National School on Neutron and X-ray Scattering
August 15-29, 2004
Argonne National Laboratory

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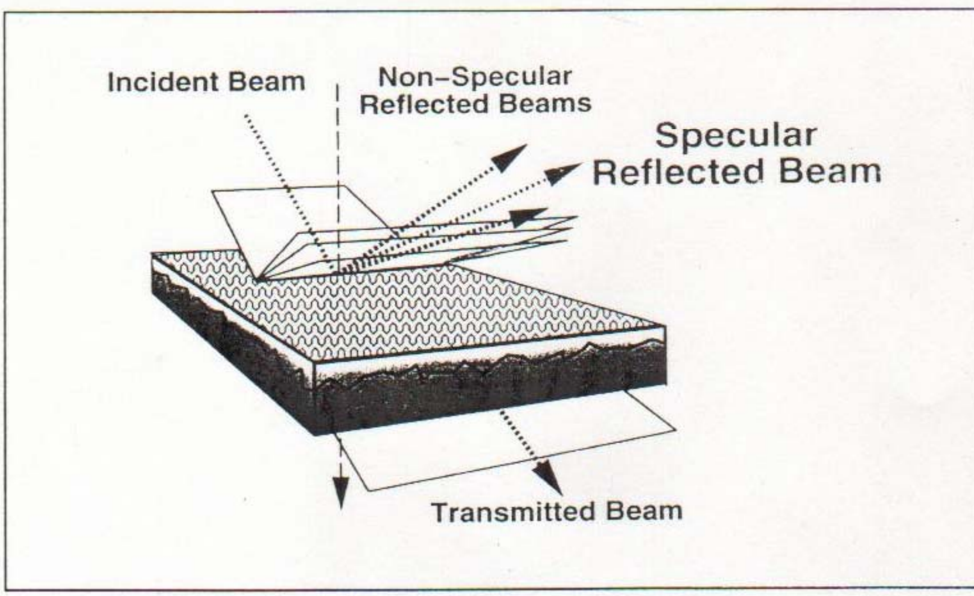
Fundamentals of X-Ray and Neutron Reflectometry



(Figure after N.F. Berk)

C.F.Majkrzak

National Institute of Standards and Technology

NCNR Researchers with a Major Interest in Reflectometry

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PROBES OF THE MICROSTRUCTURE OF SURFACES AND INTERFACES

photons, electrons, neutrons, atom and ion beams, miniature mechanical devices

* DIRECT IMAGING (REAL SPACE)

  e.g.:

  - optical microscopy (~ 1000 x magnification)
  - scanning electron microscopy (SEM) (orders of magnitude higher magnification than possible with light)
  - transmission electron microscopy (TEM)
  - atomic force microscopy (AFM)

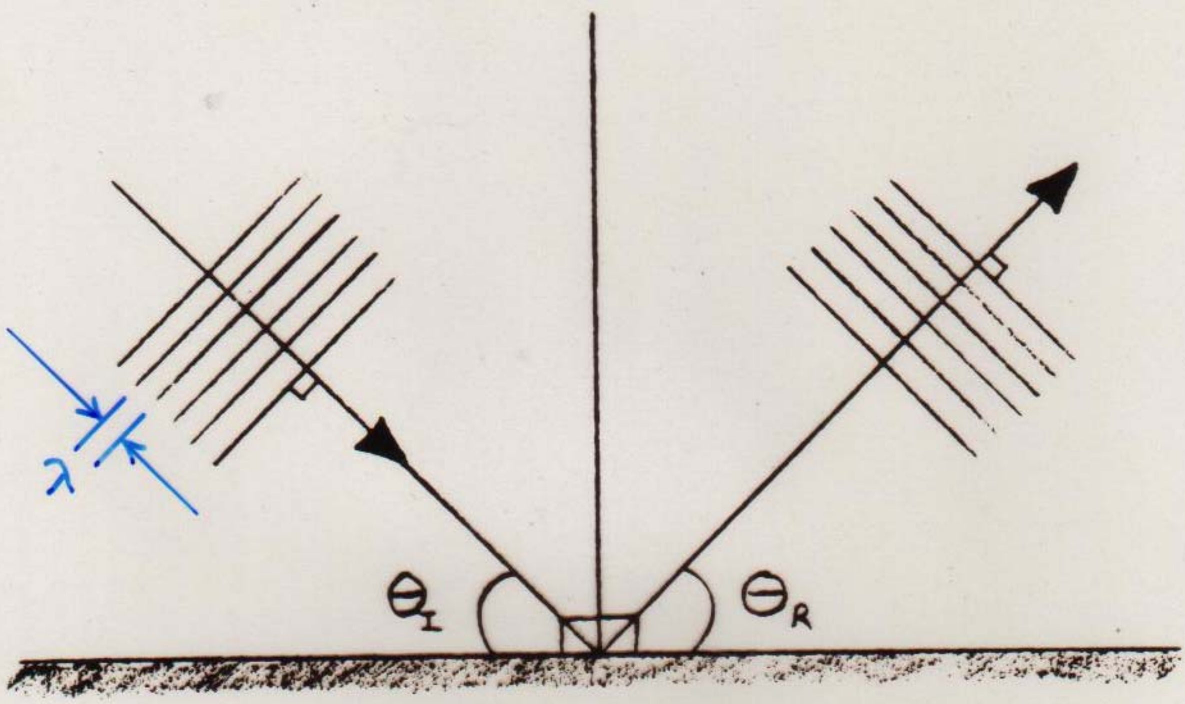
* DIFFRACTION (RECIPROCAL SPACE)

  e.g.:

  - low energy electron diffraction (LEED)
  - spin polarized LEED (SPLEED)
  - reflection high energy electron diffraction (RHEED)
  - ellipsometry (optical polarimetry)
  - x-ray reflectometry
  - neutron reflectometry

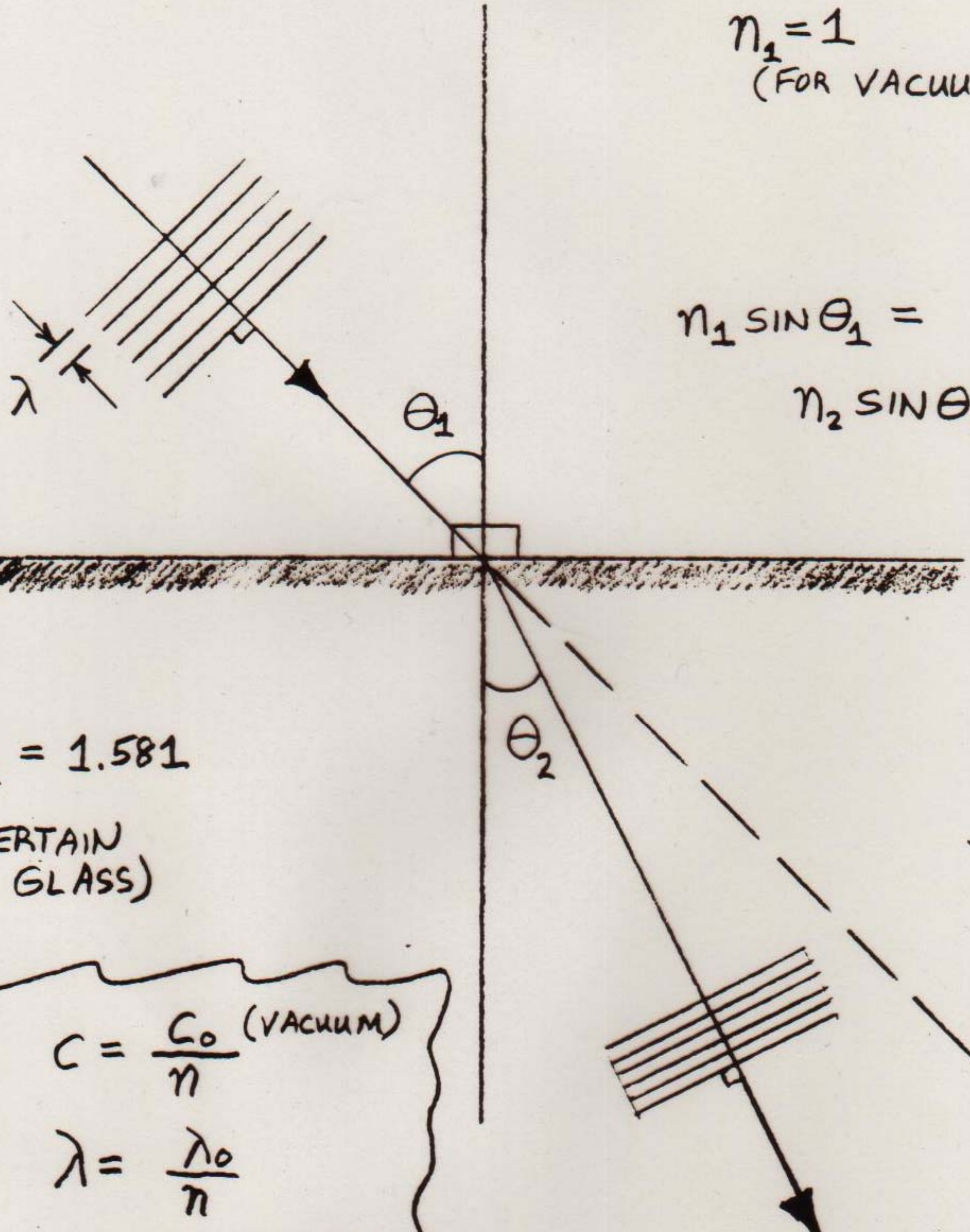
For quantitative measurements of depth profiles along a normal to the surface, x-ray and neutron reflectometry are particularly useful because of their relatively weak interactions with condensed matter and the fact that these interactions can be described accurately by a comparatively simple theory. In the case of electron diffraction, on the other hand, the potential is non-local and the scattering is non-spherical, relatively strong and highly energy-dependent. For atom diffraction, the description of the interaction potential can be even more complicated.

"SPECULAR" OR "MIRROR" REFLECTION OF A WAVE



ANGLE OF INCIDENCE Θ_I
= ANGLE OF REFLECTION Θ_R

$\eta_1 = 1$
(FOR VACUUM)



$\eta_1 \sin\theta_1 = \eta_2 \sin\theta_2$

.g.) $\eta_2 = 1.581$
(CERTAIN GLASS)

WAVE SPEED	$c = \frac{c_0}{\eta}$ (VACUUM)
WAVE-LENGTH	$\lambda = \frac{\lambda_0}{\eta}$
WAVE-VECTOR	$k = \eta k_0 = \frac{2\pi\nu}{c}$

FREQUENCY ν = CONSTANT

REFRACTIVE INDEX η DEPENDS ON MATERIAL <u>AND</u> WAVELENGTH OF THE LIGHT

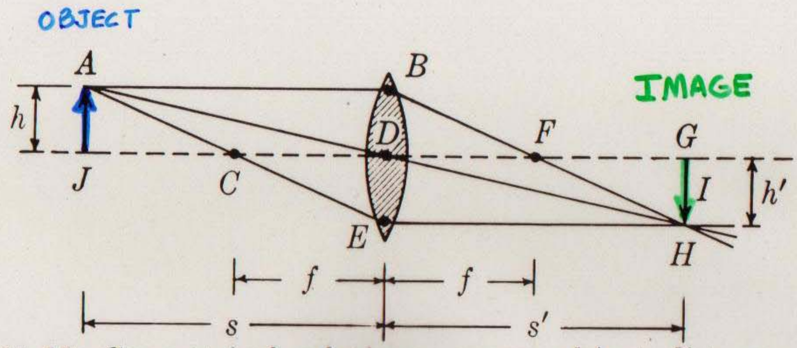


Figure 44-10. Geometrical relations among object distance s, image distance s', and focal length f.
(from Weidner & Sells, Elementary Classical Physics)

$$\boxed{1/f = 1/s + 1/s'}$$

$$h/s = h'/s'$$

The ratio of image-object *distances*, s'/s, is equal to the ratio of in object *sizes*, h'/h. This ratio h'/h is known as the *lateral magnification*.

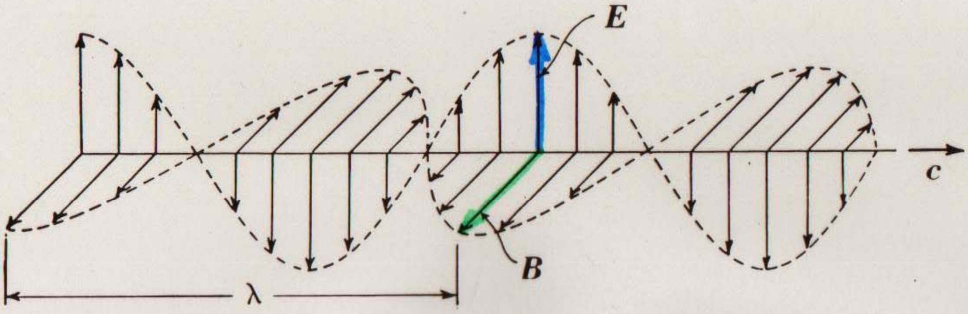
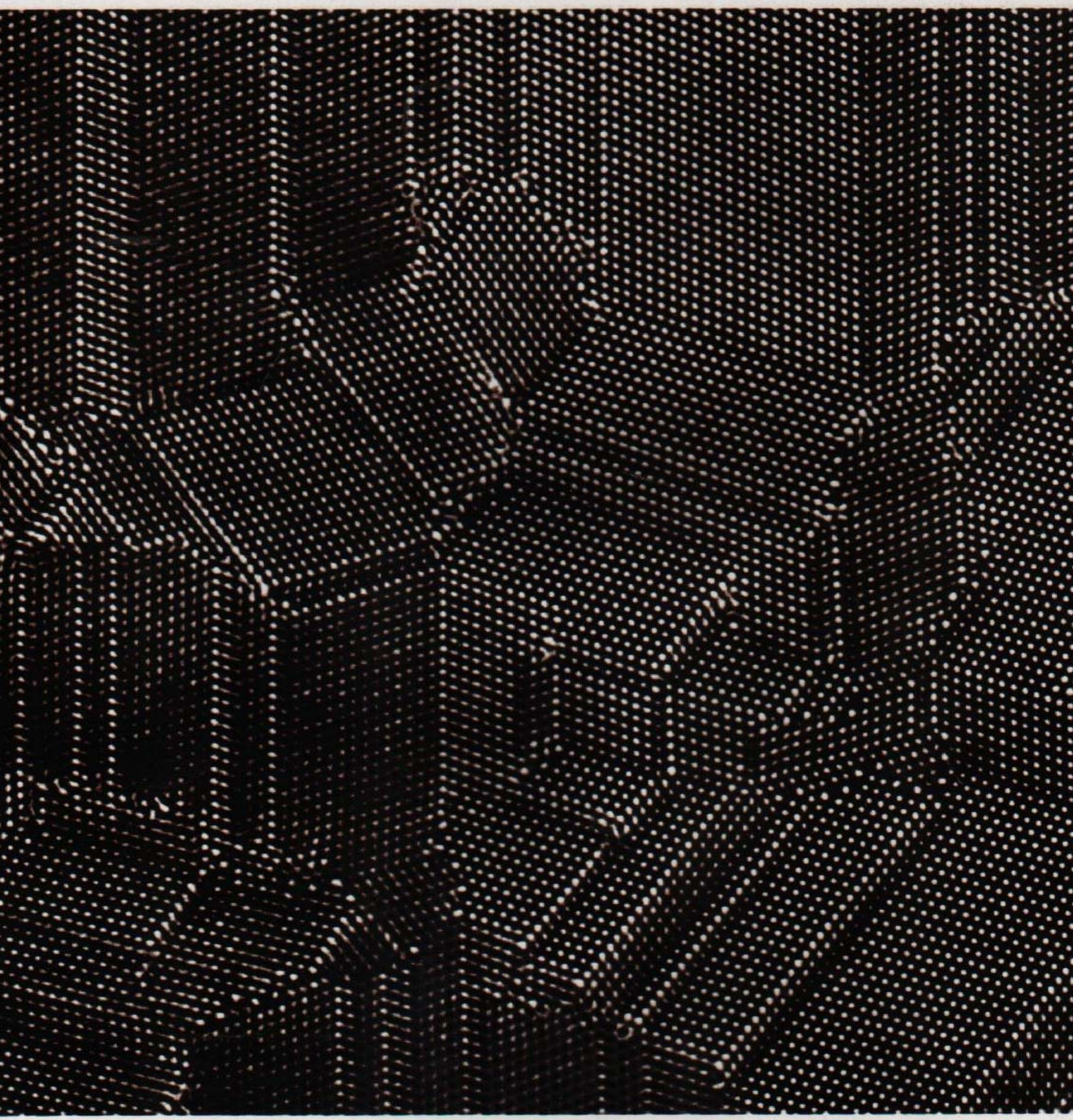


Figure 41-15. Representations of the electric and magnetic fields of a sinusoidal electromagnetic wave: (a) the field lines; (b) the sinusoidally varying amplitudes. (after Weidner & Sells, Elementary Classical Physics)

PHOTON

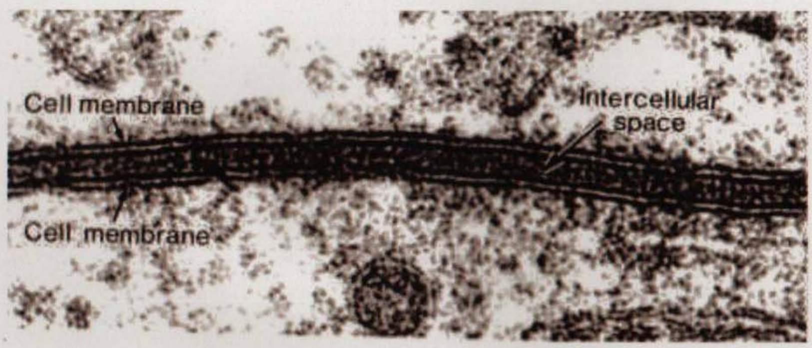
- ZERO MASS
- VELOCITY (IN VACUUM)

  $C_0 \cong 3 \times 10^8$ m/sec
- POLARIZED ELECTROMAGNETIC WAVE



Atomic resolution micrograph of multiply-twinned nanocrystalline film of Si. (C. Song)

(LAWRENCE- BERKELEY LAB.)



(AFTER BLOOM & FAWCETT, A TEXTBOOK OF HISTOLOGY)

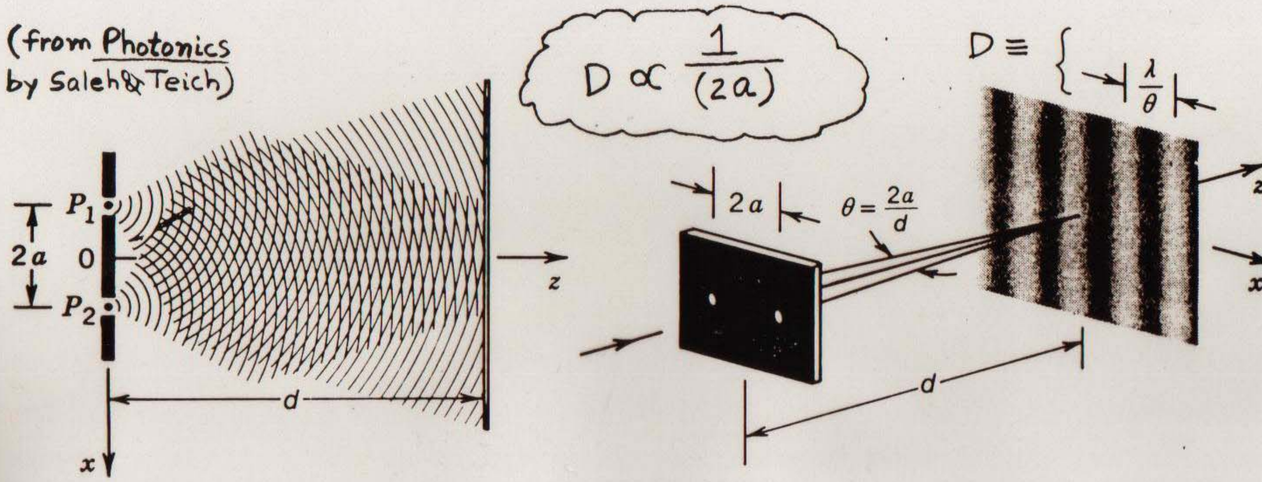
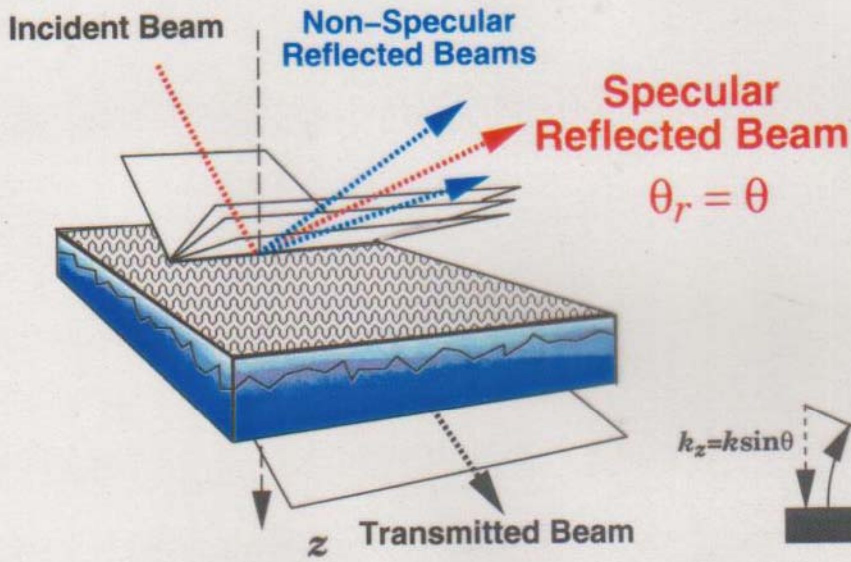


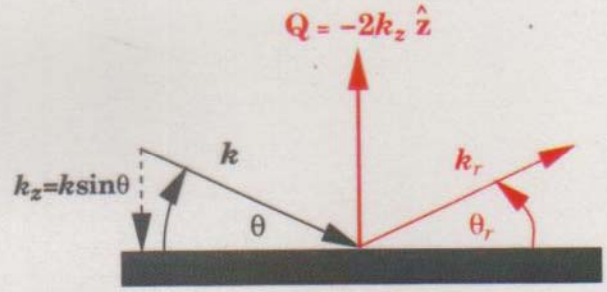
Figure 2.5-6 Interference of two spherical waves of equal intensities originating at the points P_1 and P_2. The two waves can be obtained by permitting a plane wave to impinge on two pinholes in a screen. The light intensity at an observation plane a distance d away takes the form of a sinusoidal pattern with period $\approx \lambda/\theta$.

DIFFRACTION PATTERN WHICH RESULTS FROM THE COHERENT SUPERPOSITION OF TWO WAVES (AMPLITUDES OF THE TWO WAVES ADD TOGETHER AT ANY GIVEN POINT IN SPACE)

A CHARACTERISTIC RECIPROCAL RELATIONSHIP EXISTS BETWEEN THE POSITIONS OF THE INTENSITY MAXIMA IN THE DIFFRACTION PATTERN AND THE DISTANCE SEPARATING THE OBJECTS CAUSING THE SCATTERING.

$$\text{Reflectivity} = \frac{\text{Number of reflected neutrons}}{\text{Number of incident neutrons}} = |r|^2$$





Specular reflection: $\overline{\rho}(z) = \langle\rho(x,y,z)\rangle_{xy}$

Non–Specular reflection: $\Delta\rho(x,y,z) = \rho(x,y,z) - \overline{\rho}(z)$

(AFTER N.F. BERK ET AL.)

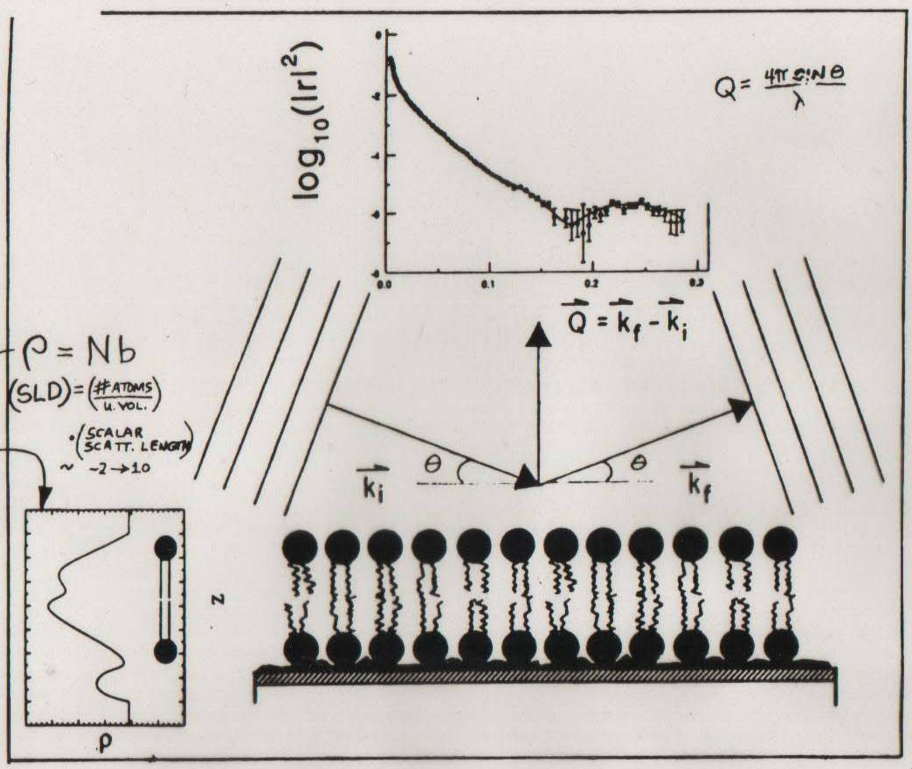

log10(|r|2)
Q = 4π sin θ / λ
0.0 0.1 0.2 0.3
Q = kf - ki
ρ = Nb
(SLD) = (#ATOMS / U. VOL.)
· (SCALAR SCATT. LENGTH)
~ -2 → 10
ki
kf
θ
z
ρ

Fig. 1

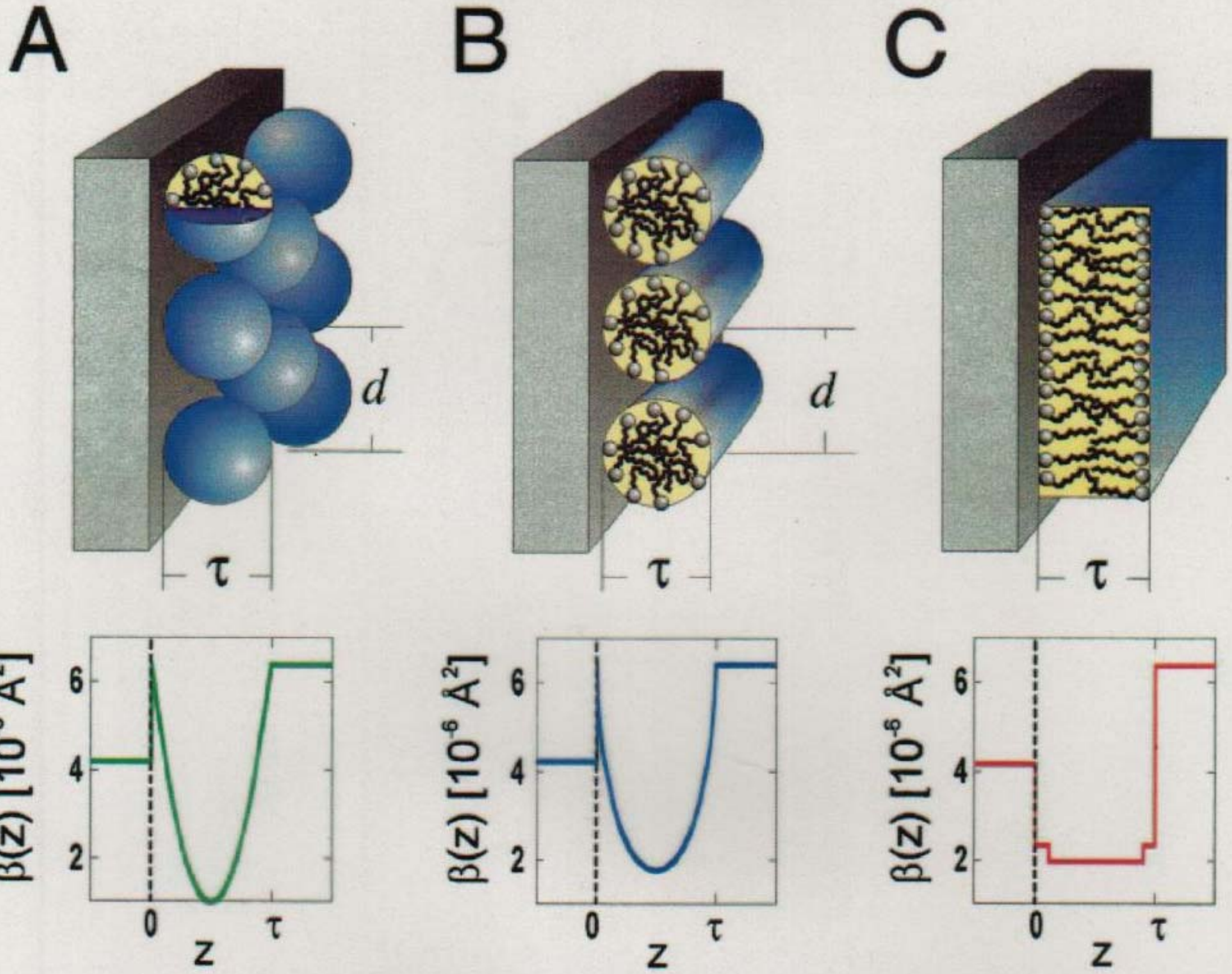


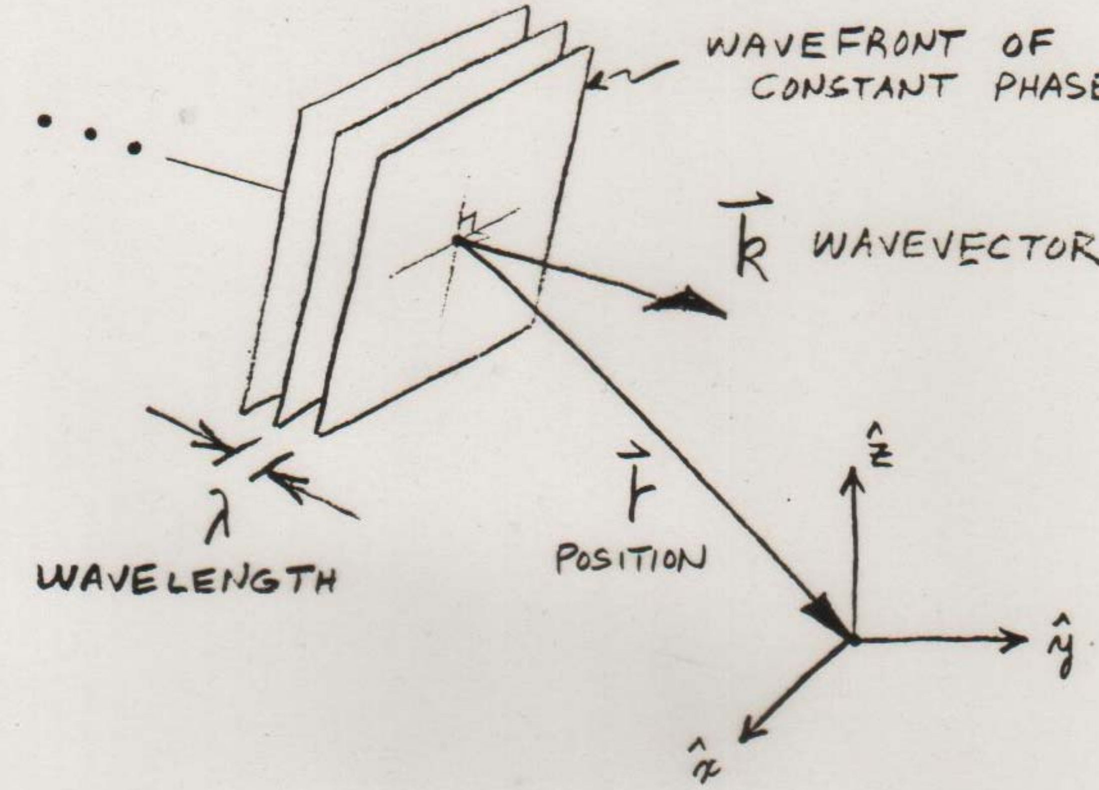
FIG. 1. (Color) Schematic diagram of adsorbed layer structures consisting of (A) spherical micelles, (B) cylindrical micelles, and (C) a bilayer, including the film thickness τ and interaggregate spacing d. Also shown are examples of neutron scattering length density profiles normal to the interface, $\beta(z)$, corresponding to each structure at the quartz/D_2O interface at a fractional surface coverage of 0.55. The head-group and alkyl tails of the surfactants have different scattering length densities, but because of the arrangement of the molecules this is only apparent in the bilayer $\beta(z)$.

single-crystal quartz block and reflected from the quartz-solution interface were recorded as a function of angle of incidence. The off-specular background, including any signal due to scattering from the bulk solution [15], was subtracted to give the reflection coefficient of the surfactant-coated interface. All solutions used were above their critical micelle or aggregation concentration, a condition which leads to a saturated adsorbed film at the solid-solution interface.

The cationic surfactant tetradecyltrimethylammonium bromide (TTAB) forms nearly spherical micellar aggregates consisting of approximately 80 molecules in bulk solution. Small angle neutron-scattering measurements [16] give mi-

FIG. 2. $200\times200\text{-nm}^2$ AFM tip deflection images of (A) spherical TTAB aggregates adsorbed onto quartz from water solution, (B) cylindrical TTAB aggregates adsorbed onto quartz from an aqueous 200mM NaBr solution, and (C) planar DDAB bilayer adsorbed onto quartz from water solution. Long-wavelength undulations visible in (B) and (C) arise from roughness in the underlying quartz.

WAVE PROPAGATING IN FREE SPACE



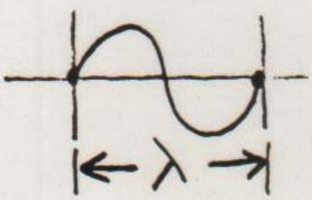
WAVEFUNCTION

$$\Psi \propto e^{i\vec{k}_0\cdot\vec{r}}$$

$$\begin{cases} \vec{k}_0 = k_{0x}\hat{x} + k_{0y}\hat{y} + k_{0z}\hat{z} \\ \vec{r} = x\hat{x} + y\hat{y} + z\hat{z} \end{cases}$$

FOR $\vec{k}_0$ ALONG $\hat{z}$, FOR EXAMPLE,

$$\Psi \propto \cos\underbrace{(k_{0z}z)}_{=\left(\frac{2\pi}{\lambda}z\right)} + i\,\sin(k_{0z}z)$$



$|\Psi|^2 \propto$ PROBABILITY OF THE NEUTRON BEING THERE

FOR ELASTIC INTERACTIONS TOTAL ENERGY OF THE NEUTRON IS CONSTANT

TOTAL ENERGY = KINETIC ENERGY
+ POTENTIAL ENERGY

= CONSTANT

WAVE EQUATION OF MOTION
(SCHROEDINGER EQUATION)

$$\underbrace{\left[\frac{-\hbar^2}{2m}\nabla^2\right.}_{K.E.} + \underbrace{\left.V(\vec{r})\right]}_{P.E.}\Psi = \underbrace{E}_{T.E.}\Psi$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

IN VACUUM

$$K.E._0 = \frac{\hbar^2 k_0^2}{2m}$$

$$V(\vec{r}) = \frac{2\pi\hbar^2}{m}\sum_{j=1} N_j b_j = \frac{2\pi\hbar^2}{m}\rho$$

NUMBER OF ATOMS OF TYPE j PER UNIT VOLUME

COHERENT SCATTERING "LENGTH" OF ATOM j

$(b = \mathrm{Re}\,b + i\,\mathrm{Im}\,b)$

ρ = "SCATTERING LENGTH DENSITY" (SLD)

IN VACUUM:

$$E_0 = \frac{\hbar^2 k_0^2}{2m} + 0$$

IN A MATERIAL MEDIUM:

$$E = \frac{\hbar^2 k^2}{2m} + \frac{2\pi\hbar^2}{m}\rho$$

CONSERVATION OF ENERGY REQUIRES $E_0 = E$

$$\therefore \quad k^2 = k_0^2 - 4\pi\rho$$

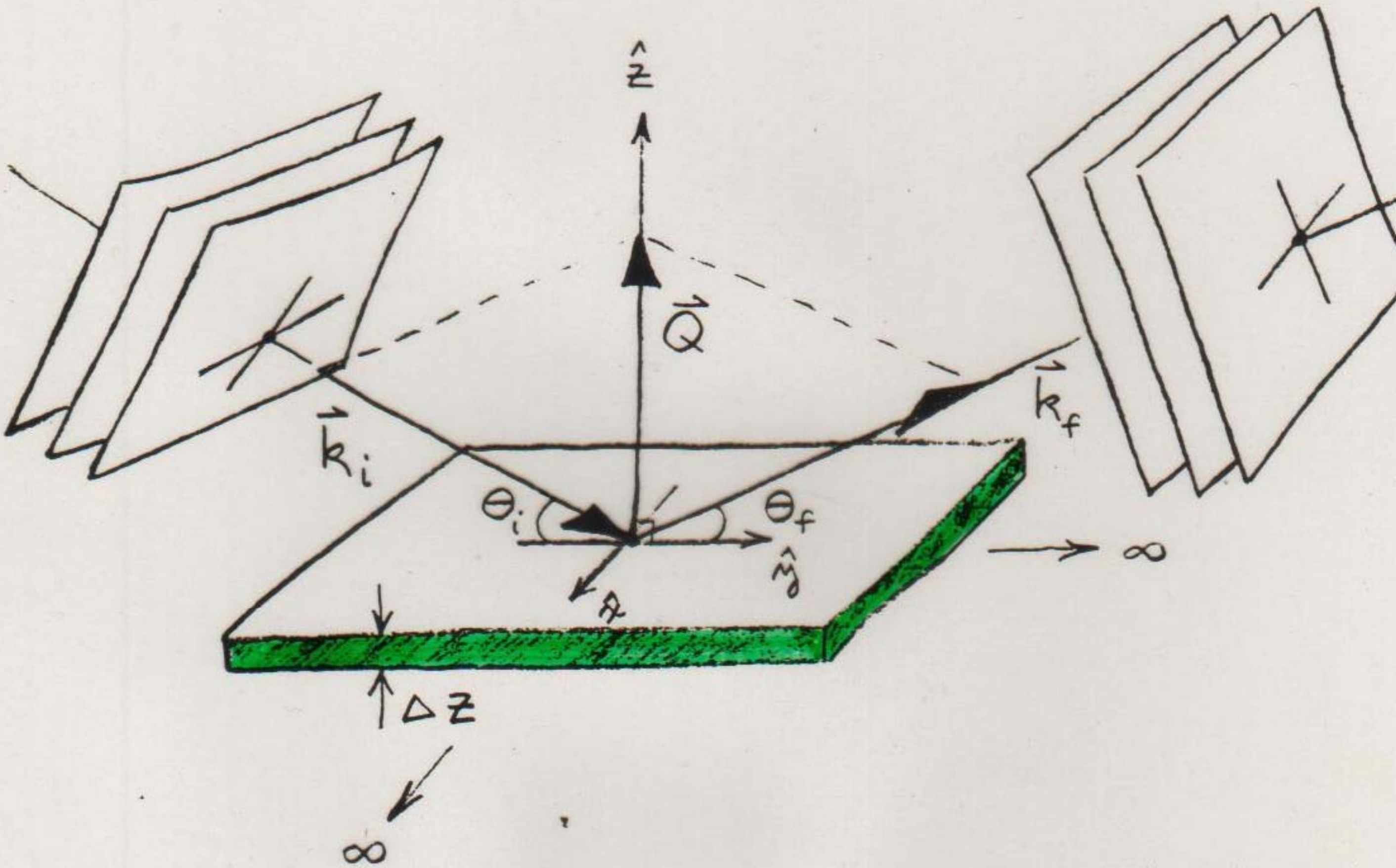
THUS

$$\left[\nabla^2 + k^2\right]\Psi = 0$$

NOTE REFRACTIVE INDEX $n \equiv \frac{k}{k_0}$:

$$n^2 = 1 - \frac{4\pi\rho}{k_0^2}$$

REFLECTION FROM AN IDEAL FILM OR SLAB OF MATERIAL



WAVEVECTOR TRANSFER $\vec{Q} = \vec{k}_f - \vec{k}_i$

$\rho = \rho(z)$ ONLY

EXPANDING $k^2 = k_0^2 - 4\pi\rho$,

$$k_x^2 + k_y^2 + k_z^2 + 4\pi\rho = k_{0x}^2 + k_{0y}^2 + k_{0z}^2 .$$

NOW IF $\rho = \rho(z)$ ONLY, THEN

$\frac{\partial \rho}{\partial x}$ AND $\frac{\partial \rho}{\partial y}$, WHICH ARE PROPORTIONAL TO THE GRADIENTS OF THE POTENTIAL OR FORCES IN THE RESPECTIVE DIRECTIONS, ARE EQUAL TO ZERO. THUS, NO FORCE ACTS ALONG THESE DIRECTIONS TO CHANGE k_x AND k_y. THEN

$k_x = k_{0x}$ AND $k_y = k_{0y}$ ARE "CONSTANTS OF THE MOTION".

SUBSTITUTING $\Psi(\vec{r}) = e^{ik_{0x}x} e^{ik_{0y}y} \psi(z)$ INTO $[\nabla^2 + k^2]\Psi = 0$ GIVES

$$\left[\frac{\partial^2}{\partial z^2} + k_z^2\right]\psi(z) = 0$$

$k_z = k_{oz}\, n(z)$:

BECAUSE THERE IS NO CHANGE IN THE POTENTIAL IN THE X- OR Y- DIRECTIONS, THERE CAN BE NO MOMENTUM CHANGE IN THESE DIRECTIONS EITHER

THE IDEAL SLAB GEOMETRY WITH $\rho = \rho(z)$ ONLY GIVES RISE TO THE COHERENT "SPECULAR" REFLECTION OF A PLANE WAVE WHICH IS DESCRIBED BY A ONE-DIMENSIONAL WAVE EQUATION :

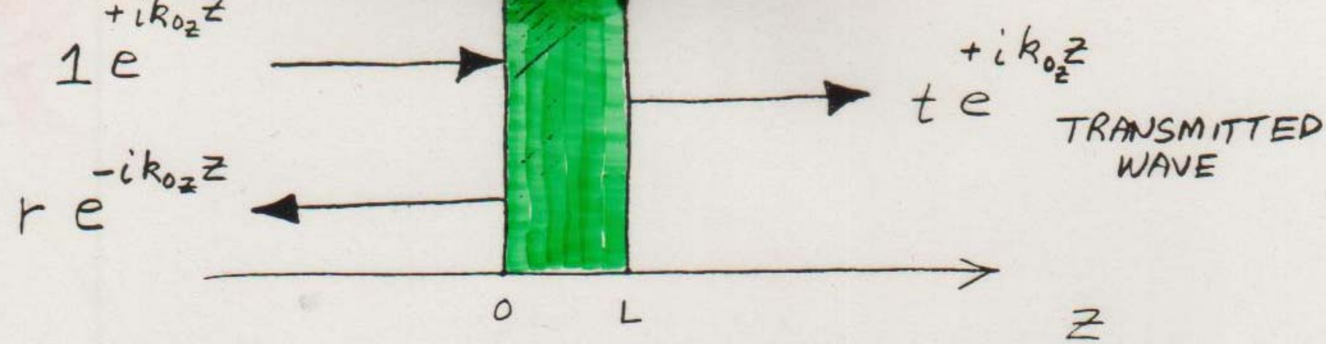
$$\left[\frac{\partial^2}{\partial z^2} + k_{oz}^2 - 4\pi\rho(z)\right]\Psi_{(z)} = 0$$

IN THIS CASE $\theta_i = \theta_f \equiv \theta$,

$|\vec{k}_i| = |\vec{k}_f|$ AND $Q = 2k \sin\theta$

$= 2k_z$

ALSO, $n_z^2 \equiv 1 - \dfrac{4\pi\rho(z)}{k_{oz}^2}$



$$Q = 2k_{0z}$$

FROM THE WAVE EQUATION, IT IS POSSIBLE TO FIND A SOLUTION FOR THE REFLECTION AMPLITUDE IN INTEGRAL FORM (SEE ARTICLE PAGES) :

$$r(Q) = \frac{4\pi}{iQ} \int_{-\infty}^{+\infty} \Psi(z)\, \rho(z)\, e^{+ik_{0z}z}\, dz$$

WHAT IS LOCALIZED AT z IN THE SLD PROFILE $\rho(z)$ IN "REAL" SPACE, IS DISTRIBUTED OVER THE REFLECTION AMPLITUDE $r(Q)$ IN THE RELATED SCATTERING OR "RECIPROCAL" SPACE

$\Psi(z)$ INSIDE THE MEDIUM IS GENERALLY UNKNOWN:

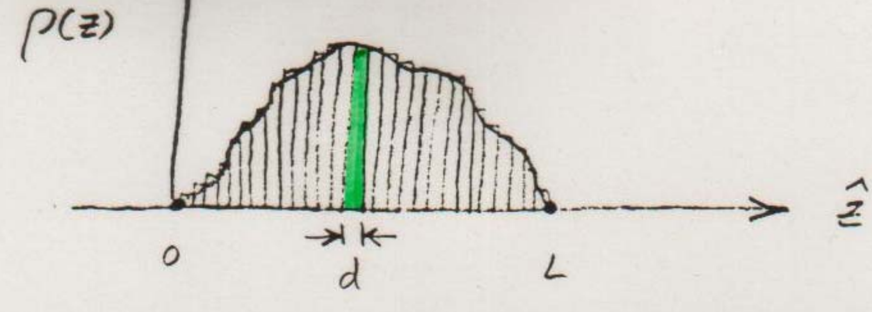
BORN APPROXIMATION REPLACES $\Psi(z)$ WITH THE INCIDENT WAVE FUNCTION $e^{+ik_{0z}z}$ BASED ON THE ASSUMPTION THAT $\Psi(z)$ IS NOT SIGNIFICANTLY DISTORTED FROM THE FREE SPACE FORM (WEAK INTERACTION): THEN

$$r(Q) \simeq \frac{4\pi}{iQ}\int_{-\infty}^{+\infty} \rho(z)\, e^{iQz}\, dz$$

FOURIER TRANSFO

FOR A REAL POTENTIAL $\rho(z)$

$$\mathrm{Re}\; r(Q) \simeq \frac{4\pi}{Q}\int_{-\infty}^{+\infty} \rho(z) \sin(Qz)\, dz$$



ARBITRARY POTENTIAL DIVIDED INTO RECTANGULAR SLABS OF WIDTH d AND CONSTANT ρ

THEN

(BORN APPROX.) $$\mathrm{Re}\, r(Q) \simeq \frac{4\pi}{Q} \int_0^L \rho(z) \sin(Qz)\, dz$$

BECOMES

$$\mathrm{Re}\, r(Q_j) \simeq \frac{4\pi}{Q_j} \sum_{\ell=1}^{N} \int_{(\ell-1)d}^{\ell d} \rho_\ell \sin(Q_j z)\, dz$$

$$= -\frac{4\pi}{Q_j^2} \sum_{\ell=1}^{N} \rho_\ell \left[\cos(Q_j z)\right]_{(\ell-1)d}^{\ell d}$$

ET OF
er FOR
DIFFERENT
VALUES OF
OR θ

$$\left\{ \begin{array}{l} \mathrm{Re}\, r_1 = \tau_{11} \rho_1 + \tau_{12} \rho_2 + \cdots + \tau_{1N} \rho_N \\ \mathrm{Re}\, r_2 = \tau_{21} \rho_1 + \tau_{22} \rho_2 + \cdots + \tau_{2N} \rho_N \\ \vdots \\ \mathrm{Re}\, r_N = \tau_{N1} \rho_1 + \tau_{N2} \rho_2 + \cdots + \tau_{NN} \rho_N \end{array} \right.$$

SOLVE SIMULTANEOUS EQUATIONS FOR ρ's GIVEN $\mathrm{Re}\, r$'s

e.g., SVD, EIGENVALUE PROBLEM FORMULATION, ...

$$\underbrace{\operatorname{Re}\, r_{BA}(Q)\left[\frac{Q^2}{8\pi \sin\left(\frac{Qd}{2}\right)}\right]}_{\equiv\, \mathcal{J}(Q)} = \sum_{j=1}^{N} \rho_j \sin\left[\frac{(2j-1)Qd}{2}\right]$$

$$\int_0^{\pi} \sin m\theta \sin n\theta \, d\theta = \begin{cases} 0 & m, n \text{ INTEGERS, } m \neq n \\ \frac{\pi}{2} & m, n \text{ INTEGERS, } m = n \end{cases}$$

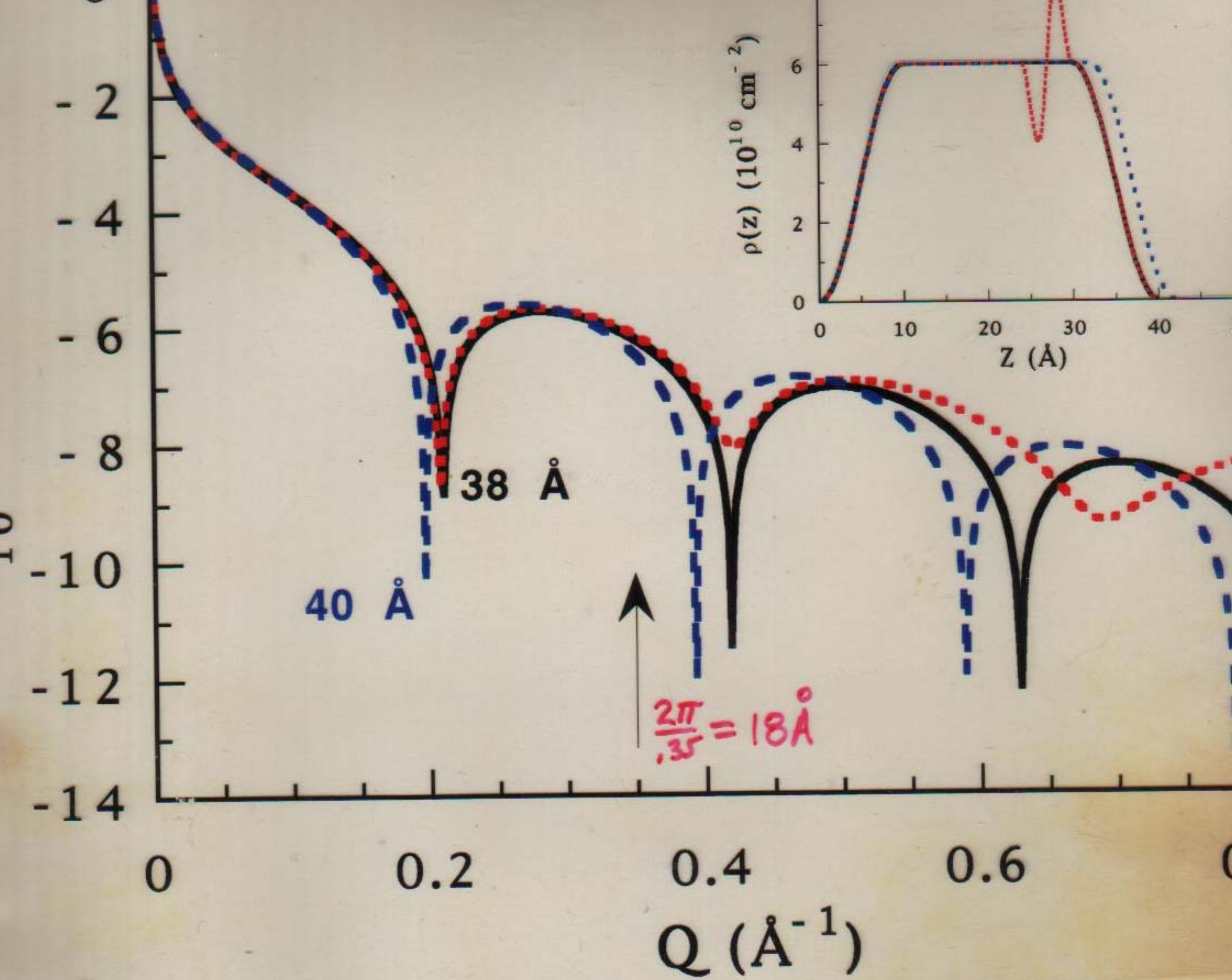
ORTHOGONALITY

$$\rho_j = \frac{d}{4\pi^2} \int_0^{\frac{\pi}{d}} Q^2 \operatorname{Re}\, r_{BA}(Q) \frac{\sin\left[\frac{(2j-1)Qd}{2}\right]}{\sin\left(\frac{Qd}{2}\right)} \, dQ$$

$2\theta = 180$

$$\left(= \frac{4\pi}{\lambda} \sin(90°)\right)$$

λ (Å)	Q_{MAX} (Å^{-1})	$D_{MIN}(\text{Å}) = \frac{2\pi}{Q_{MAX}} = \frac{\lambda}{2}$
5	2.513	2.5
10	1.256	5
50	0.251	25
100	0.125	50
500	0.025	250
1000	0.012	500
5000	0.002	2500



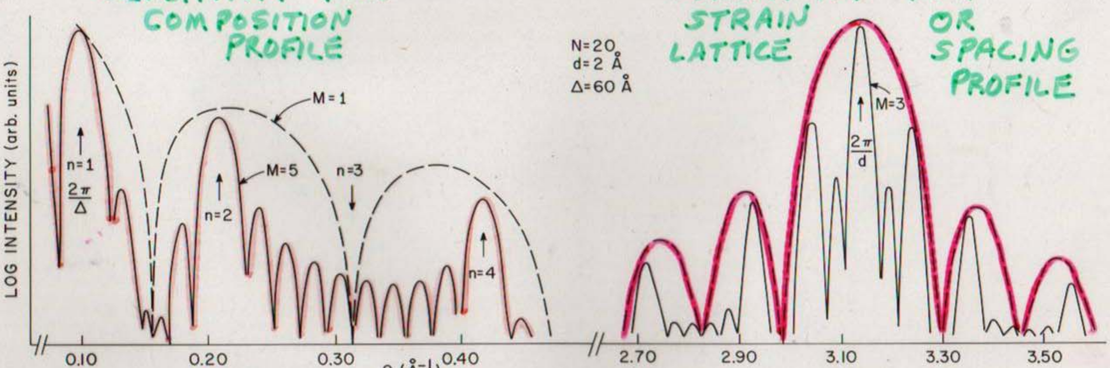
Solid, long-dash, and short-dash neutron reflectivity curves corresponding to their respective scattering length density profiles shown in the inset. This series of curves and profiles illustrates the sensitivity of the reflectivity to the overall film thickness at reflectivities approaching 10-7 whereas detailed features such as the oscillation in the long-dash profile can only be accurately discerned at reflectivities an order of magnitude or so lower, at Q-values corresponding to 2 pi/ width of the feature.

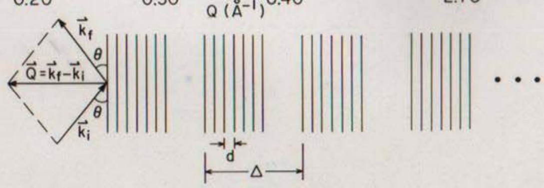
"REFLECTIVITY" REGIME

CRYSTAL "DIFFRACTION" REGIME

LOW Q : HIGHER SENSITIVITY FOR COMPOSITION PROFILE

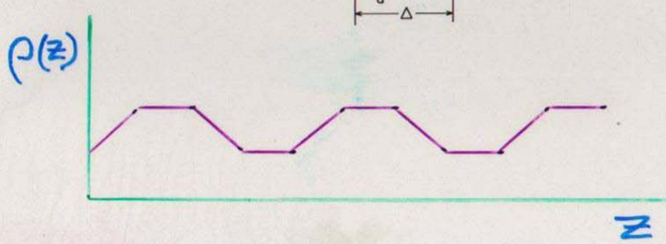
HIGH Q : HIGHER SENSITIVITY FOR STRAIN OR LATTICE SPACING PROFILE



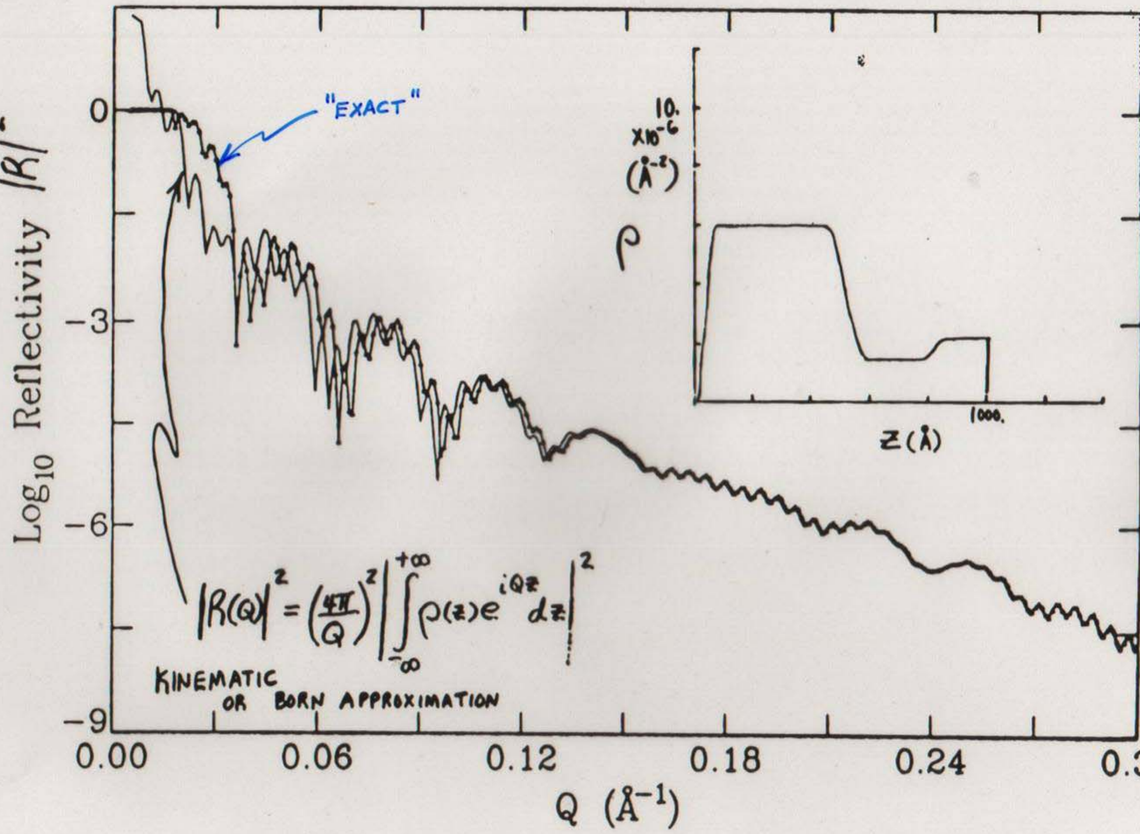


$$|R|^2_{KIN} = \left(\frac{4\pi}{Q}\right)^2 \left| \sum_{m=1}^{M} \sum_{n=1}^{N} \rho \, e^{iQ(nd+m\Delta)} \right|^2$$

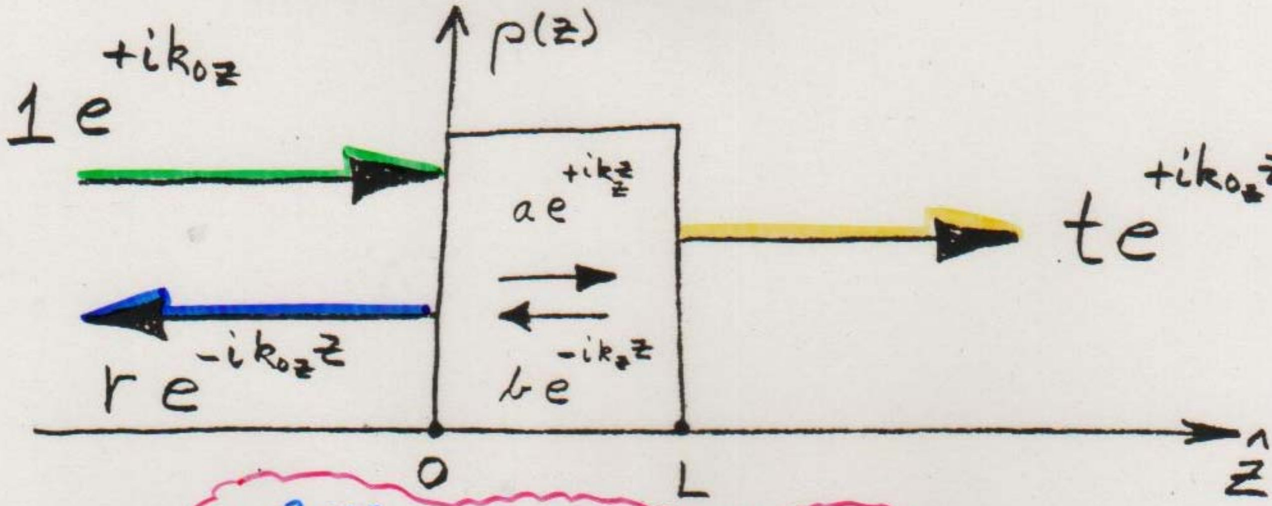
$$= \left(\frac{4\pi}{Q}\right)^2 \rho^2 \left| \frac{\sin(NQd/2)}{\sin(Qd/2)} \right|^2 \left| \frac{\sin(MQ\Delta/2)}{\sin(Q\Delta/2)} \right|^2$$



PROBLEM: BORN APPROXIMATION FAILS AT SUFFICIENTLY SMALL Q — MUST THEN USE EXACT THEORY



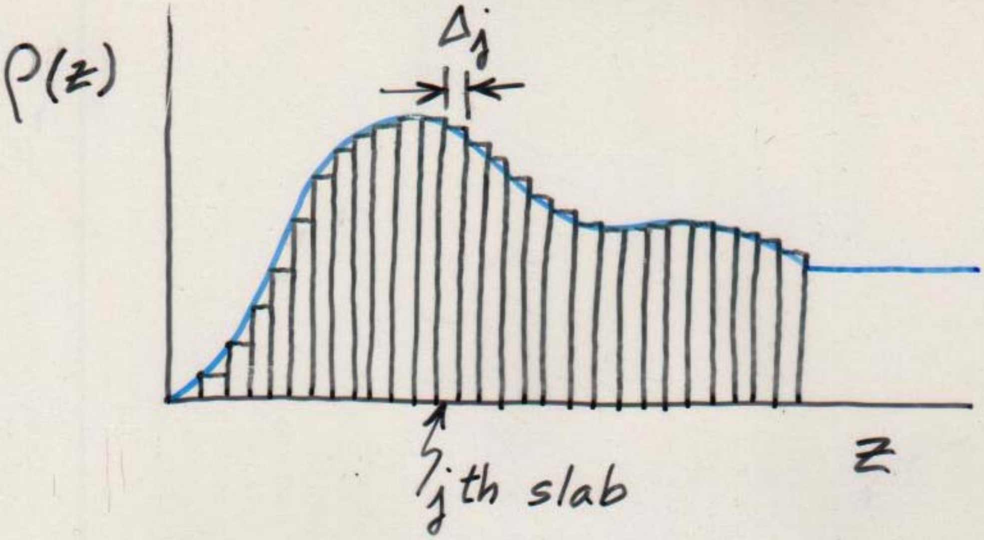
Comparison between kinematic (line) and dynamic (triangle + line) plus-state reflectivities for a density profile similar to that of Fig.2 as described in the text.



$$\frac{\partial^2 \Psi(z)}{\partial z^2} + k_z^2 \Psi(z) = 0$$

CONSERVATION OF MOMENTUM AND PARTICLE NUMBER REQUIRE THAT $\frac{\partial \Psi}{\partial z}(z)$ AND $\Psi(z)$ BE CONTINUOUS AT THE BOUNDARIES $z=0$ & $z=L$

$$\begin{pmatrix} t \\ it \end{pmatrix} e^{ik_{0z}L} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} 1+r \\ i(1-r) \end{pmatrix}$$



$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} a_N & b_N \\ c_N & d_N \end{pmatrix} \begin{pmatrix} a_{N-1} & b_{N-1} \\ c_{N-1} & d_{N-1} \end{pmatrix} \cdots \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix}$$

$$\begin{pmatrix} a_j & b_j \\ c_j & d_j \end{pmatrix} = \begin{pmatrix} \cos \delta_j & \frac{1}{n_{z_j}} \sin \delta_j \\ -n_{z_j} \sin \delta_j & \cos \delta_j \end{pmatrix}$$

$$\begin{aligned} \delta_j &= k_{0z}\, n_{z_j} \Delta_j \\ &= k_{z_j} \Delta_j \end{aligned}$$

free film

Then, once we know $\mathbf{M}_k(L)$:

$\boxed{z=L}$ $\boxed{z=0}$

$$\begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix} t(k)\mathrm{e}^{\mathrm{i}kL} = \begin{pmatrix} A_k(L) & B_k(L) \\ C_k(L) & D_k(L) \end{pmatrix} \begin{pmatrix} 1+r(k) \\ \mathrm{i}[1-r(k)] \end{pmatrix}$$

$$\boxed{r = \frac{B+C+\mathrm{i}(D-A)}{B-C+\mathrm{i}(D+A)}}$$

$$t = \frac{2\mathrm{i}\mathrm{e}^{-\mathrm{i}kL}}{B-C+\mathrm{i}(D+A)}$$

$$R = |r|^2 = \frac{\Sigma-2}{\Sigma+2}, \quad \Sigma = \mathrm{A}^2 + \mathrm{B}^2 + \mathrm{C}^2 + \mathrm{D}^2$$

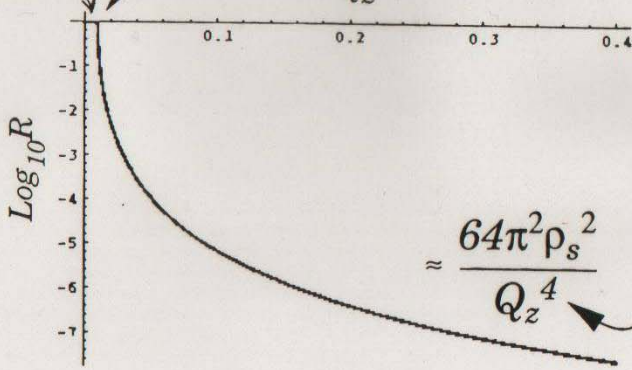
Fresnel Reflectivity

$$|r_F|^2 \equiv R_F(Q_z) = \frac{1-\sqrt{1-\frac{Q_{zc}^2}{Q^2}}}{1+\sqrt{1-\frac{Q_{zc}^2}{Q^2}}}$$

For $Q_z < Q_{zc}$, $R_F = 1$.

MIRROR REFLECTION PLATEAU

Q_{zc}



$$\approx \frac{64\pi^2\rho_s^2}{Q_z^4}$$

Analogue of SANS Porod's Law: effect of sharp edges.

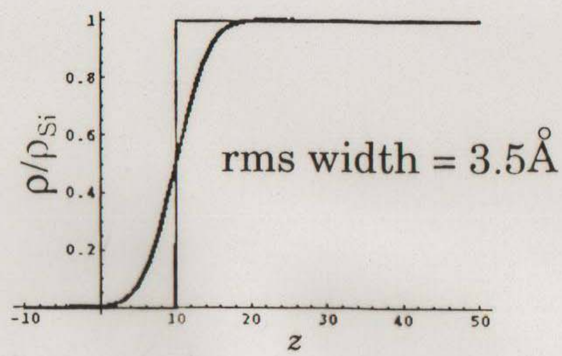
"CRITICAL Q"

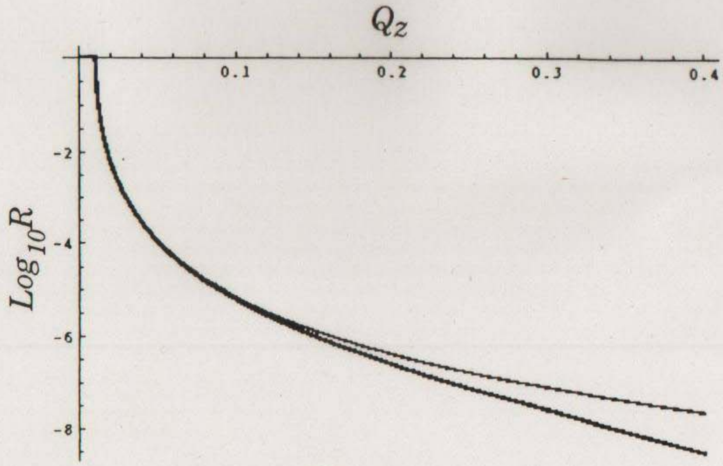
$$Q_c^2 = 16\pi\rho$$

(N.F. BERK)

"*Soft*" *substrate*

Smooth transition:
interlayer diffusion
roughness



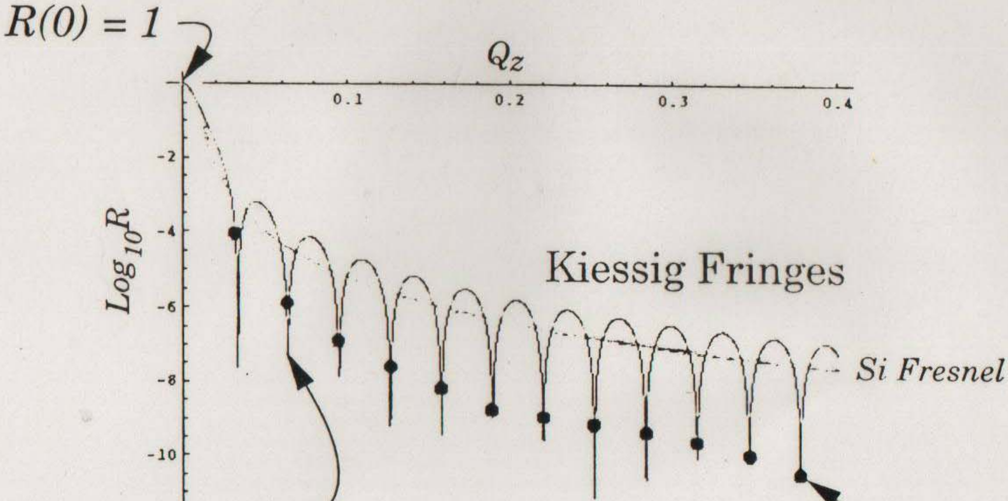


(N.F. BERK)

Uniform slab

$\rho = 2.07\ 10^{-6}\text{Å}^{-2}$

z=0 z=200Å



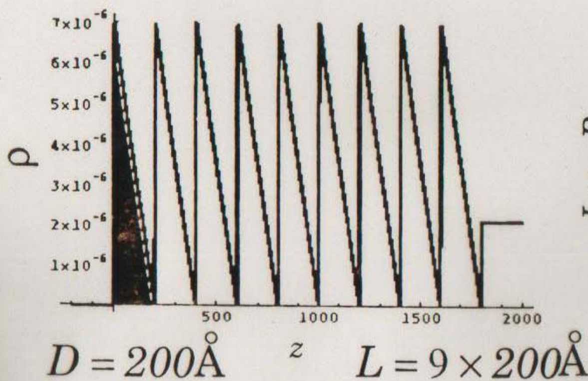
$\sqrt{Q_z{}^2 - 16\pi\rho} \ = \dfrac{2\pi}{L}$ m=1,2,...

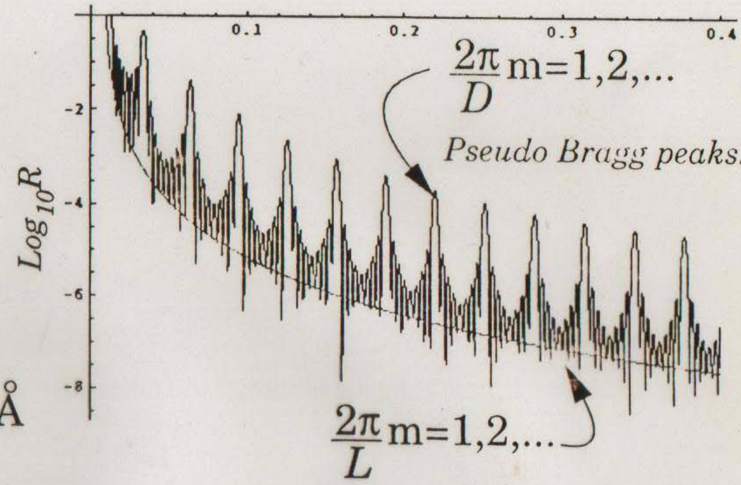
$\dfrac{2\pi}{L}$ m=1,2,...

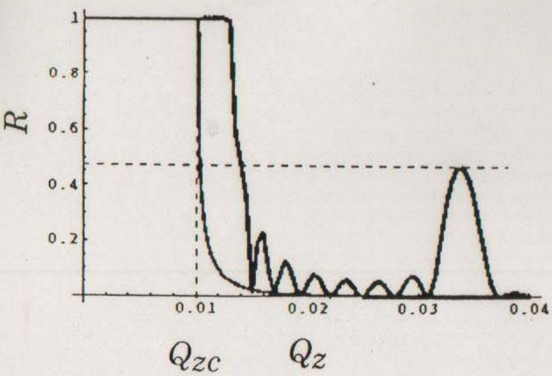
(*Kinematical*)

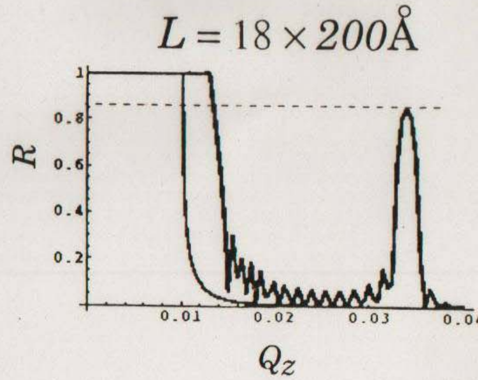
(N.F. BERK)

Multilayer on Si









(N.F. BERK)

IF ρ IS NOT EXACTLY $\rho(z)$, i.e., SOME VARIATIONS EXIST IN THE (x, y)- PLANE, THEN

$$r_{BORN} \simeq \frac{4\pi}{iQ} \int_{-\infty}^{+\infty} \langle \rho(x,y,z) \rangle_{x,y} \, e^{iQz} \, dz$$

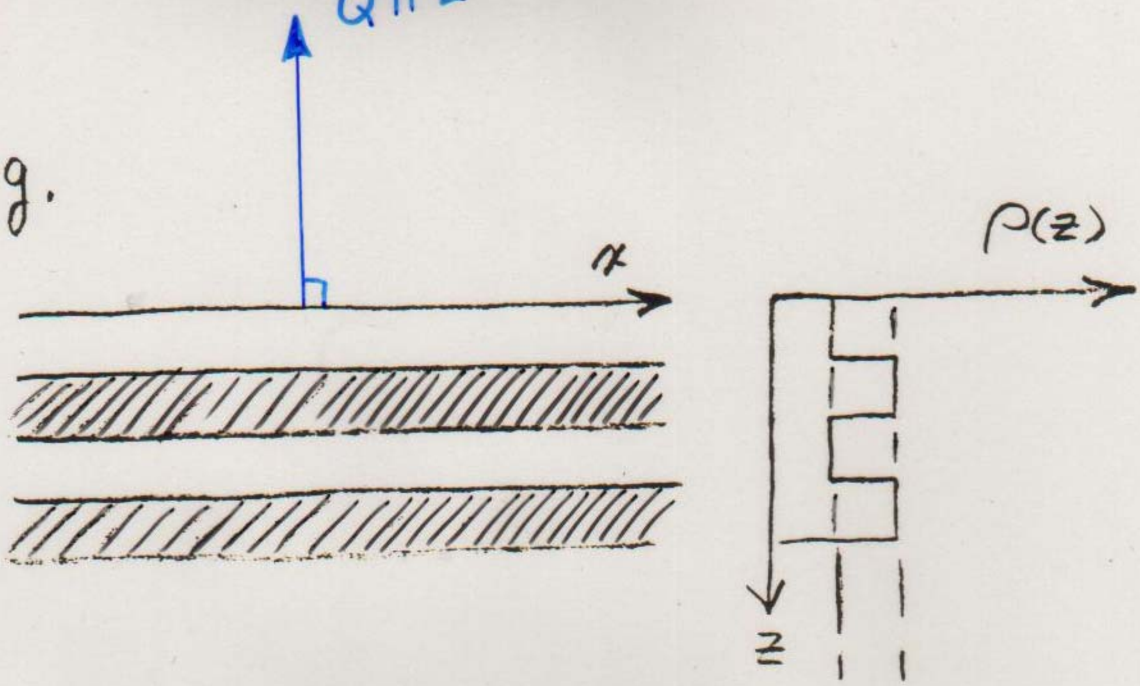
ON SPECULAR "RIDGE" WHERE $\vec{Q} = Q_z \hat{z}$

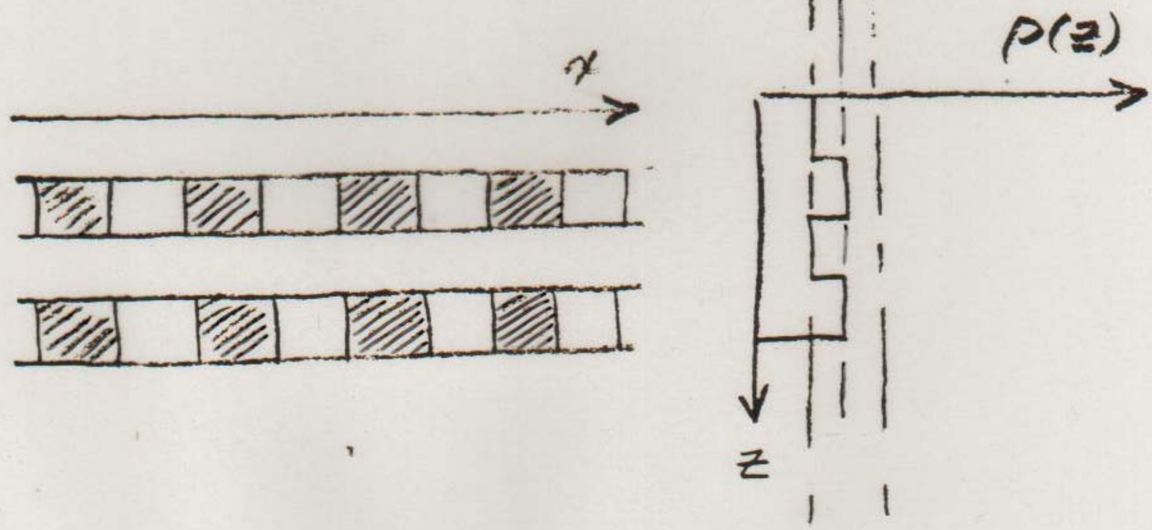
WHERE

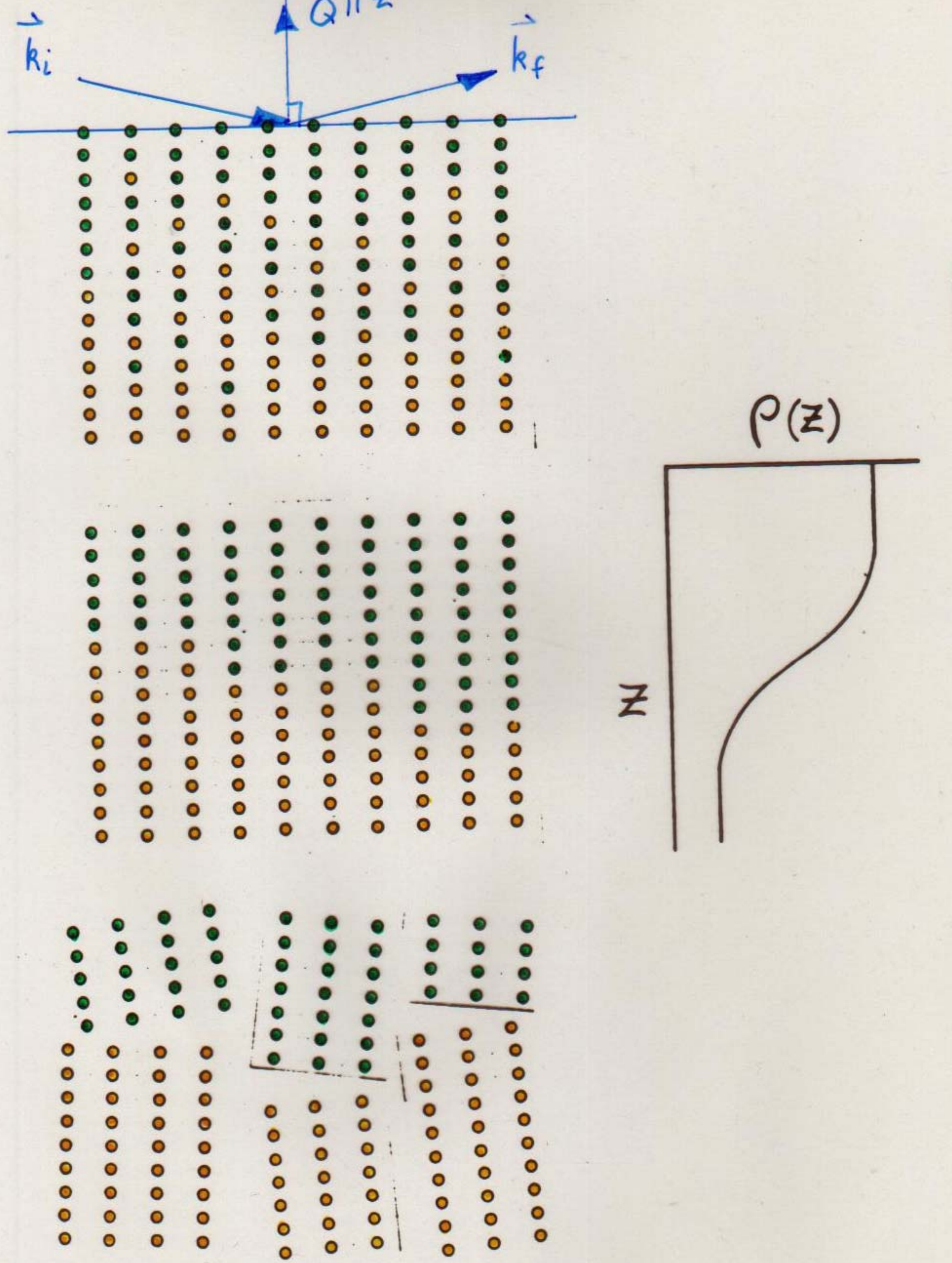
$$\langle \rho(x,y,z) \rangle_{x,y} = \frac{1}{A} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \rho(x,y,z) \, dx\,dy$$

$= \bar{\rho}(z)$ ONLY

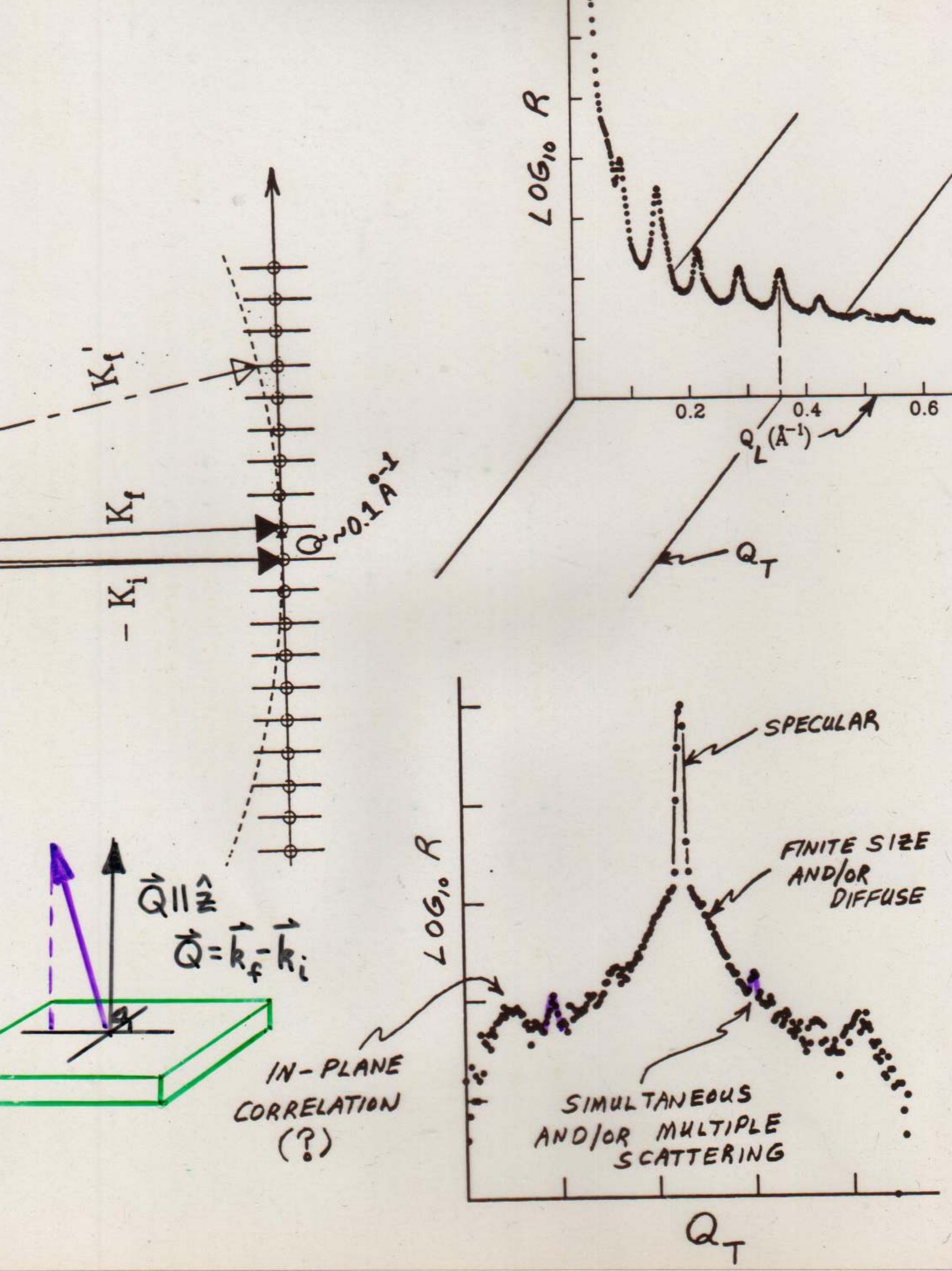
& A = NORMALIZING AREA OF THE (X,Y)- PLANE e.g.





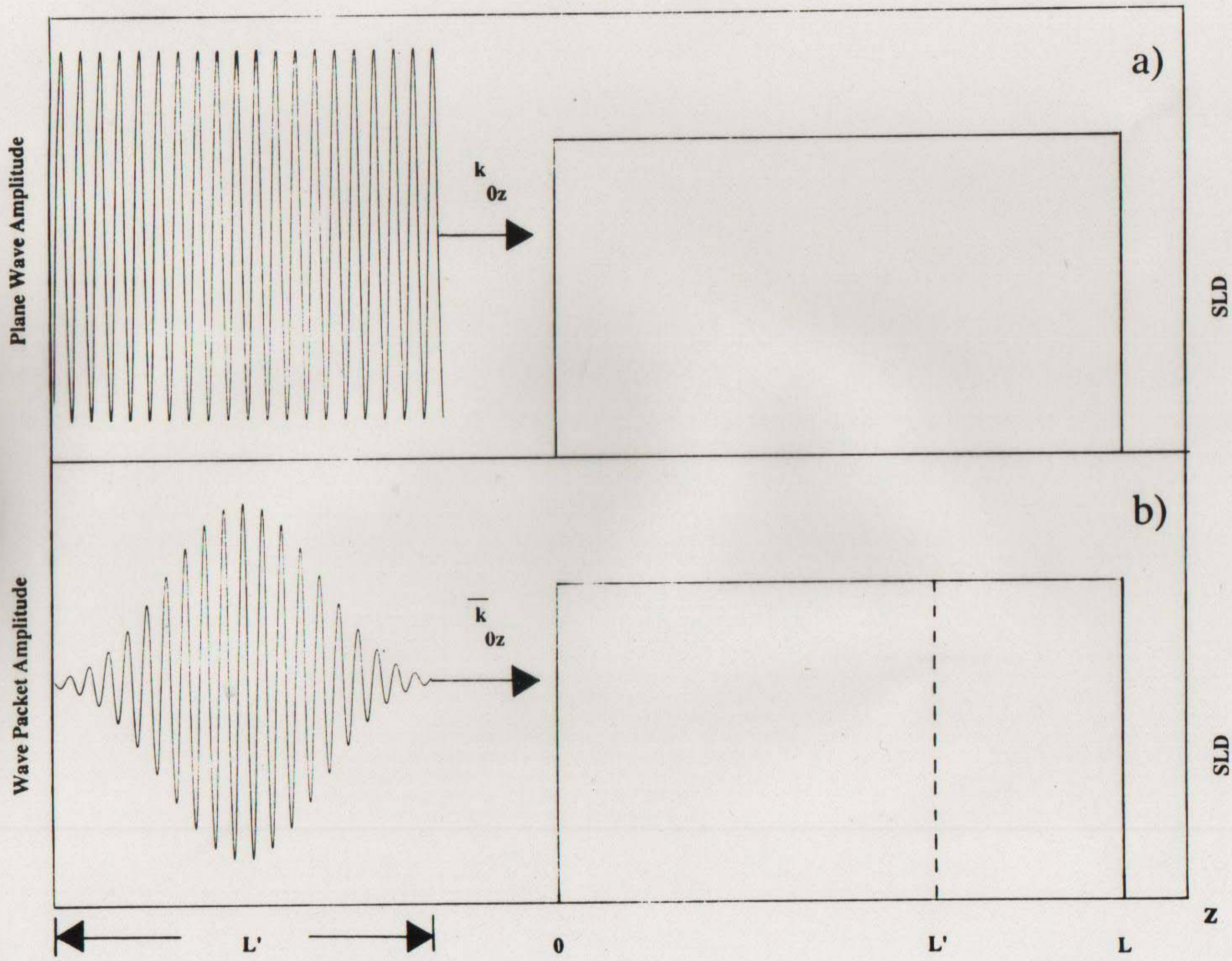


POSSIBLE MICROSTRUCTURES CORRESPONDING TO INTERFACIAL ROUGHNESS



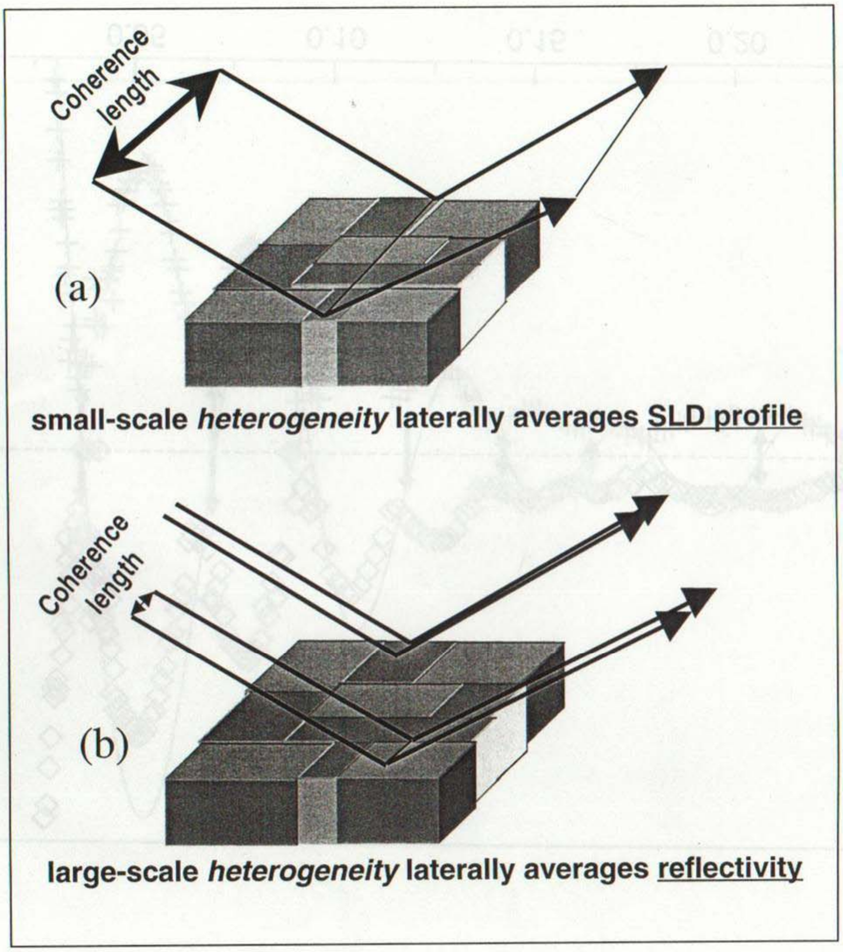
K_f'
K_f
$-K_i$
$Q \sim 0.1\ \text{Å}^{-1}$
$\vec{Q} \parallel \hat{z}$
$\vec{Q} = \vec{k}_f - \vec{k}_i$
$LOG_{10}\ R$
0.2
0.4
0.6
$Q_L\ (\text{Å}^{-1})$
Q_T
SPECULAR
FINITE SIZE AND/OR DIFFUSE
IN-PLANE CORRELATION (?)
SIMULTANEOUS AND/OR MULTIPLE SCATTERING
$LOG_{10}\ R$
Q_T

Figure 10



a)
Plane Wave Amplitude
k_{0z}
SLD
b)
Wave Packet Amplitude
$\bar{k}_{0z}$
SLD
L'
0
L'
L
Z

Figure 7.

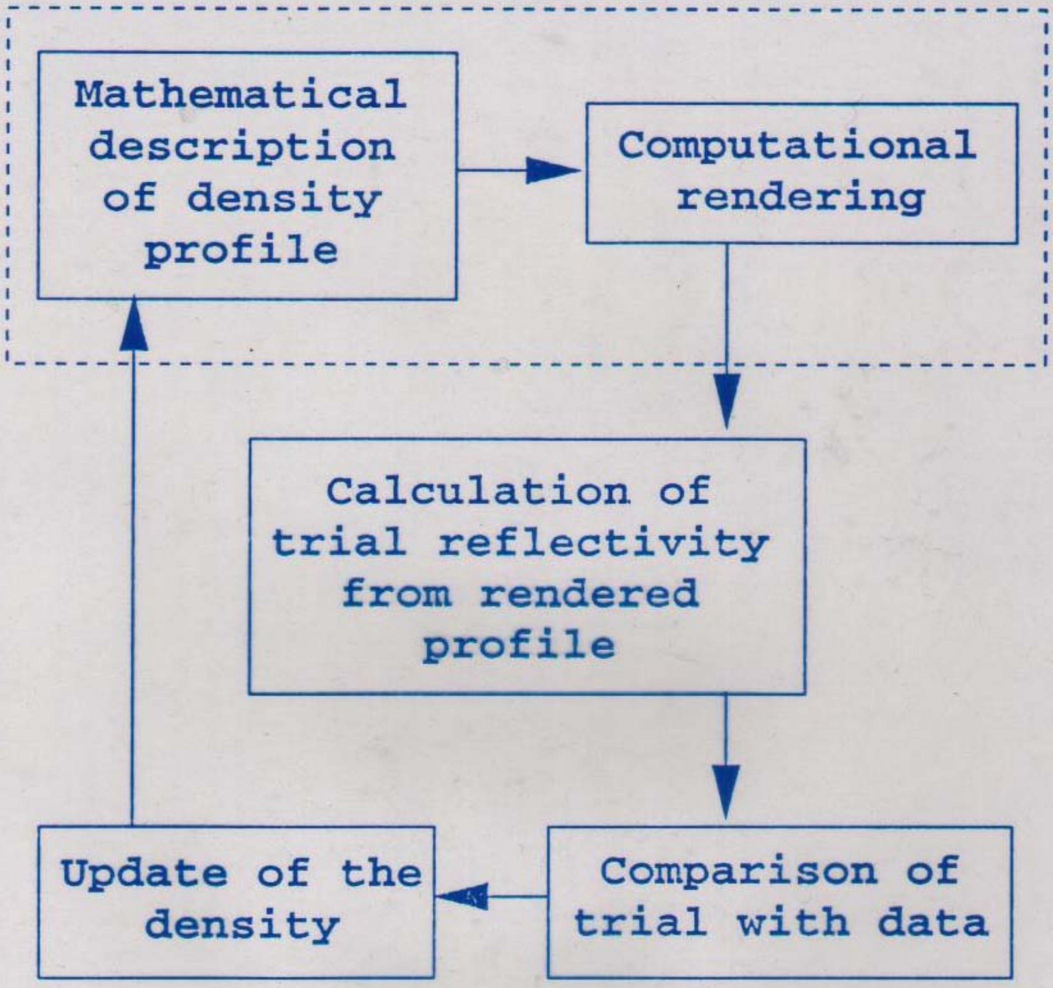


Coherence length
(a)
small-scale heterogeneity laterally averages SLD profile
Coherence length
(b)
large-scale heterogeneity laterally averages reflectivity

- SINCE ONLY $|\Psi|^2$ IS A MEASURABLE QUANTITY, CANNOT <u>DIRECTLY</u> OBTAIN REFLECTION AMPLITUDE r, BUT ONLY THE <u>REFLECTIVITY</u> $|r|^2$: $r = |r|e^{i\phi}$: $|r|^2 = |r|e^{-i\phi}|r|e^{+i\phi}$

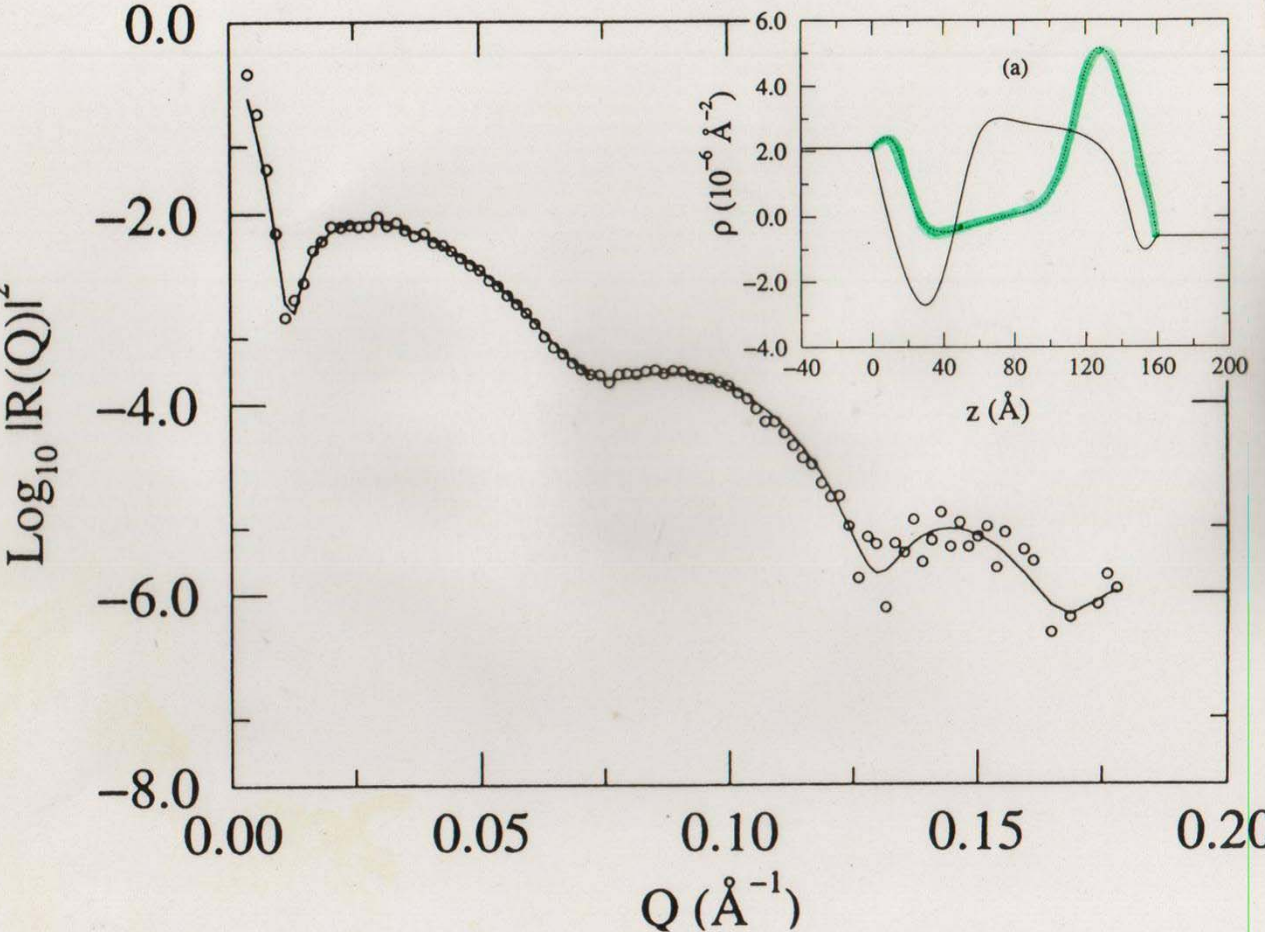
$$\boxed{|r|^2 = \frac{\text{REFLECTED } \underline{\text{INTENSITY}}}{\text{INCIDENT } \underline{\text{INTENSITY}}}}$$

⇨ HENCE, TO OBTAIN $\rho(z)$ FROM $|r(Q)|^2$ REQUIRES A CURVE FITTING ANALYSIS



- BOTH MODEL - DEPENDENT & MODEL - INDEPENDENT FITTING METHODS CAN BE USED

(FIGURE AFTER BERK & MAJKRZAK)



0.0
−2.0
−4.0
−6.0
−8.0
Log10 |R(Q)|2
0.00
0.05
0.10
0.15
0.20
Q (Å−1)
(a)
6.0
4.0
2.0
0.0
−2.0
−4.0
ρ (10−6 Å−2)
−40
0
40
80
120
160
200
z (Å)

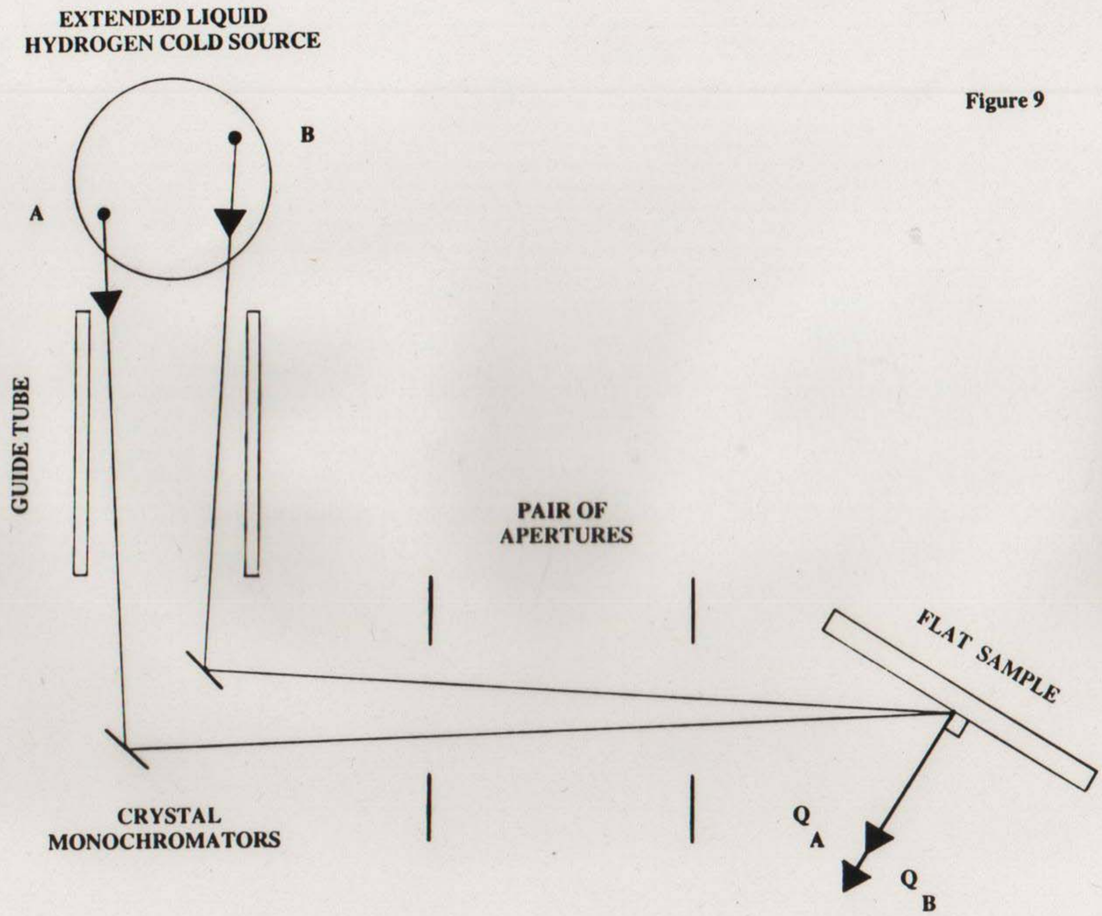
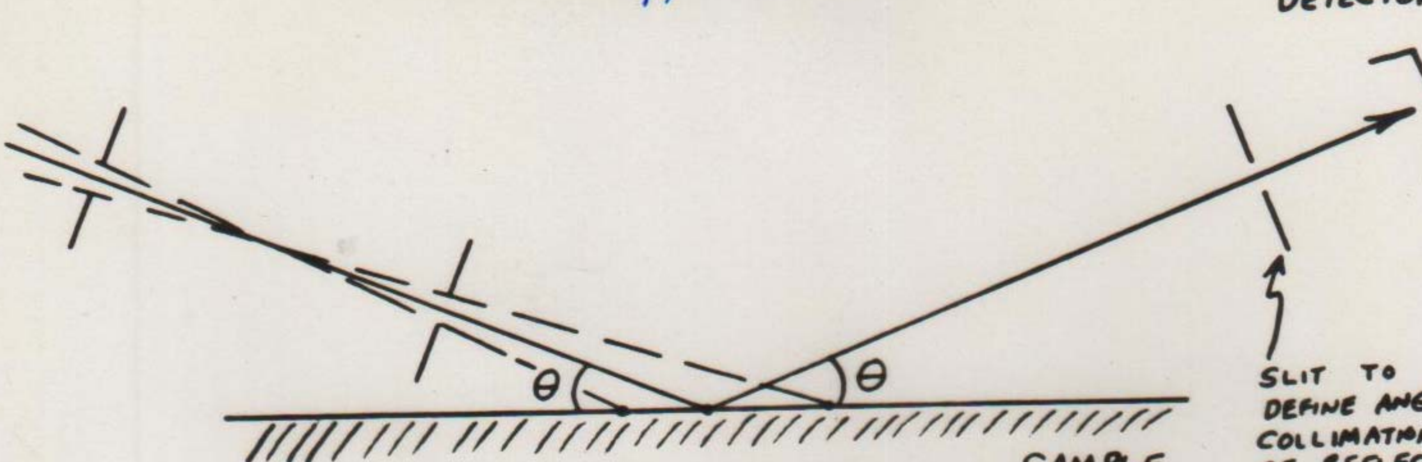

EXTENDED LIQUID
HYDROGEN COLD SOURCE
B
A
GUIDE TUBE
PAIR OF
APERTURES
FLAT SAMPLE
CRYSTAL
MONOCHROMATORS
Q
A
Q
B

Figure 9

$$\frac{\quad}{\lambda}$$



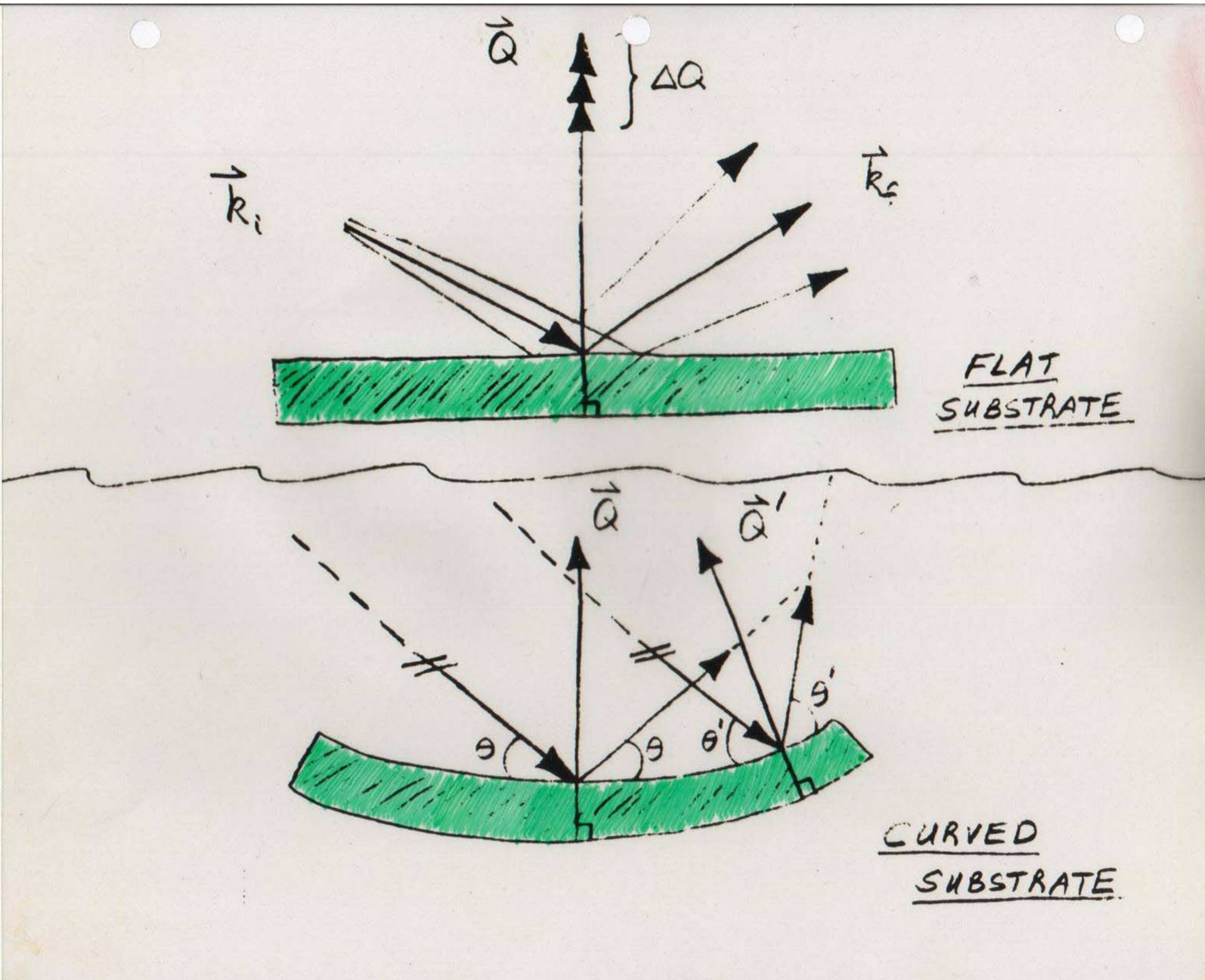
$$\Delta Q_{\text{LONGITUDINAL}} \simeq \frac{\Delta\lambda}{\lambda} Q + \sqrt{\left(\frac{4\pi}{\lambda}\right)^2 - Q^2}\ \Delta\theta$$

TYPICAL VALUES $\begin{cases} \dfrac{\Delta\lambda}{\lambda} \simeq 0.01 \\ \Delta\theta \simeq 1 \text{ min of arc} \end{cases}$

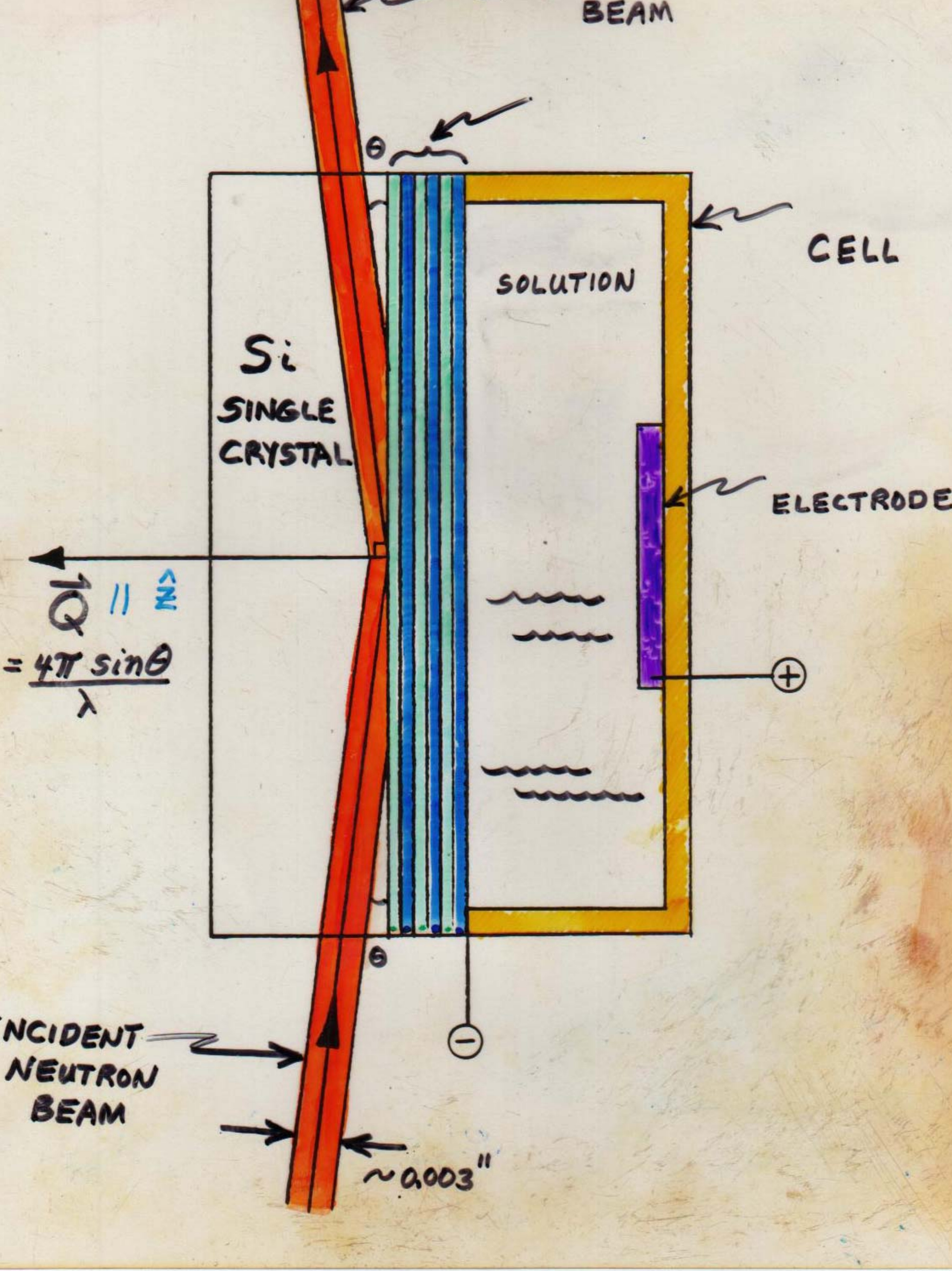
KEEP $\dfrac{\Delta Q}{Q} \simeq$ CONSTANT

$$R_{\text{OBS.}}(Q_0) \simeq \left(\frac{0.9394}{\Gamma}\right) \int_{-\Gamma}^{+\Gamma} R_{\text{ACT.}}(Q)\, e^{-\left(\frac{2.7725}{\Gamma^2}\right)(Q-Q_0)^2}\, dQ$$

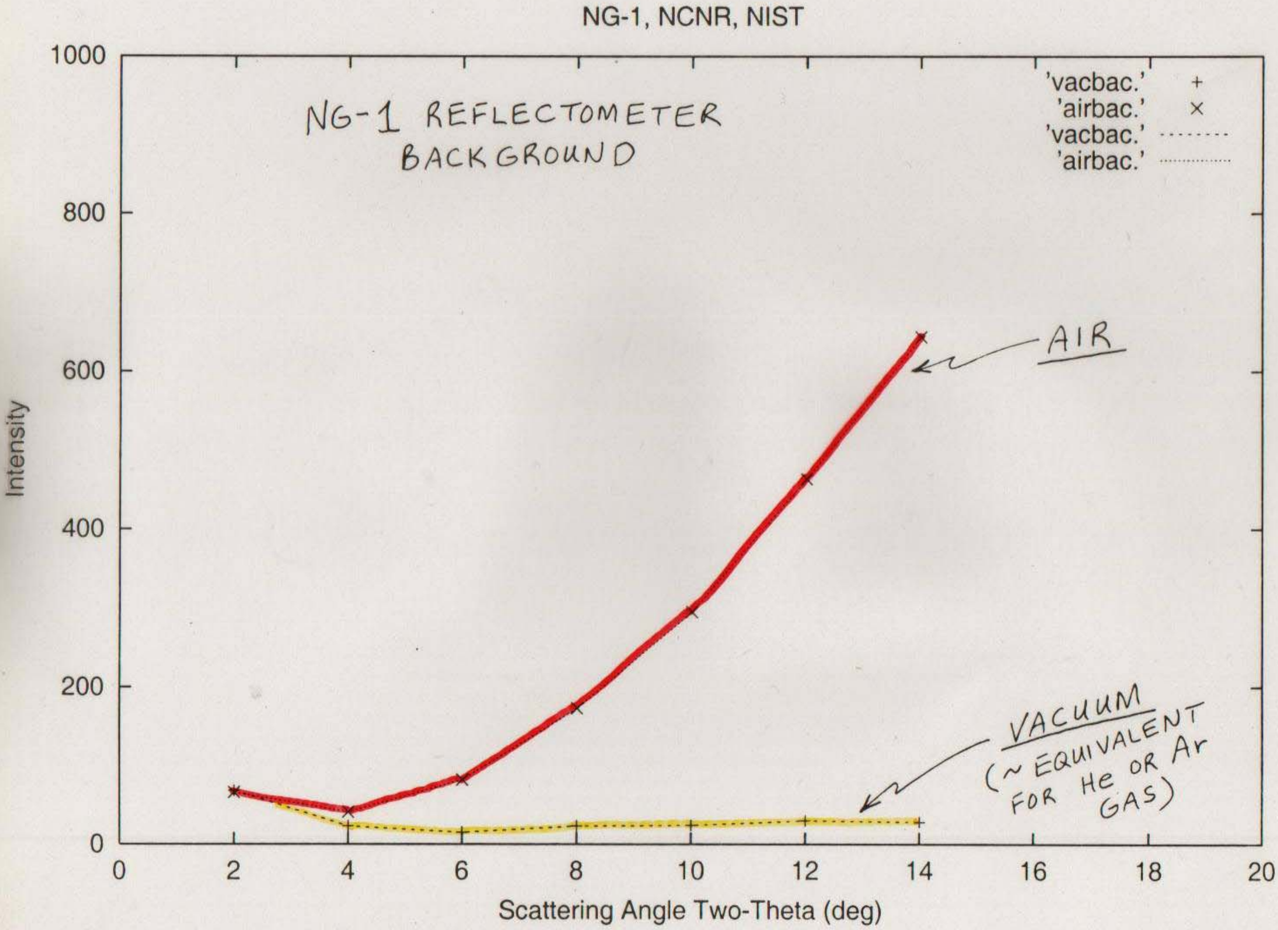
(ASSUMING A GAUSSIAN DISTRIBUTION OF Q-VA

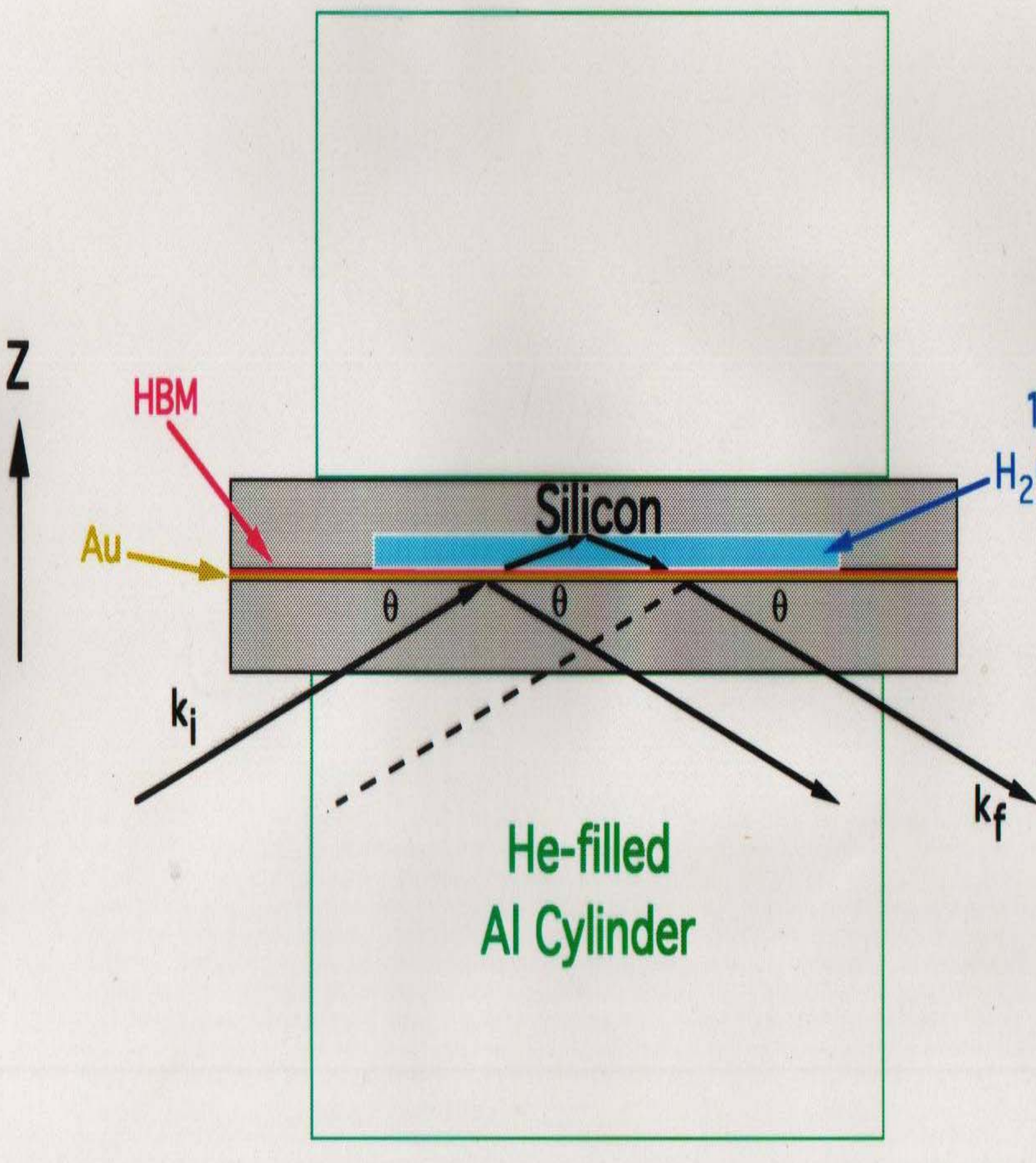


$\vec{Q}$
ΔQ
$\vec{k}_i$
$\vec{k}_f$
FLAT SUBSTRATE
$\vec{Q}$
$\vec{Q}'$
θ
θ
θ'
θ'
CURVED SUBSTRATE

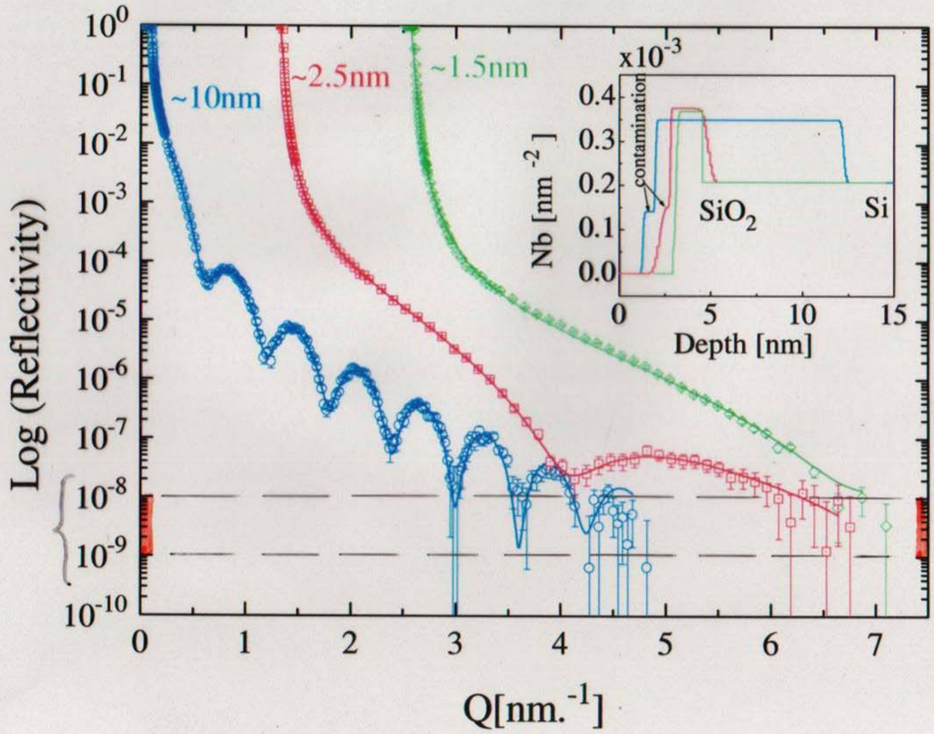

BEAM
CELL
SOLUTION
Si
SINGLE
CRYSTAL
ELECTRODE
θ
$\vec{Q} \parallel \hat{z}$
$= \frac{4\pi \sin\theta}{\lambda}$
+
−
INCIDENT
NEUTRON
BEAM
~0.003"

6/2/00


NG-1, NCNR, NIST
NG-1 REFLECTOMETER BACKGROUND
'vacbac.' +
'airbac.' ×
'vacbac.'
'airbac.'
AIR
VACUUM
(~ EQUIVALENT FOR He OR Ar GAS)
Intensity
Scattering Angle Two-Theta (deg)
0
200
400
600
800
1000
2
4
6
8
10
12
14
16
18
20



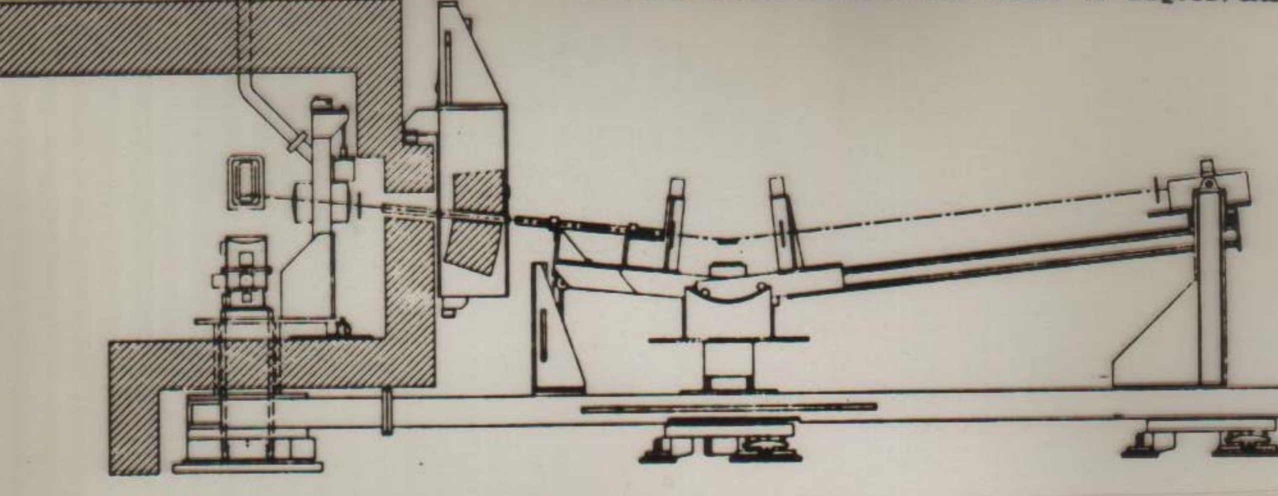
S.KRUEGER et al.

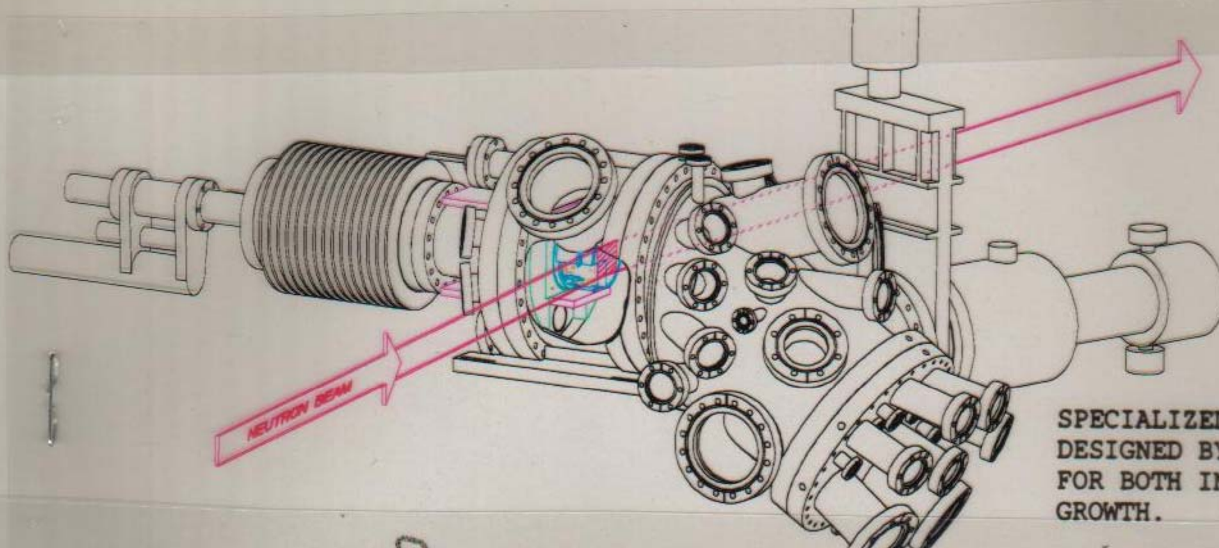


~10nm
~2.5nm
~1.5nm
Log (Reflectivity)
Q[nm.$^{-1}$]
x10^{-3}
contamination
Nb [nm^{-2}]
SiO$_2$
Si
Depth [nm]

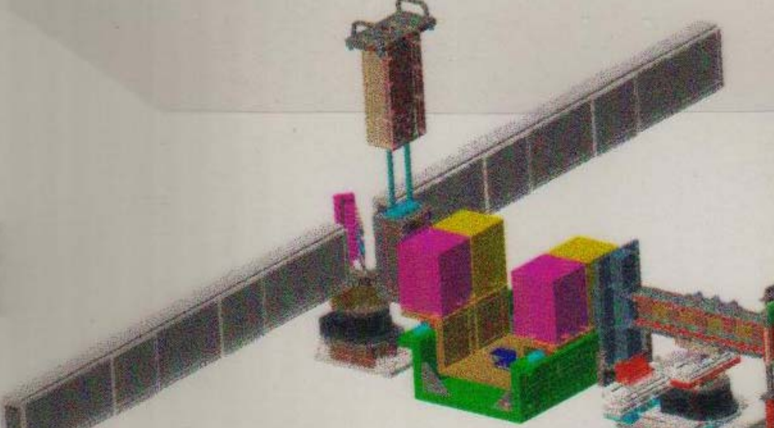
J. DURA et al.

NG-7 REFLECTOMETER DESIGNED BY S.SATIJA AND THE EXCELLE
NCNR ENGINEERING AND DESIGN GROUP. THE HORIZONTAL SAMP
PLANE GEOMETRY ALLOWS FOR STUDY OF LIQUID/GAS INTERFACE



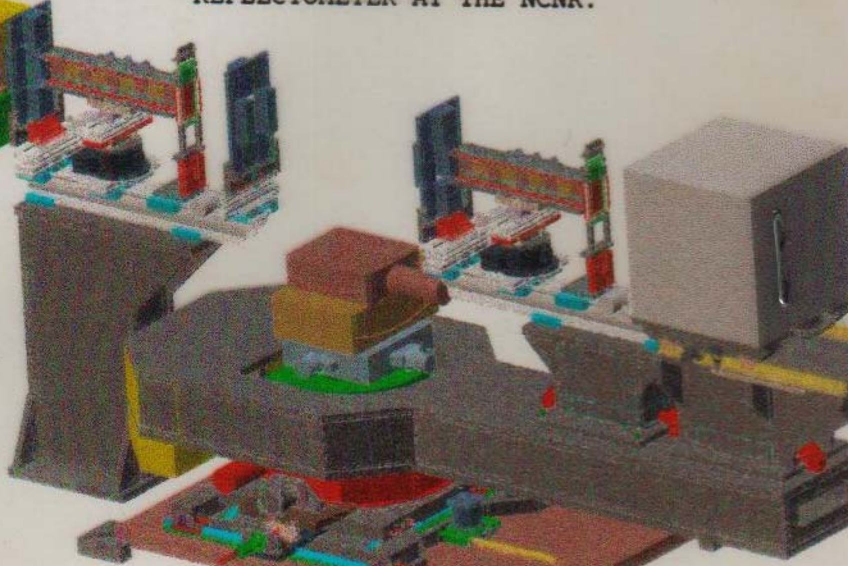


SPECIALIZED UHV/MBE CHAM
DESIGNED BY J.DURA ET AL
FOR BOTH IN- & EX-SITU F
GROWTH.



NEUTRON REFLECTOMETER WITH POLARIZED BEAM
CAPABILITY PROPOSED TO NIH BY A CONSORTIUM
BIOLOGICAL RESEARCHERS AND LED BY S.WHITE
UC IRVINE: MODELLED AFTER THE EXISTING NG-
REFLECTOMETER AT THE NCNR.

THE TWO EXISTING REFLECTOMETERS
AT THE NCNR HAVE BEEN OVERSUBSRIBED
TO BY A FACTOR OF 4 IN A RECENT PEER-
REVIEW OF PROPOSALS FOR BEAM TIME.



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* Magnetic Multilayers, Ed. by L.H.Bennett and R.E.Watson; article on "Neutron and X-Ray Diffraction Studies of Magnetic Multilayers" by C.F.Majkrzak, J.F.Ankner, N.F.Berk, and D.Gibbs, World Scientific, 1994, p.299 (contains introductory material on neutron and x-ray reflectometry not specific to magnetic materials alone)

* Neutron Reflectometry Studies of Thin Films and Multilayered Materials, C.F.Majkrzak, Acta Physica Polonica A 96, 81(1999) -- this article can also be found at the website: http://www.ncnr.nist.gov -- along with some additional information on analysing neutron reflectivity data (click on "Summer School Course Materials")

- PHASE-SENSITIVE NEUTRON REFLECTOMETRY, C.F. MAJKRZAK, N.F. BERK, AND U.A. PEREZ-SALAS, LANGMUIR 19, 7796 (2003).

- PHASE SENSITIVE REFLECTOMETRY AND THE UNAMBIGUOUS DETERMINATION OF SCATTERING LENGTH DENSITY PROFILES, C.F. MAJKRZAK AND N.F. BERK, PHYSICA B 336, 27(2003).

- www.ncnr.nist.gov — SEE ANNUAL REPORTS AND SUMMER SCHOOL COURSE MATERIALS

- POLARIZED NEUTRON REFLECTOMETRY, C.F. MAJKRZAK, K.V. O'DONOVAN AND N.F. BERK

- STRUCTURAL INVESTIGATIONS OF MEMBRANES OF INTEREST IN BIOLOGY BY NEUTRON REFLECTOMETRY, C.F. MAJKRZAK, N.F. BERK, S. KRUEGER AND U. PEREZ-SALAS