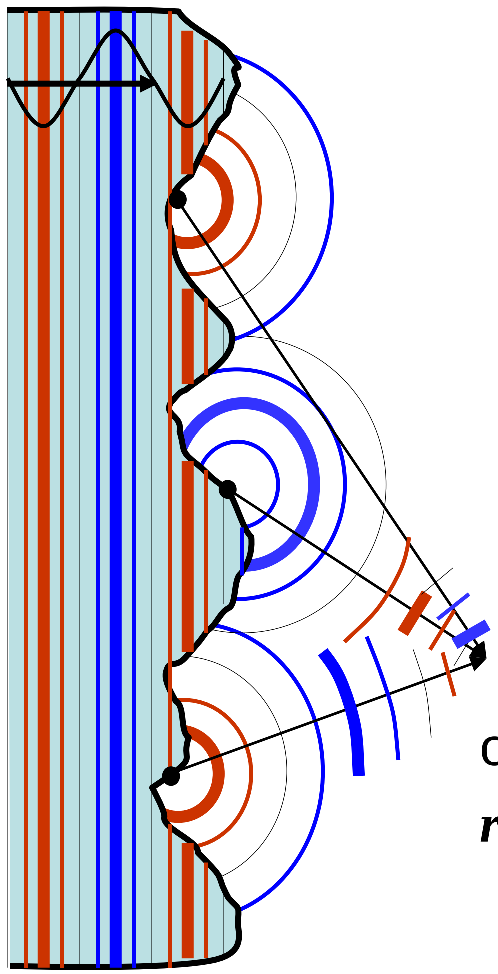


$$ARS(\theta) \sim g(k_x)\cdot\cos\theta = g\left(\frac{2\pi}{\lambda}\sin\theta\right)\cdot\cos\theta$$



- 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

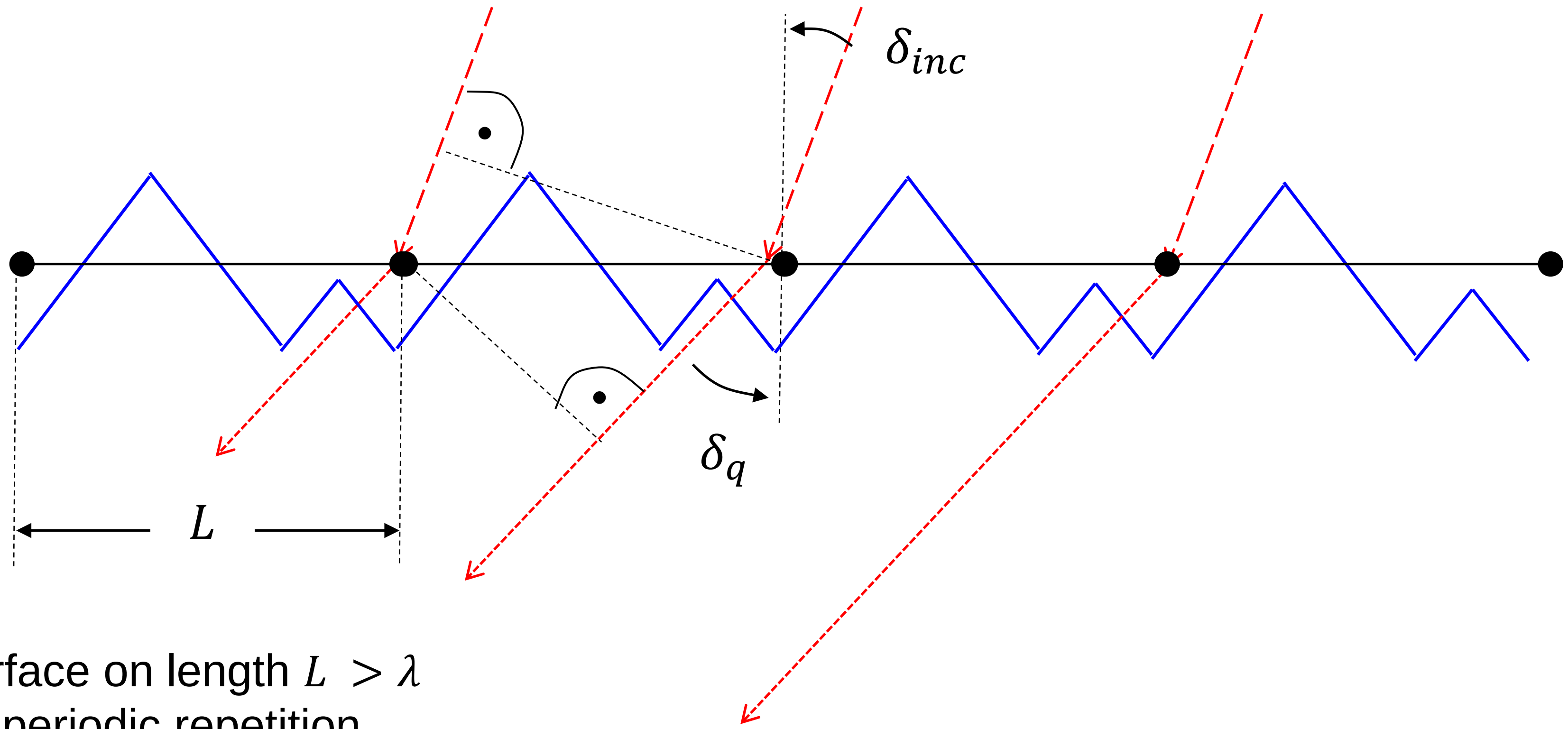
Two choices of aperture function $U_0(x,y)$:

- **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

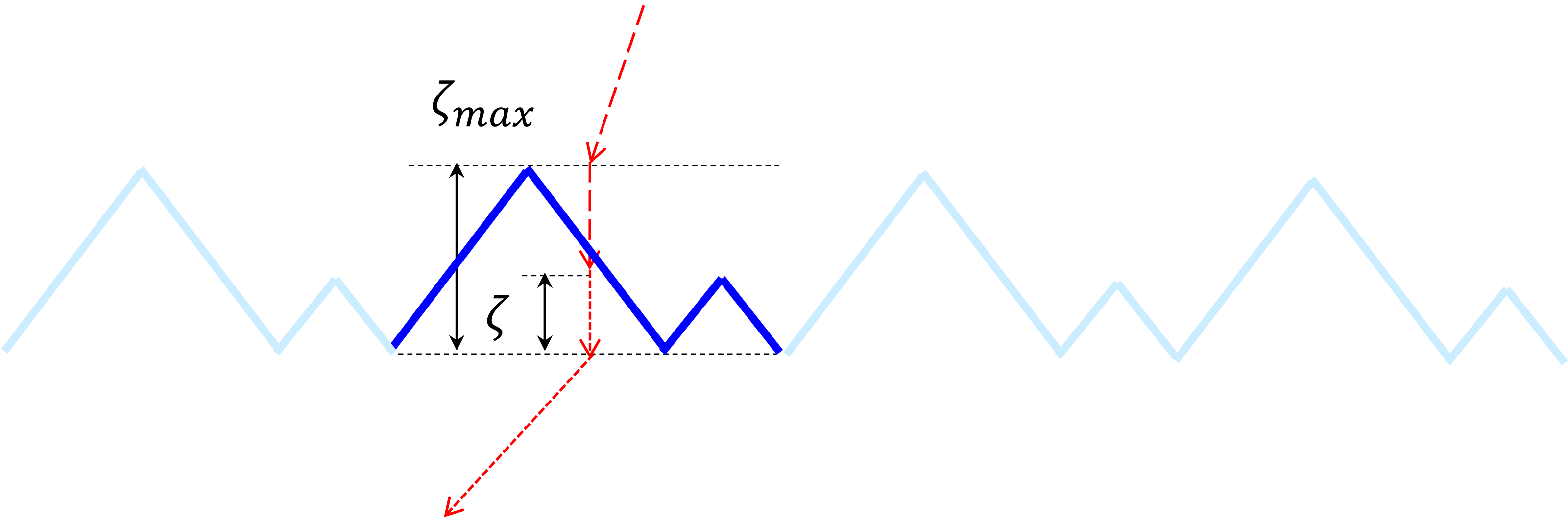


Scan surface on length $L > \lambda$
Assume periodic repetition
Periodicity L diffracts into orders q
Angles given by grating equation

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

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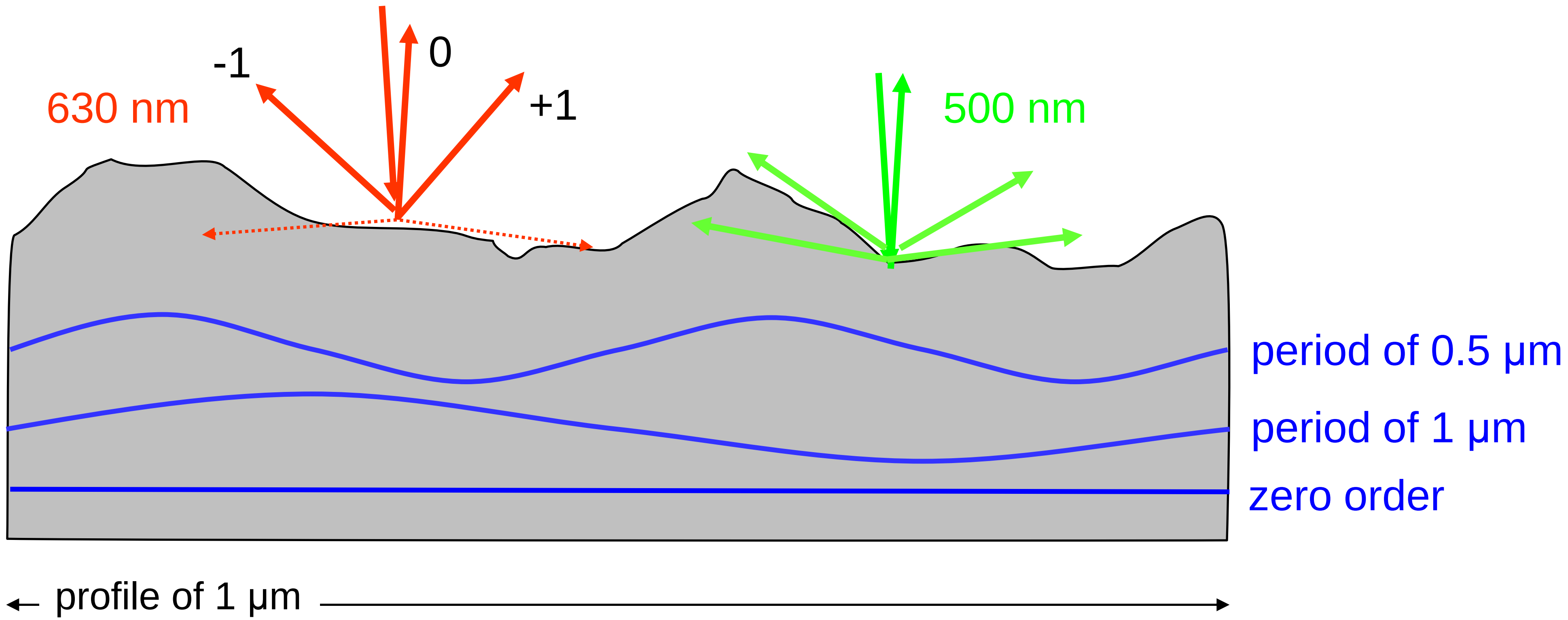
Fourier theory predicts mode amplitudes,
including zero order (specular beam) and evanescent modes

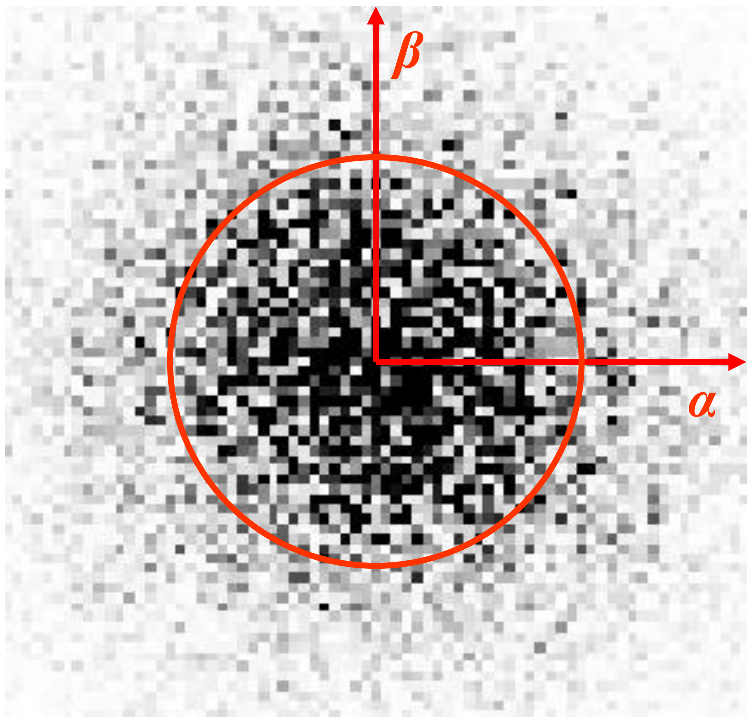
Grating analogy: λ > period: specular reflection, no diffraction



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

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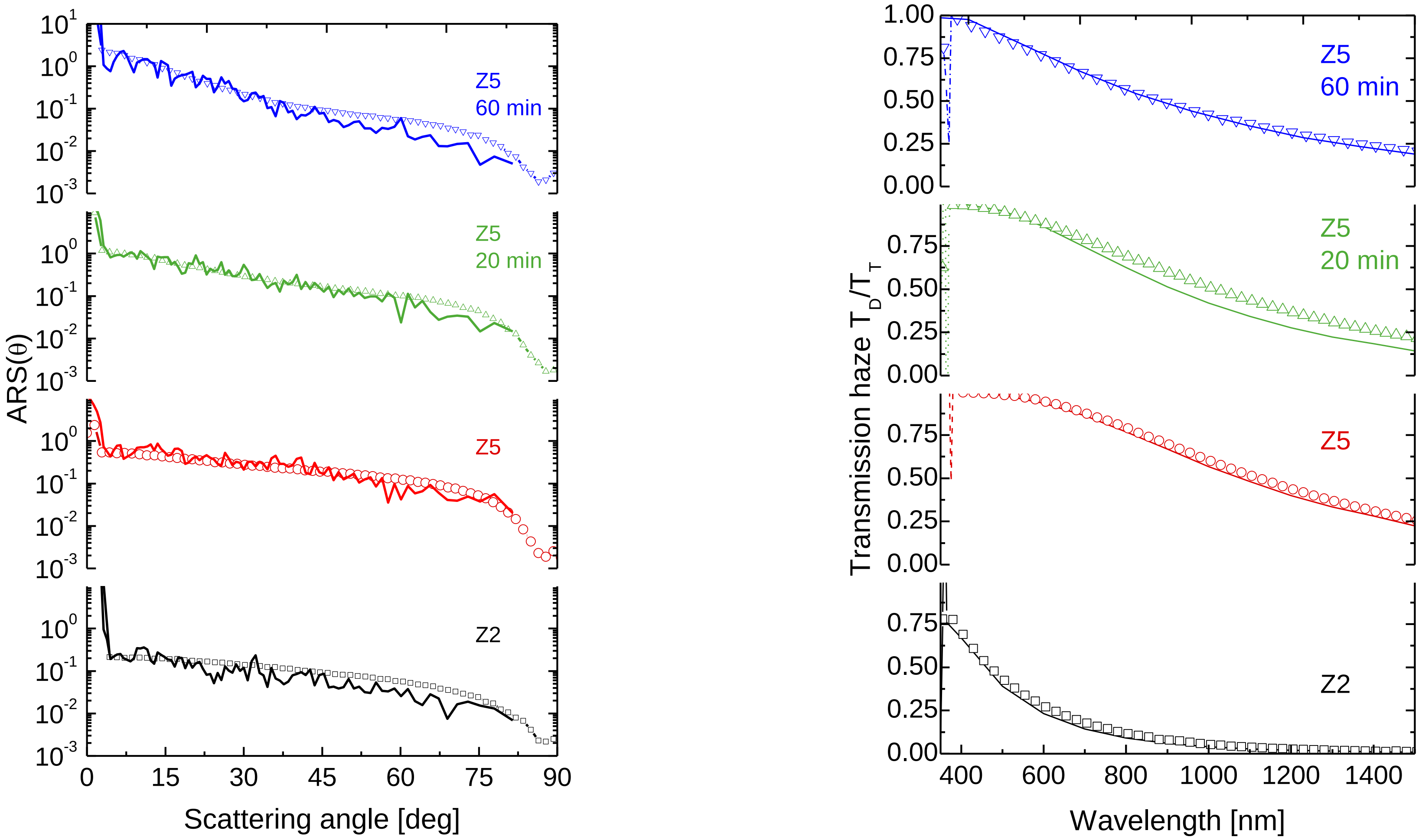
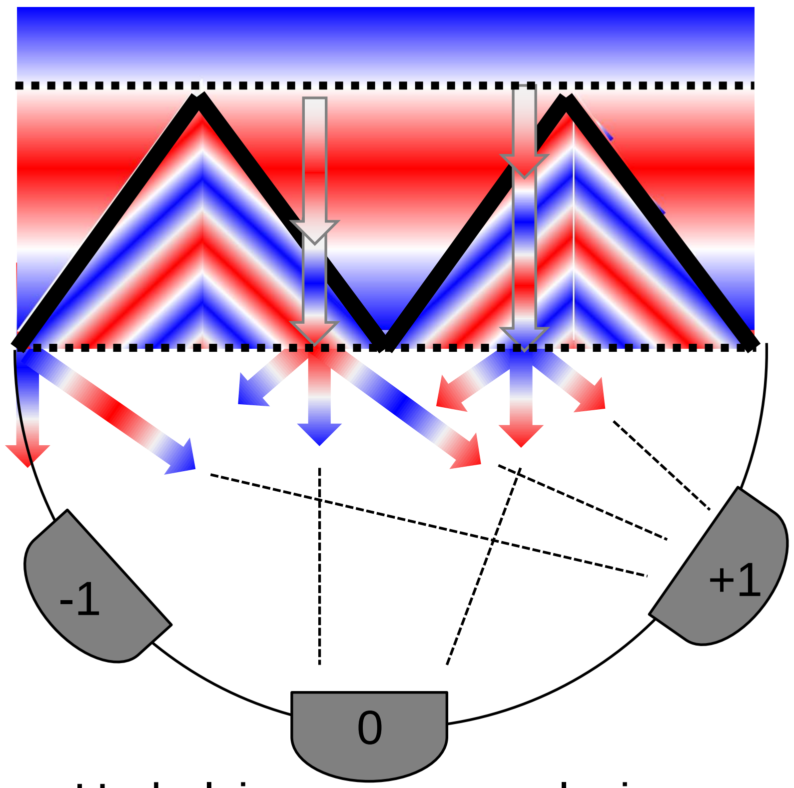


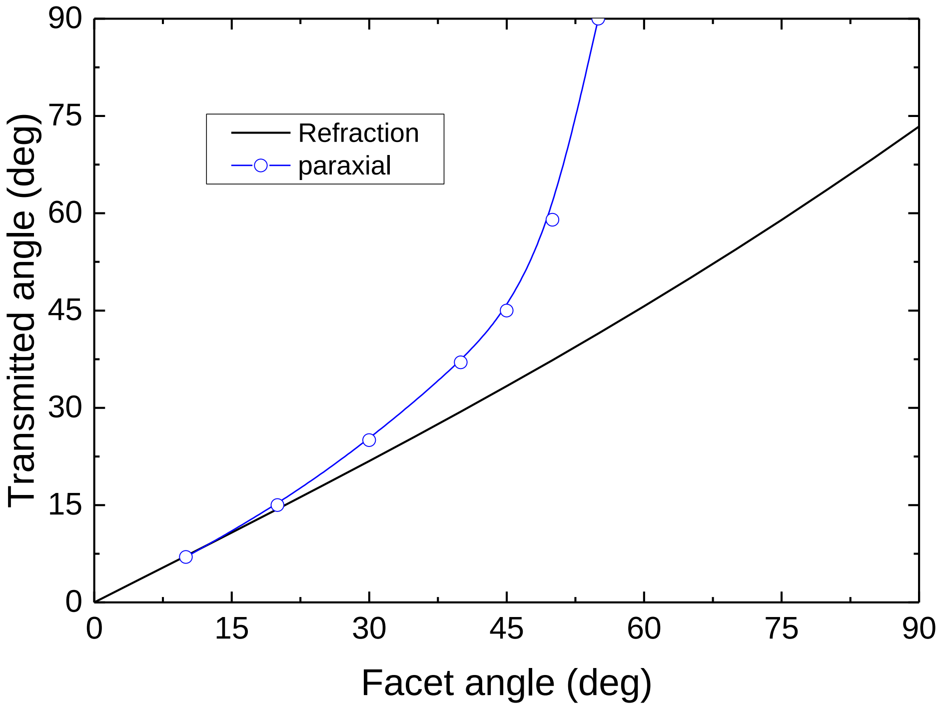
Excellent agreement for ARS at 514 nm and for spectral haze, no empiric parameters

Domine, JAP (2009)

Caveat: paraxial error for large angles

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

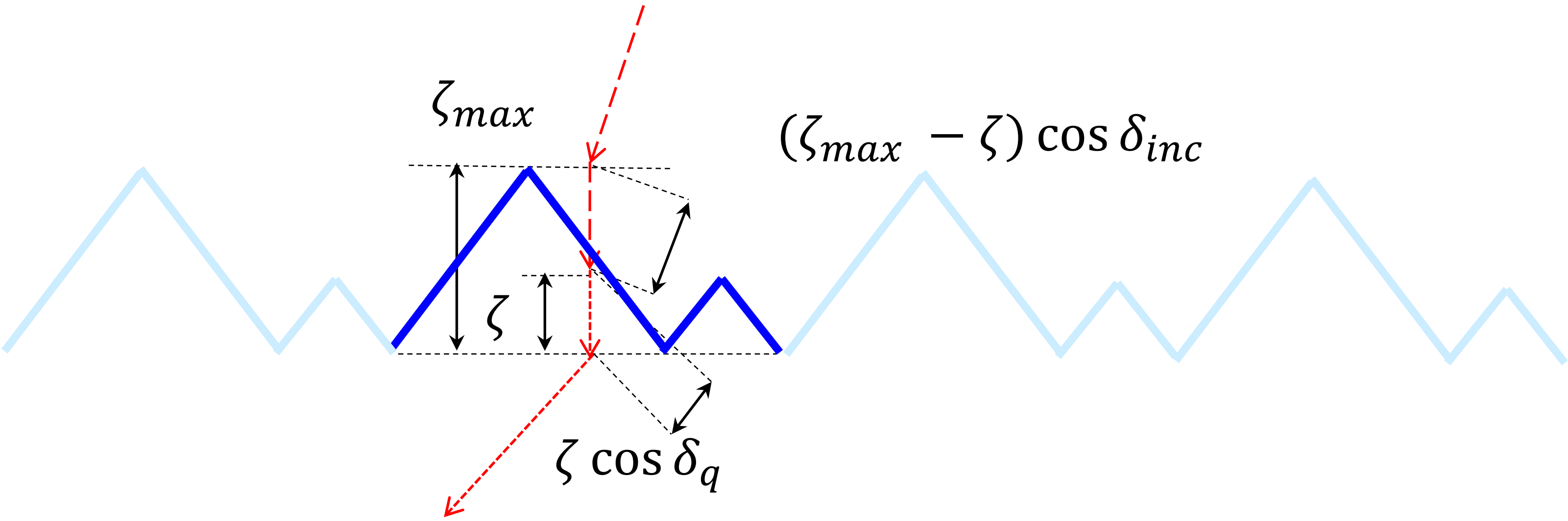




Underlying reason: replacing roughness zone with
flat phase screen ignores interference within roughness

D. Dominè, PhD thesis (2009)

Removal of paraxial error

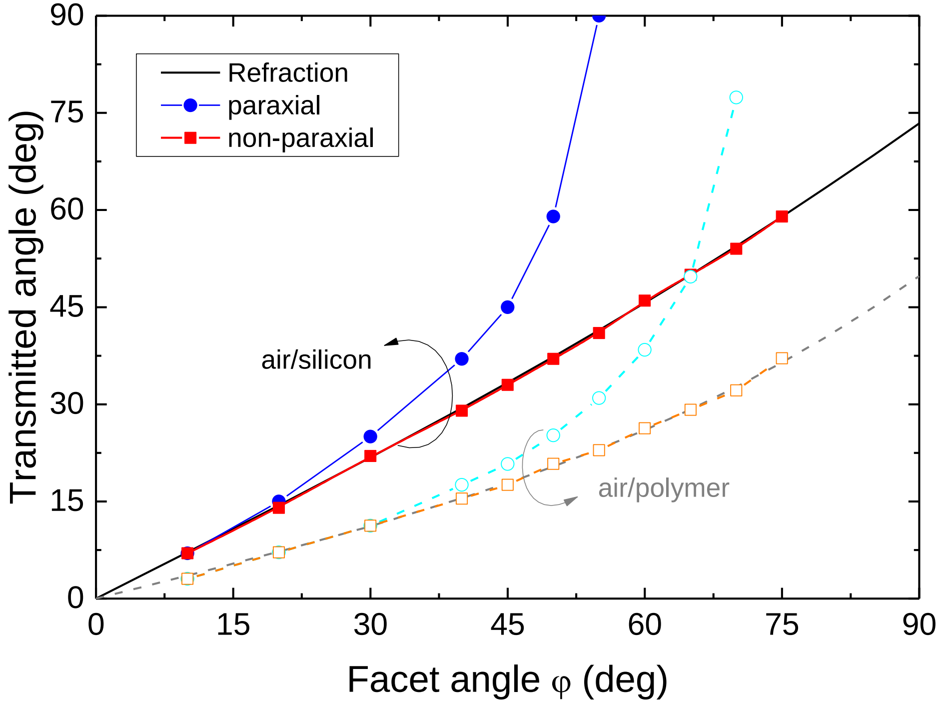


Use projections of surface profile along incoming and outgoing beams

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

Harvey, JOSAA (2006)
(defined for reflection)

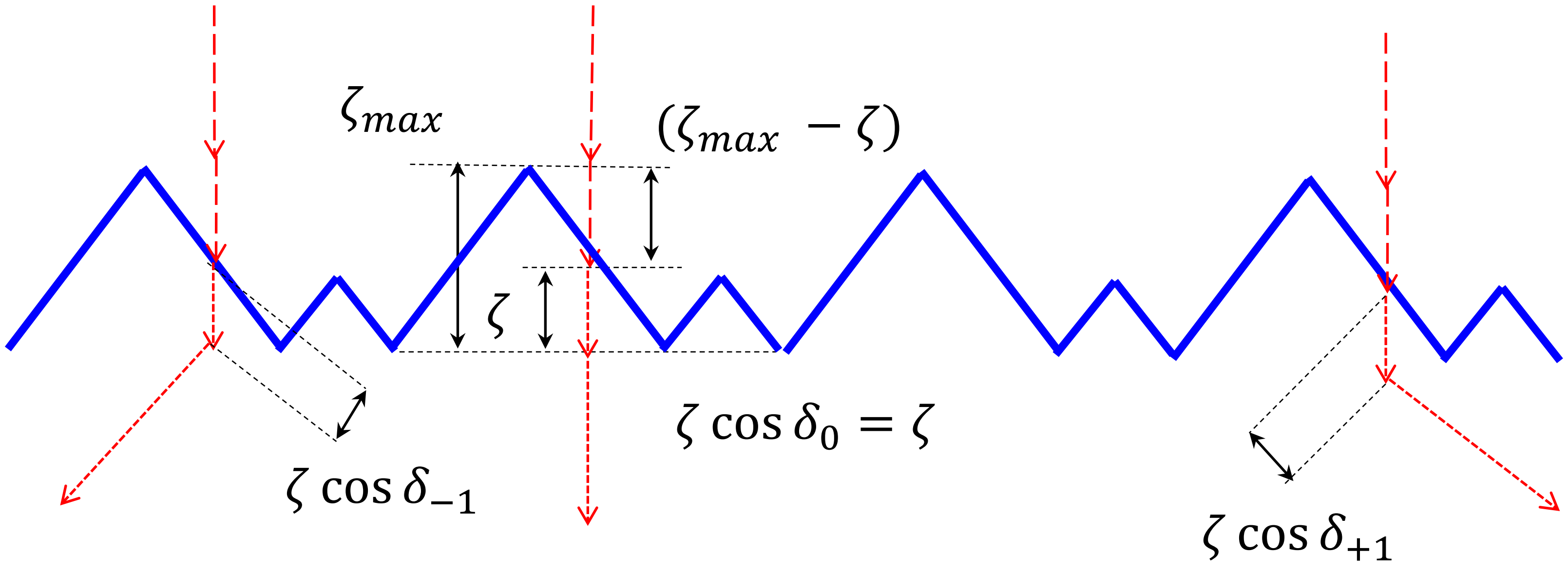
Removal of paraxial error



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



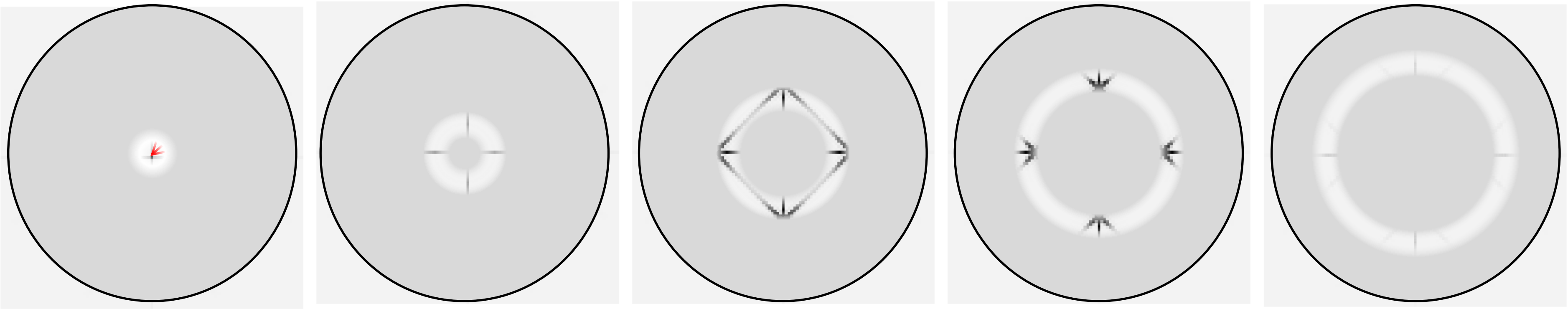
Consider perpendicular incidence
Define U_t for $q = 0$, calculate FFT_0 (fast)
Define U_t for $q = +1$ (shallower structure), calculate FFT_1 (fast)
etc.

FFT_1 is also applicable for $q = -1$ and more generally for $|q| = 1$ in case of 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

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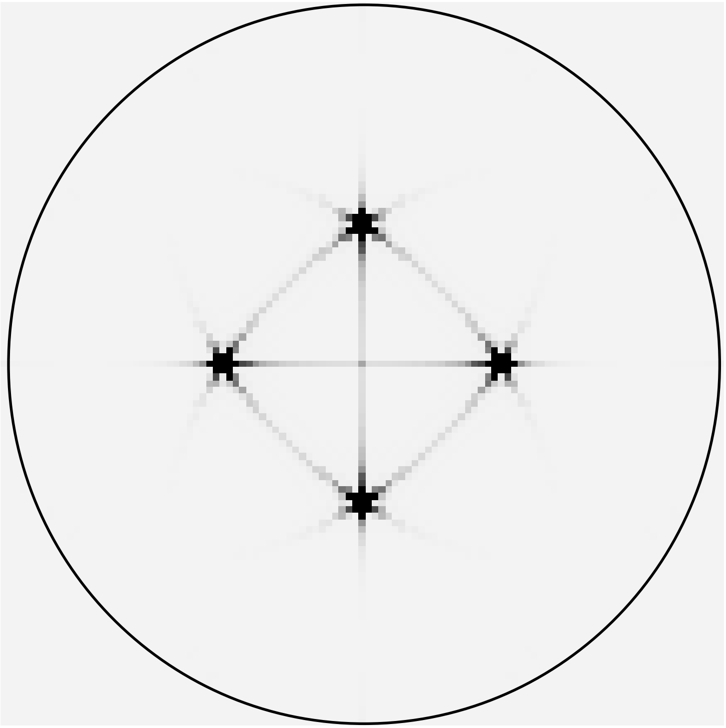
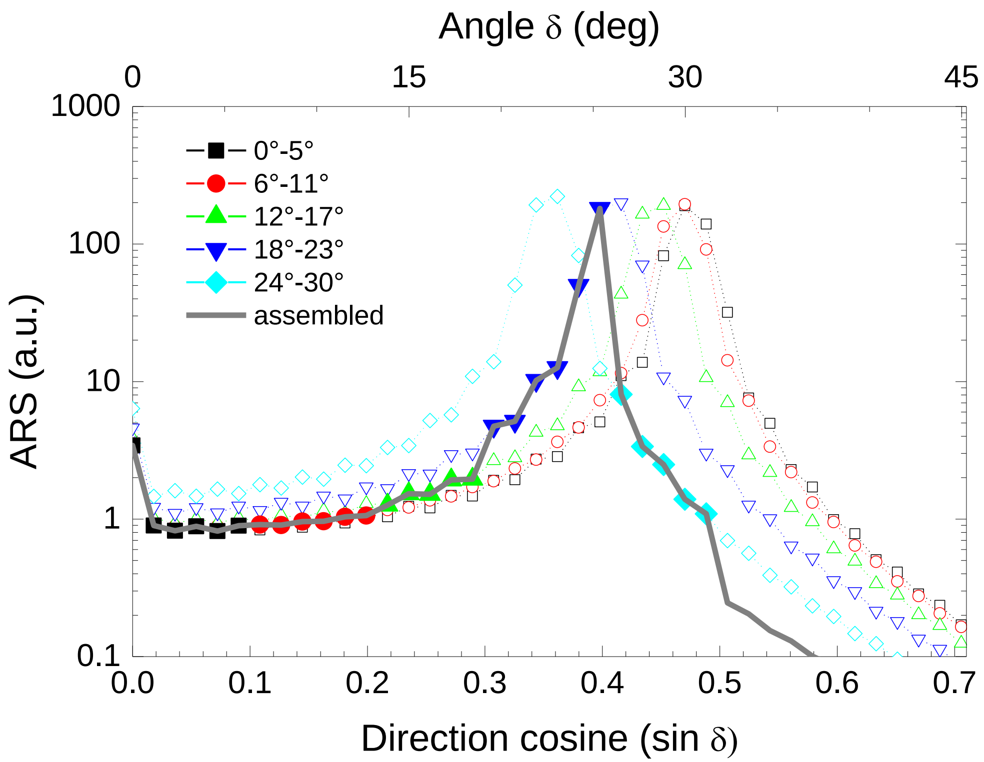
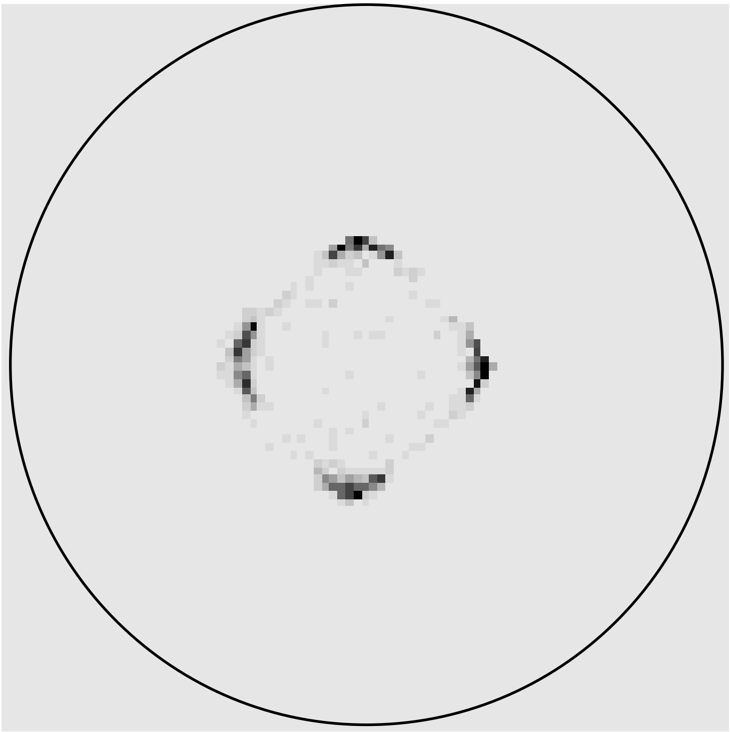




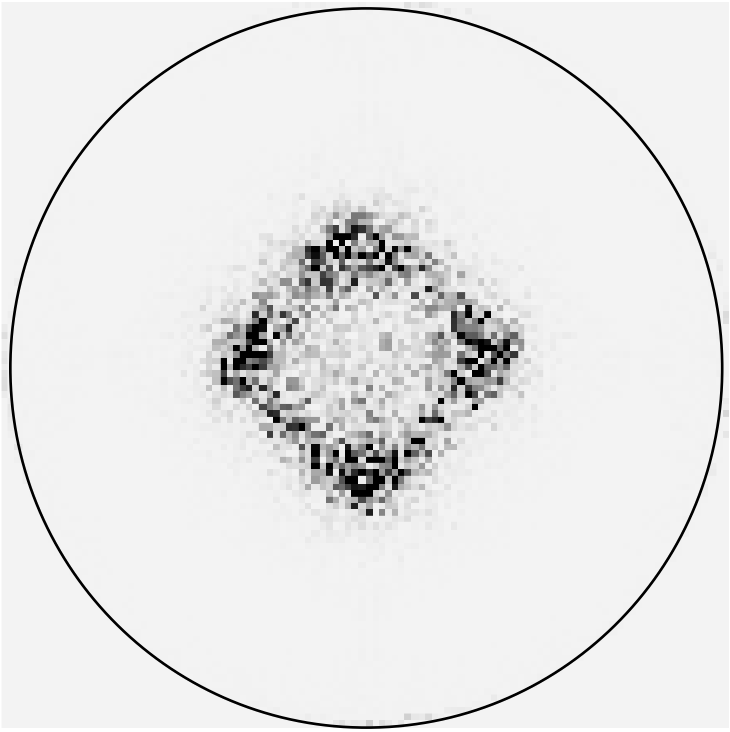
10 FFTs of 512x512 array; 12 sec with Mathematica on my laptop

Ray tracing or Fourier model?

Compare predictions for AFM profile of large pyramids



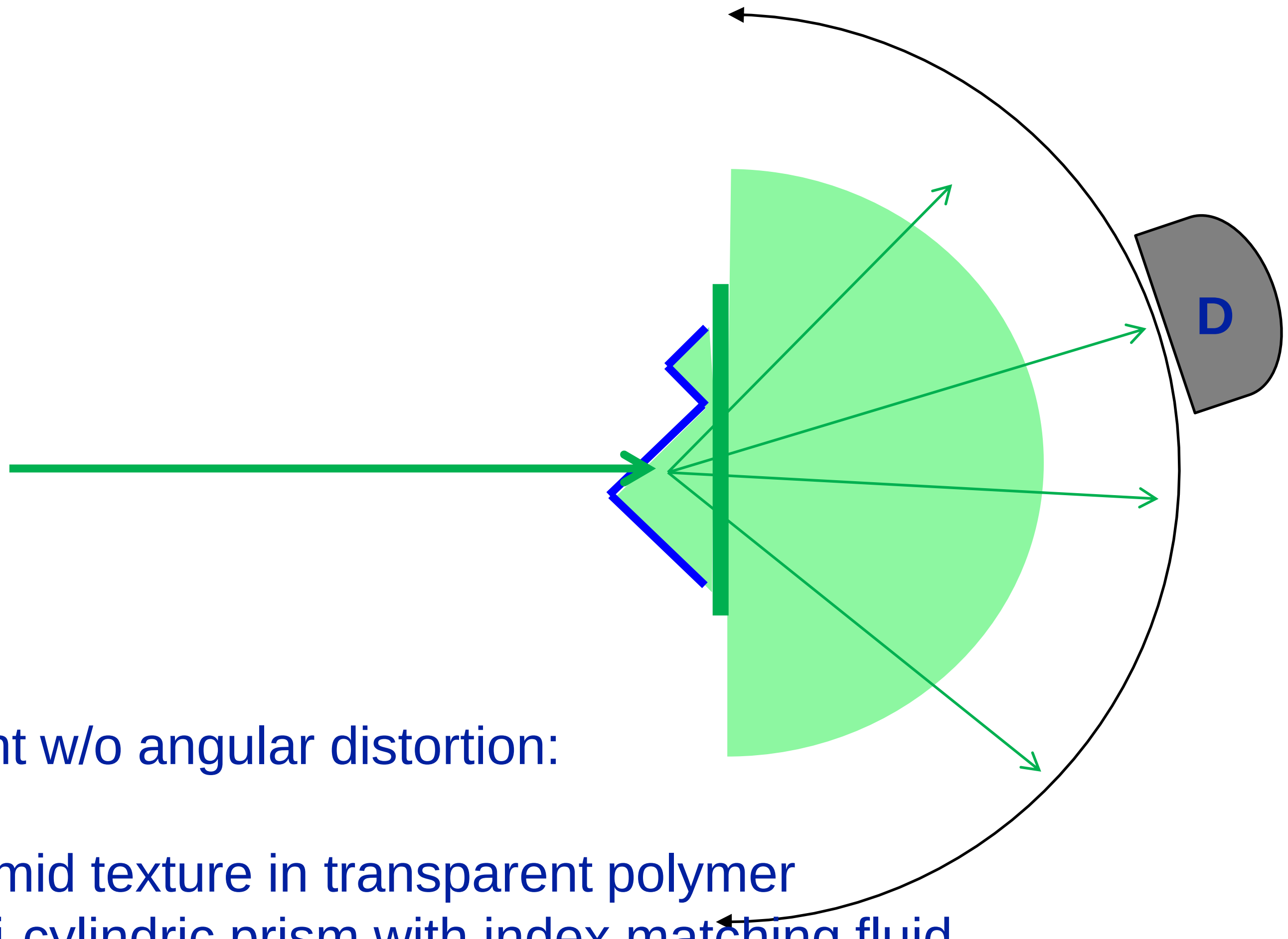
Ray tracing: four clear peaks



Fourier: broader peaks w. connection

PV-lab
IEM NEUCHATEL

Comparison with measurement (n =1.5)

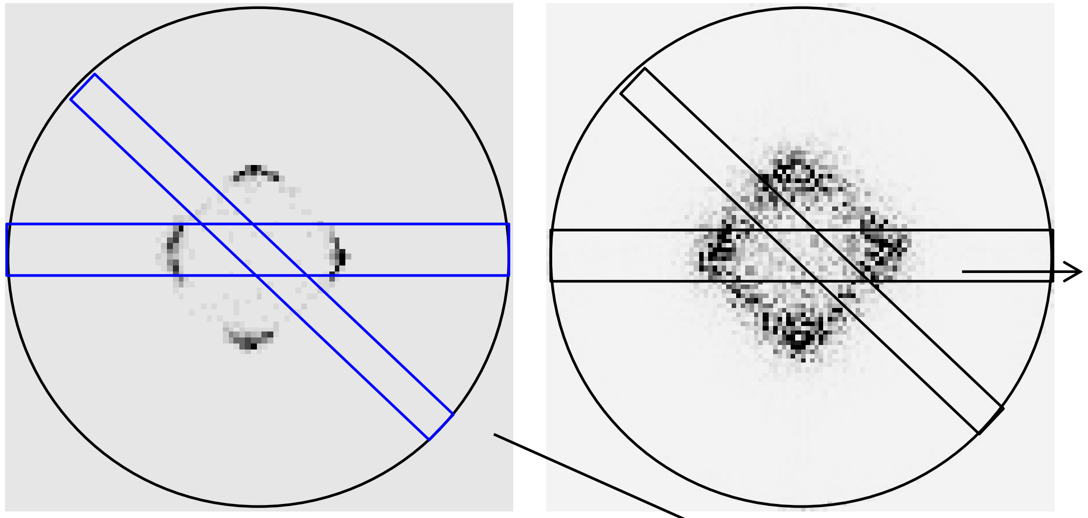


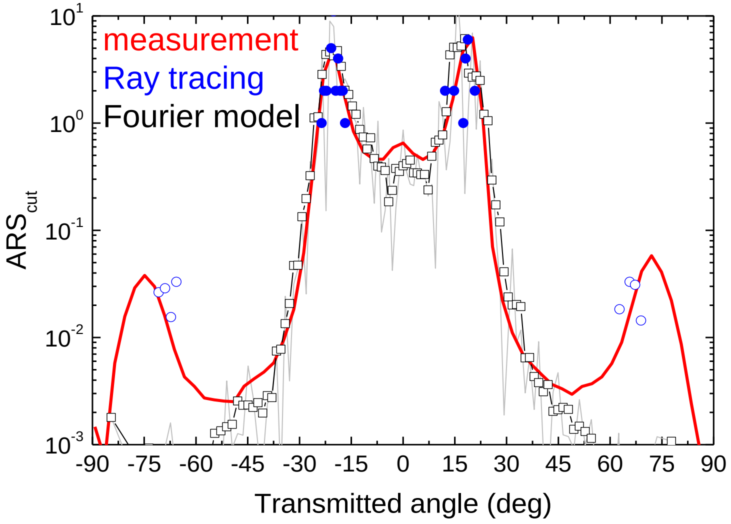
measuremeant w/o angular distortion:

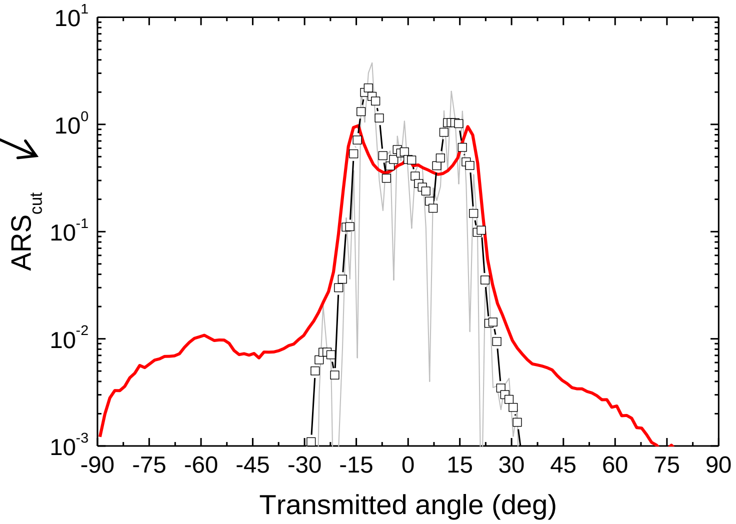
replicate pyramid texture in transparent polymer
attach to hemi-cylindric prism with index matching fluid

Replica:
Escarre, SolMat (2012)

Comparison with measurement





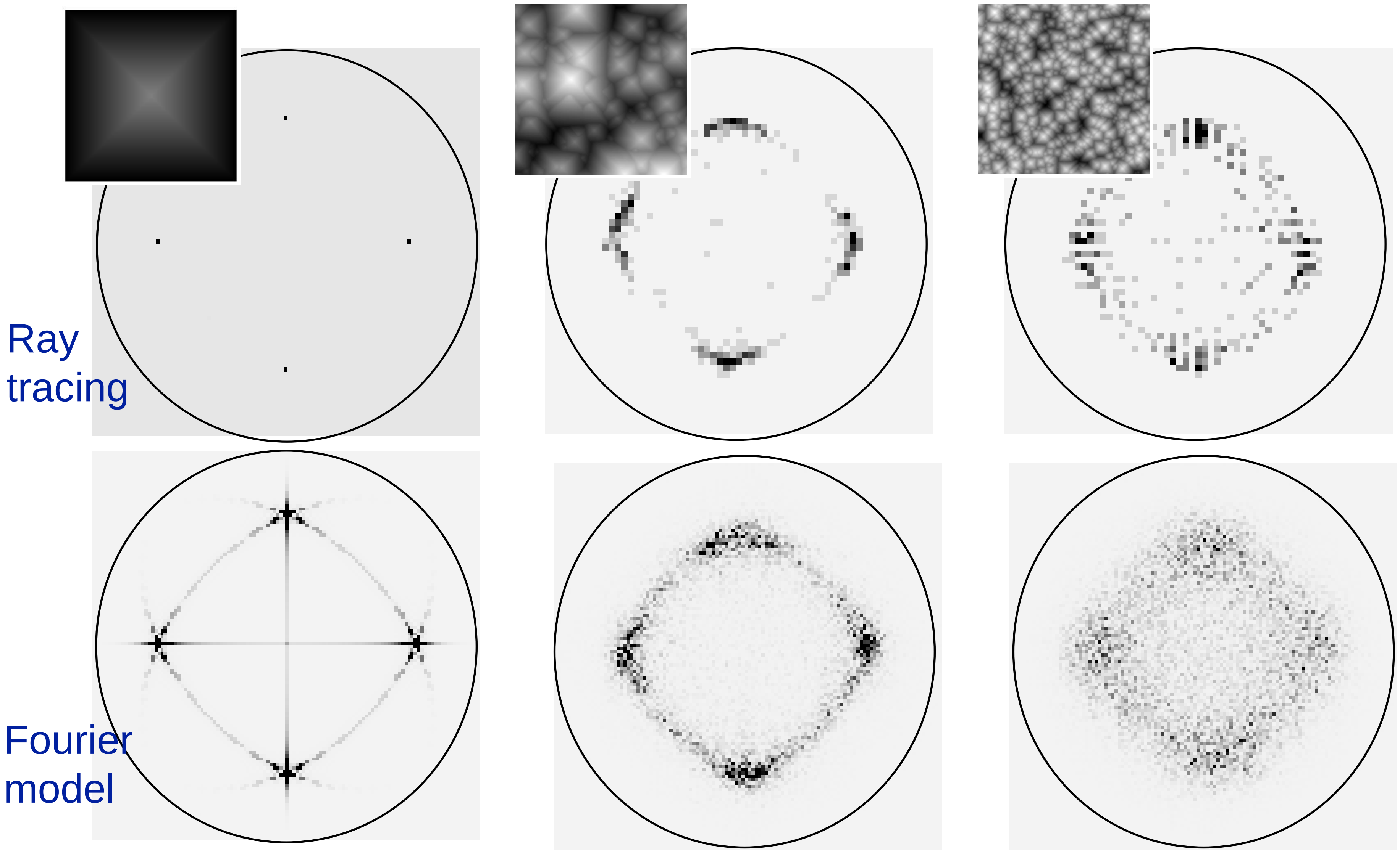


Ray tracing:
- peak positions reproduced
- 2^{nd} rebound at high angles
- little or no signal along diagonal

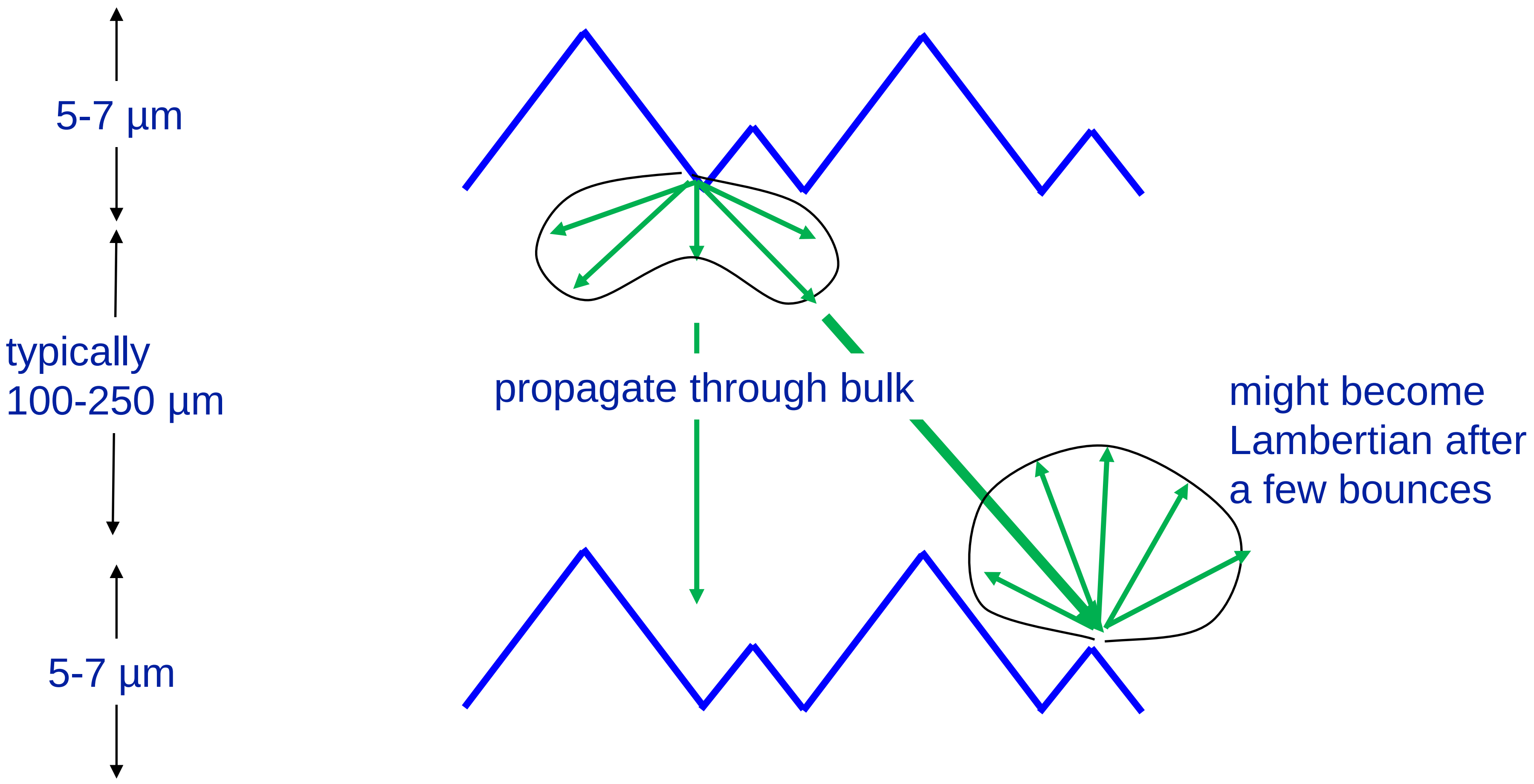
Fourier model
- Main peaks reproduced over 4 orders
- Diagonal over 3 orders
- But: no 2^{nd} rebound

Refraction vs. diffraction into silicon (n =3.5)

F.-J. Haug



Use in a combined modelling approach



Back reflector

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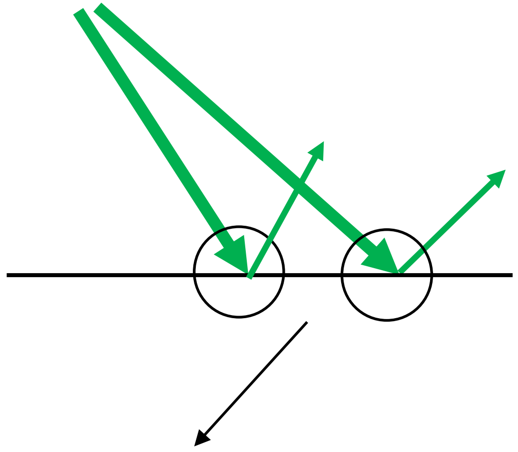
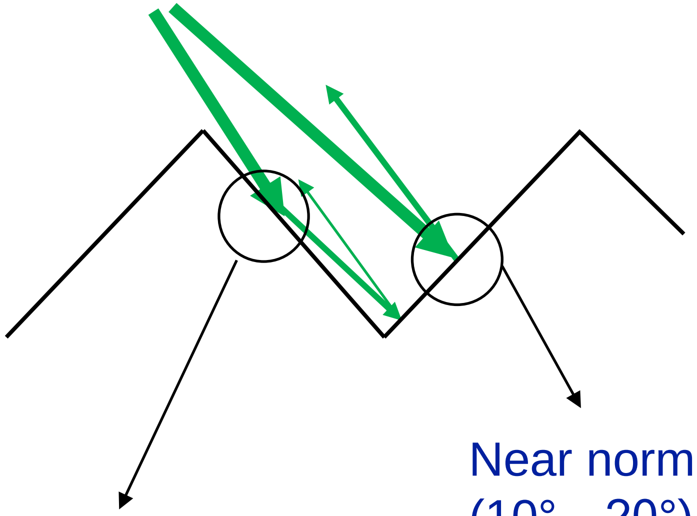
Flat



Incidence btw. 40° and 60°

Textured



Grazing incidence
(70°…80°)

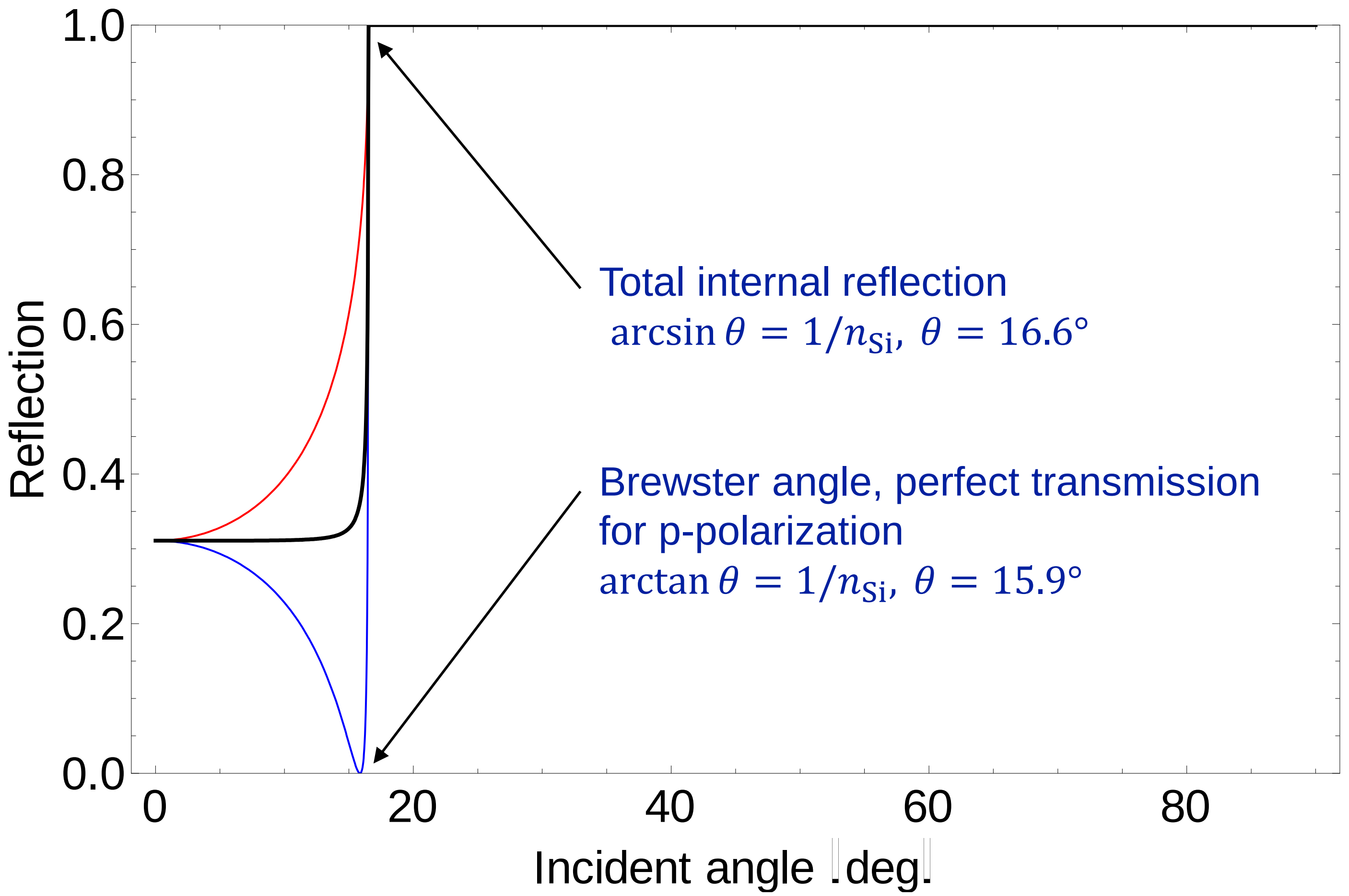
Near normal incidence
(10°…20°)

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

Angular reflection from wafer into air

F.-J. Haug

at 1200 nm



more information: Holman, JAP (2013)

Back surface with metal contact

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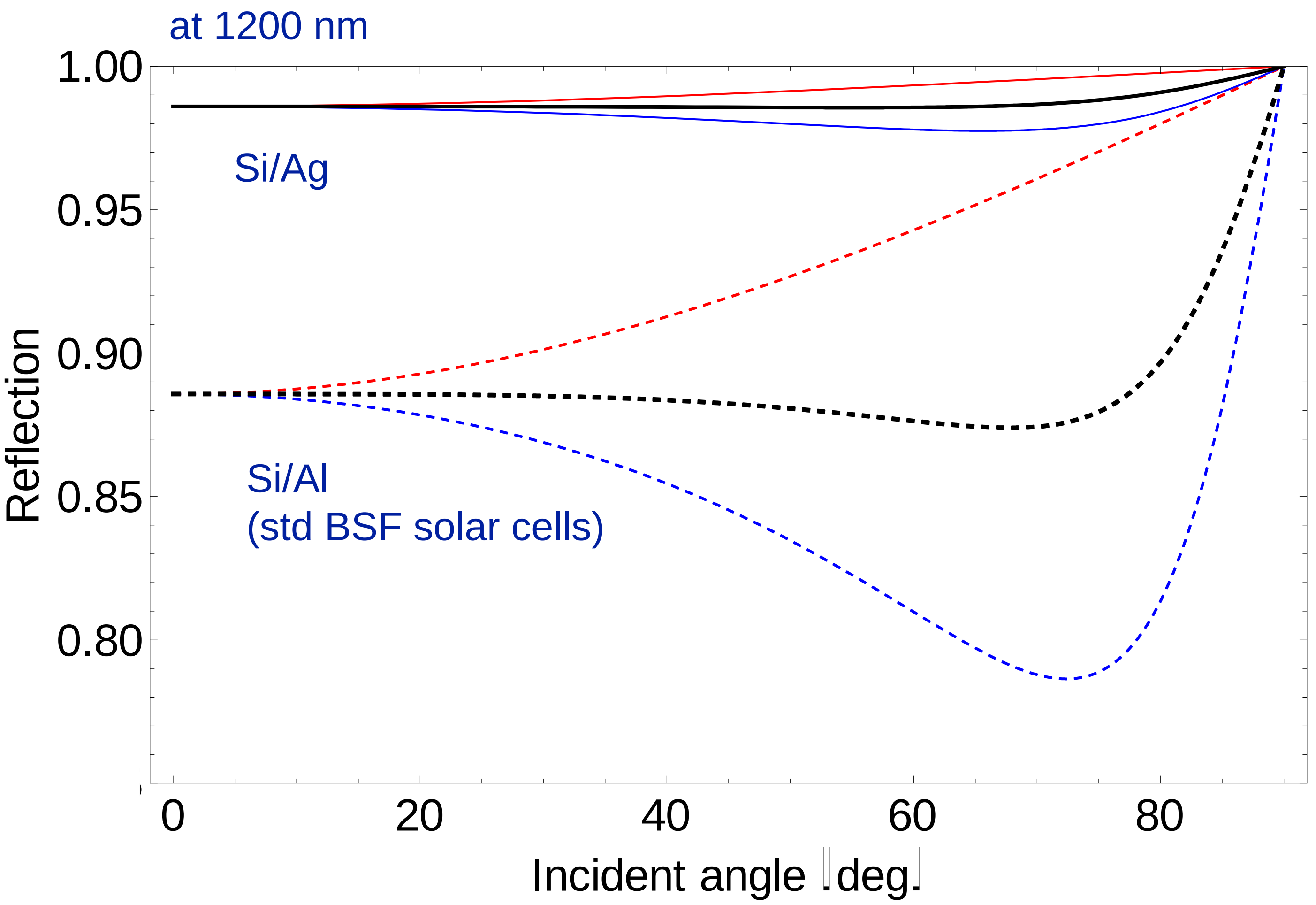
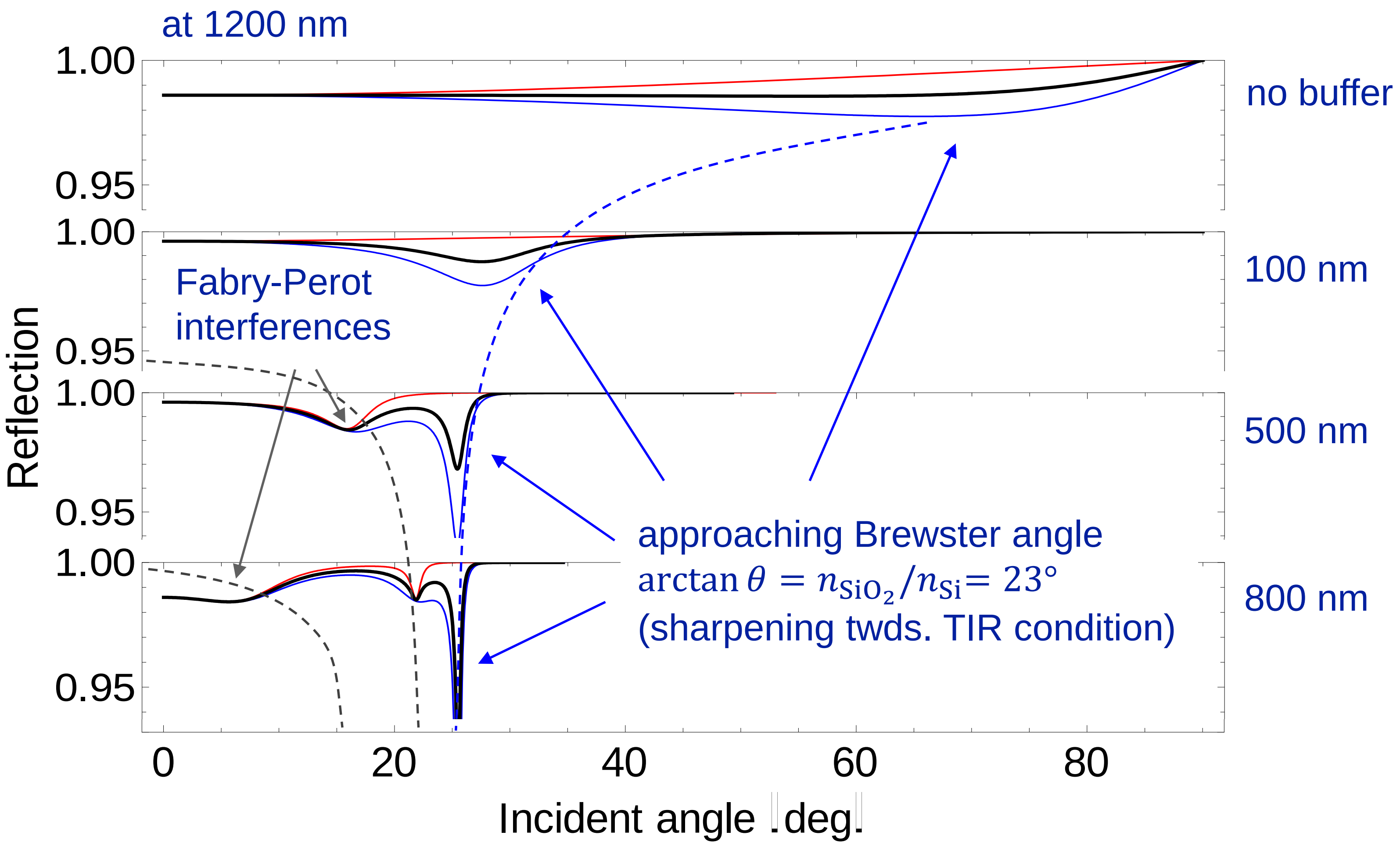


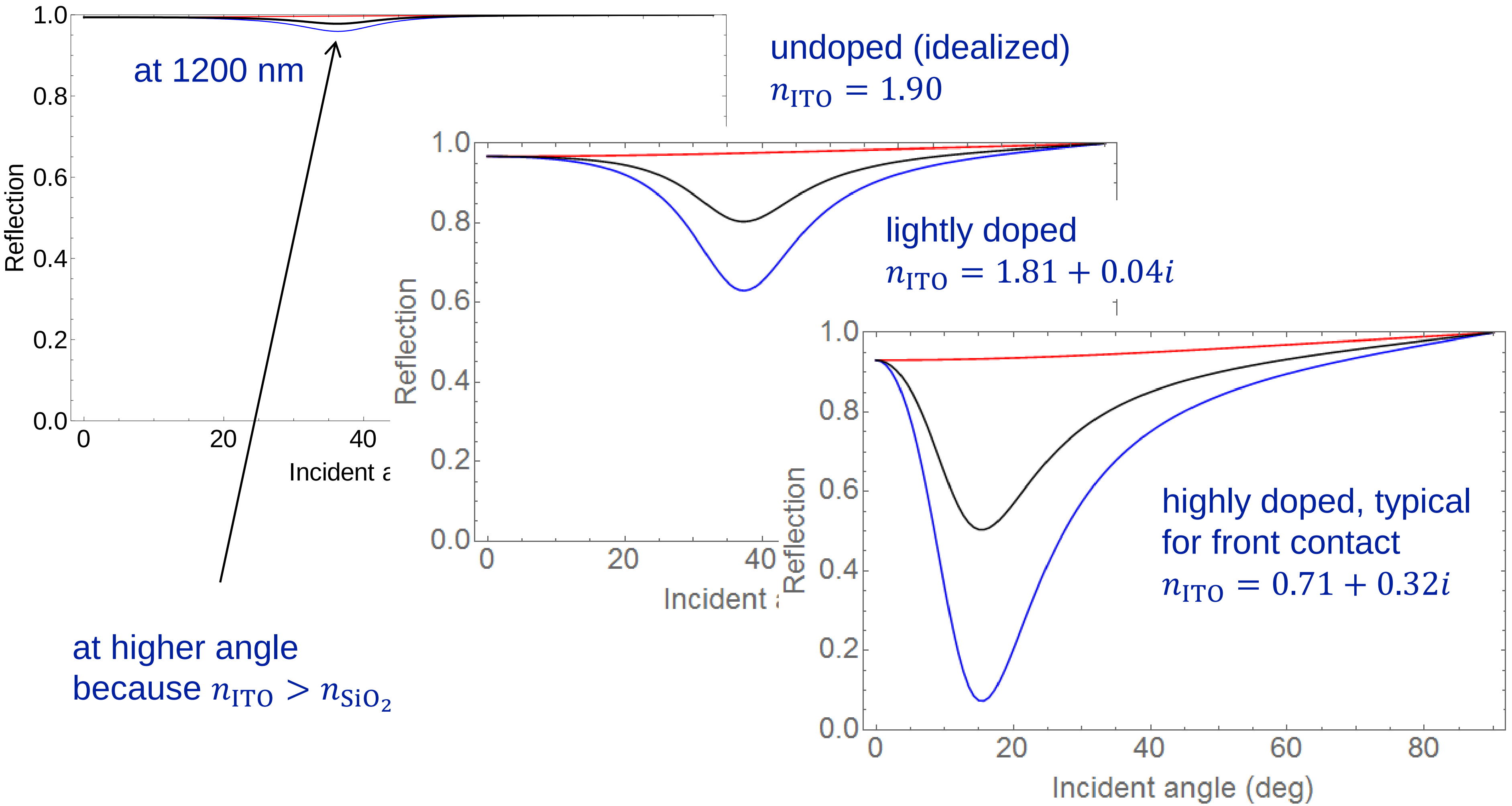
better for low angles (even with Al), much worse for high angles (no TIR any more)
Technological constraint: massive recombination at semiconductor/metal interfaces

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)



at 1200 nm

undoped (idealized)
$n_{\text{ITO}} = 1.90$

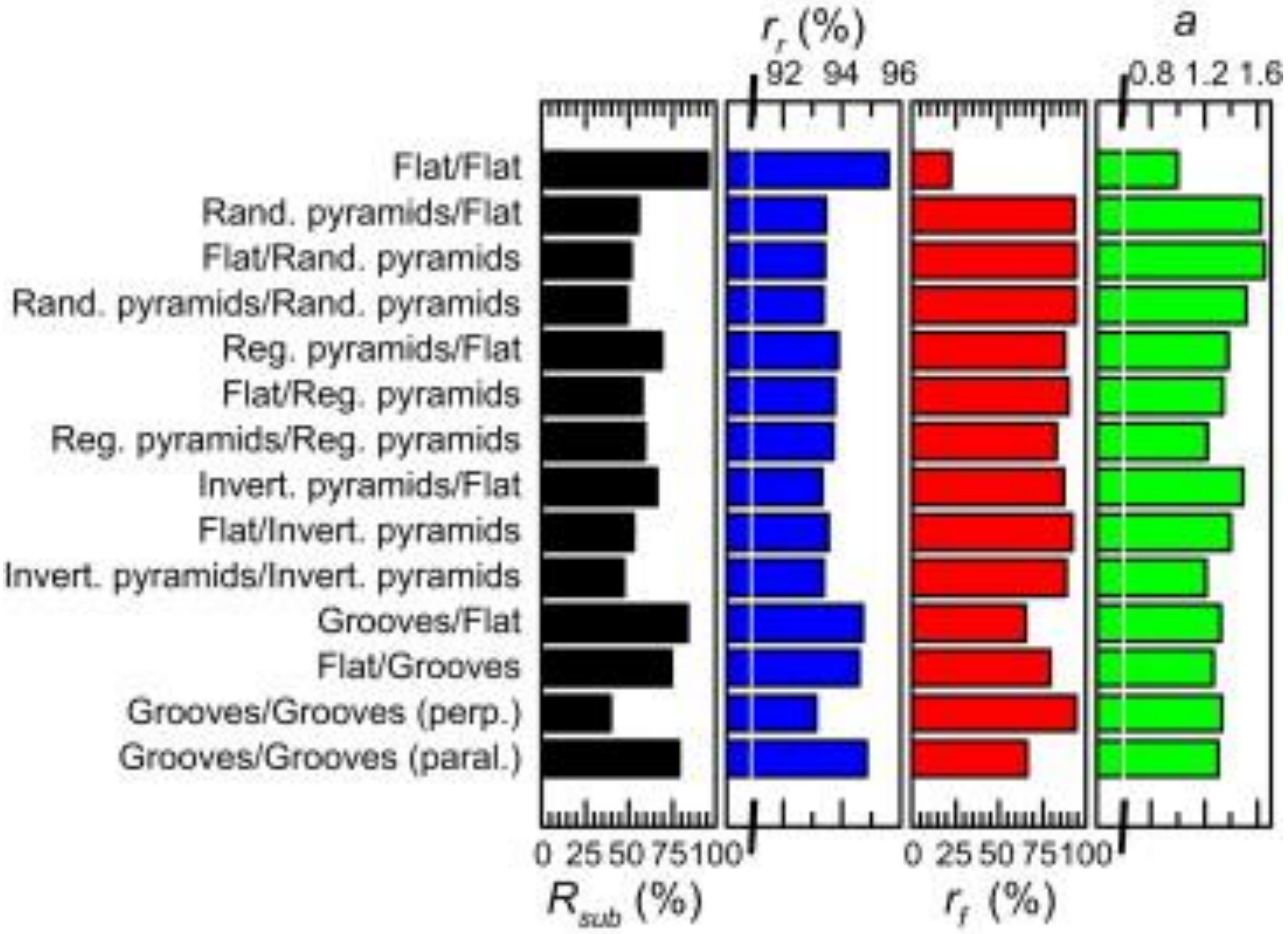
lightly doped
$n_{\text{ITO}} = 1.81 + 0.04i$

highly doped, typical for front contact
$n_{\text{ITO}} = 0.71 + 0.32i$

at higher angle
because $n_{\text{ITO}} > n_{\text{SiO}_2}$

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