matrix method smilgies 4/2002

refractive indices at given photon energy (from CXRO)

$n0 := 1$ air

$n1 := \left(1 - 1.971\cdot10^{-5}\right) + i\cdot1.083\cdot10^{-6}$ Pd

$n2 := \left(1 - 1.2777\cdot10^{-5}\right) + i\cdot8.2374\cdot10^{-7}$ Cr

$n3 := \left(1 - 4.4847\cdot10^{-6}\right) + i\cdot6.1802\cdot10^{-8}$ Si substrate

z-components of wave vectors

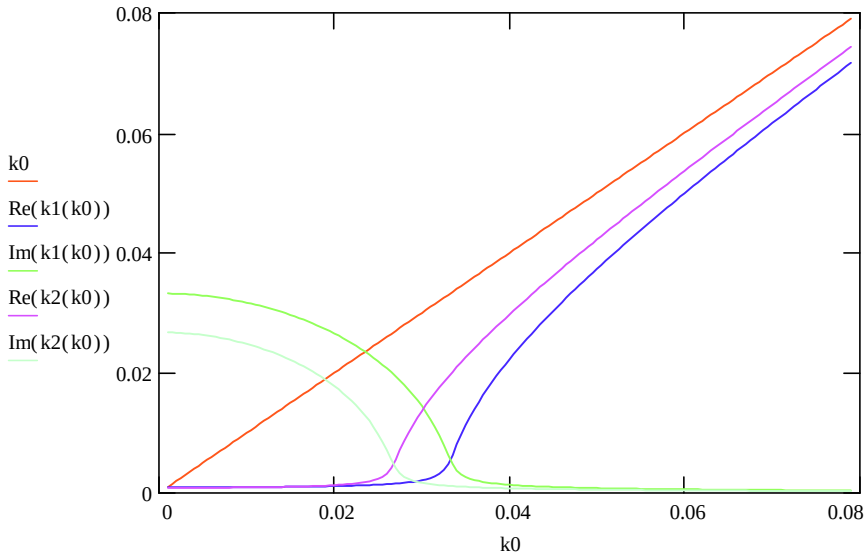
$E := 10.450$ (keV) $\quad k := \frac{2\cdot\pi}{12.4}\cdot E \quad k = 5.295$ (inverse Angstroem)

$k0 := 0.001, 0.0015 .. 0.079$

$k1(k0) := \sqrt{\left(n1^2 - 1\right)\cdot k^2 + k0^2}$

$k2(k0) := \sqrt{\left(n2^2 - 1\right)\cdot k^2 + k0^2}$

$k3(k0) := \sqrt{\left(n3^2 - 1\right)\cdot k^2 + k0^2}$



boundary matrices

$z01 := 0$ air-layer1 boundary

$z12 := 200$ boundary layer1 and 2

$z23 := 58 + z12$ boundary layer 2 and 3 (all values in Angstroem)

interface 01

$$ap01(k0) := \left(\frac{k0 + k1(k0)}{2 \cdot k0}\right) \qquad am01(k0) := \left(\frac{k0 - k1(k0)}{2 \cdot k0}\right)$$

$$bpp01(k0) := \exp(i \cdot (k1(k0) - k0) \cdot z01) \qquad bmp01(k0) := \exp(-i \cdot (k1(k0) + k0) \cdot z01)$$

$$bpm01(k0) := \exp(i \cdot (k1(k0) + k0) \cdot z01) \qquad bmm01(k0) := \exp(-i \cdot (k1(k0) - k0) \cdot z01)$$

$$M01(k0) := \begin{pmatrix} ap01(k0) \cdot bpp01(k0) & am01(k0) \cdot bmp01(k0) \\ am01(k0) \cdot bpm01(k0) & ap01(k0) \cdot bmm01(k0) \end{pmatrix}$$

interface 12

$$ap12(k0) := \left(\frac{k1(k0) + k2(k0)}{2 \cdot k1(k0)}\right) \qquad am12(k0) := \left(\frac{k1(k0) - k2(k0)}{2 \cdot k1(k0)}\right)$$

$$bpp12(k0) := \exp(i \cdot (k2(k0) - k1(k0)) \cdot z12) \qquad bmp12(k0) := \exp(-i \cdot (k2(k0) + k1(k0)) \cdot z12)$$

$$bpm12(k0) := \exp(i \cdot (k2(k0) + k1(k0)) \cdot z12) \qquad bmm12(k0) := \exp(-i \cdot (k2(k0) - k1(k0)) \cdot z12)$$

$$M12(k0) := \begin{pmatrix} ap12(k0) \cdot bpp12(k0) & am12(k0) \cdot bmp12(k0) \\ am12(k0) \cdot bpm12(k0) & ap12(k0) \cdot bmm12(k0) \end{pmatrix}$$

interface 23

$$ap23(k0) := \left(\frac{k2(k0) + k3(k0)}{2 \cdot k2(k0)}\right) \qquad am23(k0) := \left(\frac{k2(k0) - k3(k0)}{2 \cdot k2(k0)}\right)$$

$$bpp23(k0) := \exp(i \cdot (k3(k0) - k2(k0)) \cdot z23) \qquad bmp23(k0) := \exp(-i \cdot (k3(k0) + k2(k0)) \cdot z23)$$

$$bpm23(k0) := \exp(i \cdot (k3(k0) + k2(k0)) \cdot z23) \qquad bmm23(k0) := \exp(-i \cdot (k3(k0) - k2(k0)) \cdot z23)$$

$$M23(k0) := \begin{pmatrix} ap23(k0) \cdot bpp23(k0) & am23(k0) \cdot bmp23(k0) \\ am23(k0) \cdot bpm23(k0) & ap23(k0) \cdot bmm23(k0) \end{pmatrix}$$

transfer matrix

$$Mat(k0) := (M01(k0) \cdot M12(k0) \cdot M23(k0))$$

transmissivity

$$t(k0) := \frac{1}{(Mat(k0))_{0,0}}$$

reflectivity

$$r(k0) := \frac{(Mat(k0))_{1,0}}{(Mat(k0))_{0,0}}$$

interface

$A2(k0) := M23(k0)_{0,0} \cdot t(k0)$ $\quad$ $A1(k0) := (M12(k0) \cdot M23(k0))_{0,0} \cdot t(k0)$

$B2(k0) := M23(k0)_{1,0} \cdot t(k0)$ $\quad$ $B1(k0) := (M12(k0) \cdot M23(k0))_{1,0} \cdot t(k0)$

calculation

$R(k0) := (|r(k0)|)^2$

Fresnel reflectivities

top layer

$$R_{FT}(k0) := \left(\left| \frac{k1(k0) - k0}{k1(k0) + k0} \right| \right)^2$$

guiding layer

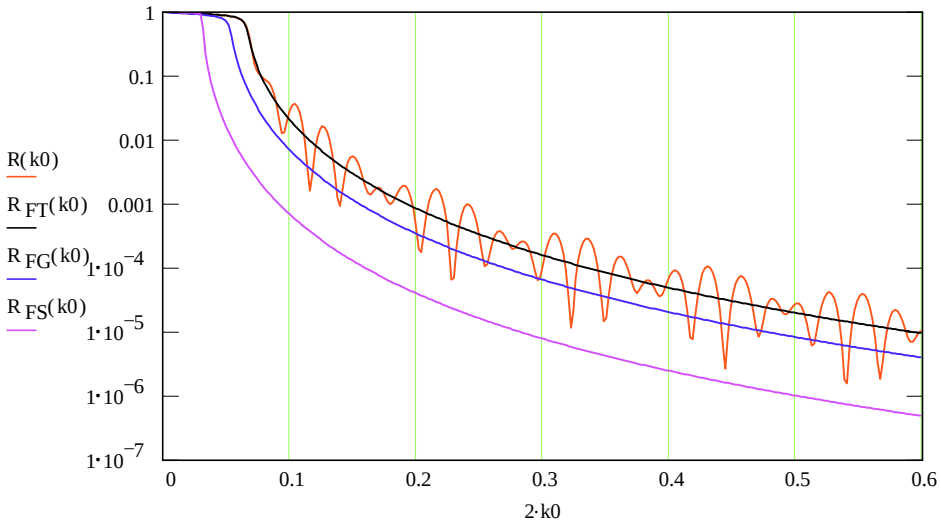
$$R_{FG}(k0) := \left(\left| \frac{k2(k0) - k0}{k2(k0) + k0} \right| \right)^2$$

substrate

$$R_{FS}(k0) := \left(\left| \frac{k3(k0) - k0}{k3(k0) + k0} \right| \right)^2$$

plot

$k0 := 0.001, 0.002 .. 0.299$



crude roughness model

$\sigma := 4$

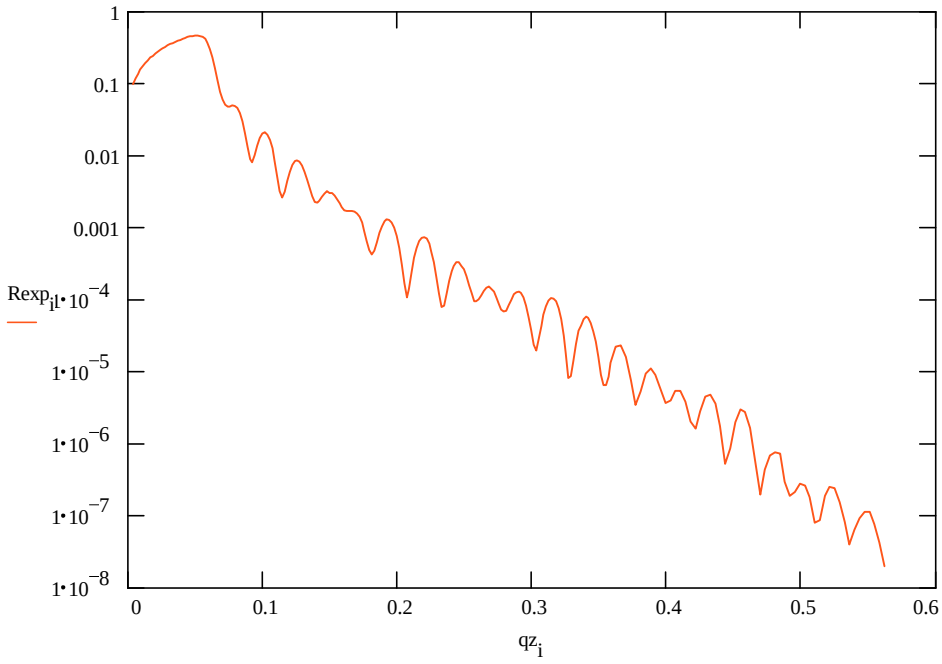
$R_{rough}(k0) := R(k0) \cdot \exp\left[-\sigma^2 \cdot (2 \cdot k0)^2 \right]$

read in data file "problem.prn" :
- create a column file [filename].prn (the extension .prn is essential !!)
- put [filename] in READPRN(filename) in a blue calculation box
- goto the FILE menue, choose "associate filename"
    - browse for filename and fill into box by clicking
    - choose filetype .prn
    - choose MathCAD varibale from list
- re-calculate READPRN() function value

$data := READPRN(problem)$

$qz := data^{<0>}$ $Rexp := data^{<1>}$

$length(qz) = 248$ $length(Rexp) = 248$ $N := length(qz)$ $i := 0 .. N - 1$



my solution

boundary locations

z01 = 0
z12 = 200
z23 = 258

layer thickness

z12 − z01 = 200
z23 − z12 = 58
σ = 4

Parratt32 fit

tPd := 201
tCr := 57
σfit := 4