Today's outline - September 16, 2021

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation
- Designing a multilayer

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation
- Designing a multilayer
- Reflection from a graded index

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation
- Designing a multilayer
- Reflection from a graded index
- Reflection from rough surfaces

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation
- Designing a multilayer
- Reflection from a graded index
- Reflection from rough surfaces
- Surface models

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation
- Designing a multilayer
- Reflection from a graded index
- Reflection from rough surfaces
- Surface models

Reading Assignment: Chapter 3.7–3.8

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation
- Designing a multilayer
- Reflection from a graded index
- Reflection from rough surfaces
- Surface models

Reading Assignment: Chapter 3.7–3.8

Homework Assignment #02:
Problems on Blackboard
due Tuesday, September 21, 2021

Today's outline - September 16, 2021

- Kinematical approximation for a thin slab
- Multilayers in the kinematical regime
- Parratt's exact recursive calculation
- Designing a multilayer
- Reflection from a graded index
- Reflection from rough surfaces
- Surface models

Reading Assignment: Chapter 3.7–3.8

Homework Assignment #02:
Problems on Blackboard
due Tuesday, September 21, 2021

Homework Assignment #03:
Chapter 3: 1,3,4,6,8
due Tuesday, October 05, 2021

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab.

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab.

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2}$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2}$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle

$$q \gg 1$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2}$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2}$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c \qquad r_{01} = \frac{q_0 - q_1}{q_0 + q_1}$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c \qquad r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1}$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2}$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2} \approx \frac{1}{(2q_0)^2}$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2} \approx \frac{1}{(2q_0)^2} = \left(\frac{Q_c}{2Q_0}\right)^2$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2} \approx \frac{1}{(2q_0)^2} = \left(\frac{Q_c}{2Q_0}\right)^2$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right) \approx \left(\frac{Q_c}{2Q_0}\right)^2 \left(1 - e^{iQ\Delta}\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2} \approx \frac{1}{(2q_0)^2} = \left(\frac{Q_c}{2Q_0}\right)^2$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right) \approx \left(\frac{Q_c}{2Q_0}\right)^2\left(1 - e^{iQ\Delta}\right)$$

$$= -\frac{16\pi\rho r_0}{4Q^2} e^{iQ\Delta/2}\left(e^{iQ\Delta/2} - e^{-iQ\Delta/2}\right)$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2} \approx \frac{1}{(2q_0)^2} = \left(\frac{Q_c}{2Q_0}\right)^2$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right) \approx \left(\frac{Q_c}{2Q_0}\right)^2\left(1 - e^{iQ\Delta}\right)$$

$$= -\frac{16\pi\rho r_0}{4Q^2} e^{iQ\Delta/2}\left(e^{iQ\Delta/2} - e^{-iQ\Delta/2}\right) = -i\left(\frac{4\pi\rho r_0\Delta}{Q}\right)\frac{\sin(Q\Delta/2)}{Q\Delta/2} e^{iQ\Delta/2}$$

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1$$

$$|r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2} \approx \frac{1}{(2q_0)^2} = \left(\frac{Q_c}{2Q_0}\right)^2$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right) \approx \left(\frac{Q_c}{2Q_0}\right)^2\left(1 - e^{iQ\Delta}\right)$$

$$= -\frac{16\pi\rho r_0}{4Q^2}e^{iQ\Delta/2}\left(e^{iQ\Delta/2} - e^{-iQ\Delta/2}\right) = -i\left(\frac{4\pi\rho r_0\Delta}{Q}\right)\frac{\sin(Q\Delta/2)}{Q\Delta/2}e^{iQ\Delta/2}$$

Since $Q\Delta \ll 1$ for a thin slab

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1 \qquad |r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2} \approx \frac{1}{(2q_0)^2} = \left(\frac{Q_c}{2Q_0}\right)^2$$

$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right) \approx \left(\frac{Q_c}{2Q_0}\right)^2 \left(1 - e^{iQ\Delta}\right)$$

$$= -\frac{16\pi\rho r_0}{4Q^2} e^{iQ\Delta/2}\left(e^{iQ\Delta/2} - e^{-iQ\Delta/2}\right) = -i\left(\frac{4\pi\rho r_0\Delta}{Q}\right)\cancel{\frac{\sin(Q\Delta/2)}{Q\Delta/2}}\cancel{e^{iQ\Delta/2}}$$

Since $Q\Delta \ll 1$ for a thin slab

Kinematical reflection from a thin slab

Recall the reflection coefficient for a thin slab. If the slab is thin and we are well above the critical angle refraction effects can be ignored and we are in the "kinematical" regime.

$$q \gg 1 \qquad |r_{01}| \ll 1 \qquad \alpha > \alpha_c$$

$$r_{01} = \frac{q_0 - q_1}{q_0 + q_1}\frac{q_0 + q_1}{q_0 + q_1} = \frac{q_0^2 - q_1^2}{(q_0 + q_1)^2} \approx \frac{1}{(2q_0)^2} = \left(\frac{Q_c}{2Q_0}\right)^2$$

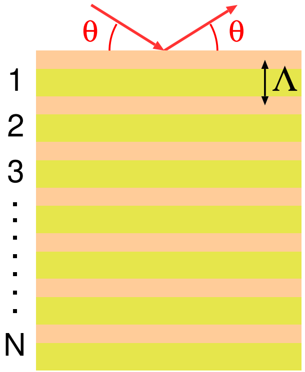
$$r_{slab} = \frac{r_{01}\left(1 - p^2\right)}{1 - r_{01}^2 p^2} \approx r_{01}\left(1 - p^2\right) \approx r_{01}\left(1 - e^{iQ\Delta}\right) \approx \left(\frac{Q_c}{2Q_0}\right)^2\left(1 - e^{iQ\Delta}\right)$$

$$= -\frac{16\pi\rho r_0}{4Q^2} e^{iQ\Delta/2}\left(e^{iQ\Delta/2} - e^{-iQ\Delta/2}\right) = -i\left(\frac{4\pi\rho r_0\Delta}{Q}\right)\cancel{\frac{\sin(Q\Delta/2)}{Q\Delta/2}}\cancel{e^{iQ\Delta/2}}$$

$$\approx -i\frac{\lambda\rho r_0\Delta}{\sin\alpha} = r_{thin\,slab}$$

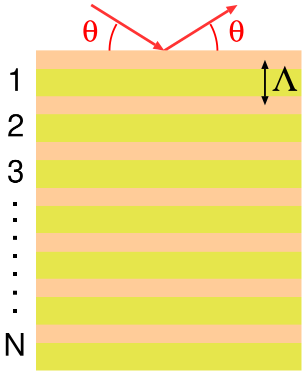
Since $Q\Delta \ll 1$ for a thin slab

Multilayers in the kinematical regime



N repetitions of a bilayer of thickness Λ composed of two materials, A and B which have a density contrast $(\rho_A > \rho_B)$.

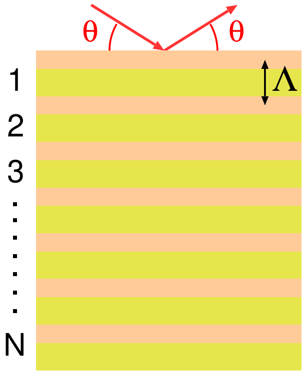
Multilayers in the kinematical regime



N repetitions of a bilayer of thickness Λ composed of two materials, A and B which have a density contrast $(\rho_A > \rho_B)$.

r_1 is the reflectivity of a single bilayer

Multilayers in the kinematical regime

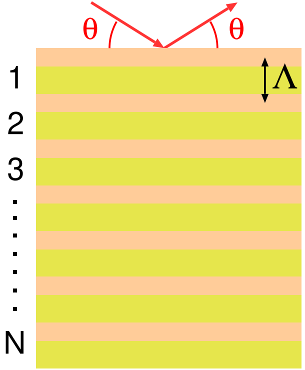


N repetitions of a bilayer of thickness Λ composed of two materials, A and B which have a density contrast ($\rho_A > \rho_B$).

r_1 is the reflectivity of a single bilayer

β is the average absorption per bilayer

Multilayers in the kinematical regime



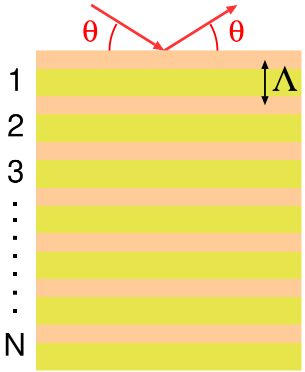
N repetitions of a bilayer of thickness Λ composed of two materials, A and B which have a density contrast ($\rho_A > \rho_B$).

r_1 is the reflectivity of a single bilayer

β is the average absorption per bilayer

$\zeta = Q\Lambda/2\pi$ is a dimensionless parameter related to the phase shift of a single bilayer

Multilayers in the kinematical regime



N repetitions of a bilayer of thickness Λ composed of two materials, A and B which have a density contrast ($\rho_A > \rho_B$).

r_1 is the reflectivity of a single bilayer

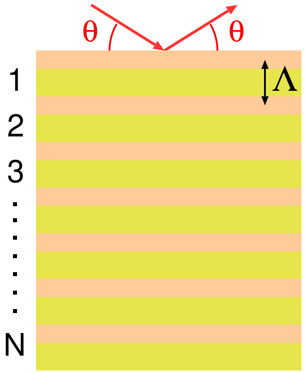
β is the average absorption per bilayer

$\zeta = Q\Lambda/2\pi$ is a dimensionless parameter related to the phase shift of a single bilayer

Form a stack of N bilayers

$$r_N(\zeta) = \sum_{\nu=0}^{N-1} r_1(\zeta) e^{i2\pi\zeta\nu} e^{-\beta\nu}$$

Multilayers in the kinematical regime



N repetitions of a bilayer of thickness Λ composed of two materials, A and B which have a density contrast $(\rho_A > \rho_B)$.

r_1 is the reflectivity of a single bilayer

β is the average absorption per bilayer

$\zeta = Q\Lambda/2\pi$ is a dimensionless parameter related to the phase shift of a single bilayer

Form a stack of N bilayers

$$r_N(\zeta) = \sum_{\nu=0}^{N-1} r_1(\zeta) e^{i2\pi\zeta\nu} e^{-\beta\nu} = r_1(\zeta) \frac{1 - e^{i2\pi\zeta N} e^{-\beta N}}{1 - e^{i2\pi\zeta} e^{-\beta}}$$

Reflectivity of a bilayer

The reflectivity from a single bilayer can be evaluated using the reflectivity developed for a slab but replacing the density of the slab material with the difference in densities of the bilayer components

Reflectivity of a bilayer

The reflectivity from a single bilayer can be evaluated using the reflectivity developed for a slab but replacing the density of the slab material with the difference in densities of the bilayer components

$$\rho \quad \longrightarrow \quad \rho_{AB} = \rho_A - \rho_B$$

Reflectivity of a bilayer

The reflectivity from a single bilayer can be evaluated using the reflectivity developed for a slab but replacing the density of the slab material with the difference in densities of the bilayer components and assuming that material A is a fraction Γ of the bilayer thickness

$$\rho \quad \longrightarrow \quad \rho_{AB} = \rho_A - \rho_B$$

$$r_1(\zeta) = -i\frac{\lambda r_0 \rho_{AB}}{\sin\theta} \int_{-\Gamma\Lambda/2}^{+\Gamma\Lambda/2} e^{i2\pi\zeta z/\Lambda} dz$$

Reflectivity of a bilayer

The reflectivity from a single bilayer can be evaluated using the reflectivity developed for a slab but replacing the density of the slab material with the difference in densities of the bilayer components and assuming that material A is a fraction Γ of the bilayer thickness

$$\rho \quad \longrightarrow \quad \rho_{AB} = \rho_A - \rho_B$$

$$r_1(\zeta) = -i\frac{\lambda r_0 \rho_{AB}}{\sin\theta}\int_{-\Gamma\Lambda/2}^{+\Gamma\Lambda/2} e^{i2\pi\zeta z/\Lambda} dz$$

$$= -i\frac{\lambda r_0 \rho_{AB}}{\sin\theta}\frac{\Lambda}{i2\pi\zeta}\left[e^{i\pi\zeta\Gamma} - e^{-i\pi\zeta\Gamma}\right]$$

Reflectivity of a bilayer

The reflectivity from a single bilayer can be evaluated using the reflectivity developed for a slab but replacing the density of the slab material with the difference in densities of the bilayer components and assuming that material A is a fraction Γ of the bilayer thickness

$$\rho \quad \longrightarrow \quad \rho_{AB} = \rho_A - \rho_B$$

$$r_1(\zeta) = -i\frac{\lambda r_0 \rho_{AB}}{\sin\theta} \int_{-\Gamma\Lambda/2}^{+\Gamma\Lambda/2} e^{i2\pi\zeta z/\Lambda} dz$$

$$e^{ix} - e^{-ix} = 2i\sin x$$

$$= -i\frac{\lambda r_0 \rho_{AB}}{\sin\theta} \frac{\Lambda}{i2\pi\zeta}\left[e^{i\pi\zeta\Gamma} - e^{-i\pi\zeta\Gamma}\right]$$

$$Q = 4\pi\sin\theta/\lambda = 2\pi\zeta/\Lambda$$

Reflectivity of a bilayer

The reflectivity from a single bilayer can be evaluated using the reflectivity developed for a slab but replacing the density of the slab material with the difference in densities of the bilayer components and assuming that material A is a fraction Γ of the bilayer thickness

$$\rho \quad \longrightarrow \quad \rho_{AB} = \rho_A - \rho_B$$

$$r_1(\zeta) = -i\frac{\lambda r_0 \rho_{AB}}{\sin\theta}\int_{-\Gamma\Lambda/2}^{+\Gamma\Lambda/2} e^{i2\pi\zeta z/\Lambda} dz$$

$$e^{ix} - e^{-ix} = 2i\sin x$$

$$= -i\frac{\lambda r_0 \rho_{AB}}{\sin\theta}\frac{\Lambda}{i2\pi\zeta}\left[e^{i\pi\zeta\Gamma} - e^{-i\pi\zeta\Gamma}\right]$$

$$Q = 4\pi\sin\theta/\lambda = 2\pi\zeta/\Lambda$$

$$r_1(\zeta) = -2ir_0\rho_{AB}\left(\frac{\Lambda^2\Gamma}{\zeta}\right)\frac{\sin(\pi\Gamma\zeta)}{\pi\Gamma\zeta}$$

Absorption coefficient of a bilayer

The total reflectivity for the multilayer is therefore:

$$r_N = -2ir_0\rho_{AB}\left(\frac{\Lambda^2\Gamma}{\zeta}\right)\frac{\sin\left(\pi\Gamma\zeta\right)}{\pi\Gamma\zeta}\frac{1-e^{i2\pi\zeta N}e^{-\beta N}}{1-e^{i2\pi\zeta}e^{-\beta}}$$

Absorption coefficient of a bilayer

The total reflectivity for the multilayer is therefore:

$$r_N = -2ir_0\rho_{AB}\left(\frac{\Lambda^2\Gamma}{\zeta}\right)\frac{\sin(\pi\Gamma\zeta)}{\pi\Gamma\zeta}\frac{1-e^{i2\pi\zeta N}e^{-\beta N}}{1-e^{i2\pi\zeta}e^{-\beta}}$$

The incident x-ray has a path length $\Lambda/\sin\theta$ in a bilayer, a fraction Γ through n_A and a fraction $(1-\Gamma)$ through n_B.

Absorption coefficient of a bilayer

The total reflectivity for the multilayer is therefore:

$$r_N = -2ir_0\rho_{AB}\left(\frac{\Lambda^2\Gamma}{\zeta}\right)\frac{\sin\left(\pi\Gamma\zeta\right)}{\pi\Gamma\zeta}\frac{1-e^{i2\pi\zeta N}e^{-\beta N}}{1-e^{i2\pi\zeta}e^{-\beta}}$$

The incident x-ray has a path length $\Lambda/\sin\theta$ in a bilayer, a fraction Γ through n_A and a fraction $(1-\Gamma)$ through n_B. The amplitude absorption coefficient, β is

Absorption coefficient of a bilayer

The total reflectivity for the multilayer is therefore:

$$r_N = -2ir_0\rho_{AB}\left(\frac{\Lambda^2\Gamma}{\zeta}\right)\frac{\sin(\pi\Gamma\zeta)}{\pi\Gamma\zeta}\frac{1-e^{i2\pi\zeta N}e^{-\beta N}}{1-e^{i2\pi\zeta}e^{-\beta}}$$

The incident x-ray has a path length $\Lambda/\sin\theta$ in a bilayer, a fraction Γ through n_A and a fraction $(1-\Gamma)$ through n_B. The amplitude absorption coefficient, β is

$$\beta = 2\left[\frac{\mu_A}{2}\frac{\Gamma\Lambda}{\sin\theta}+\frac{\mu_B}{2}\frac{(1-\Gamma)\Lambda}{\sin\theta}\right]$$

Absorption coefficient of a bilayer

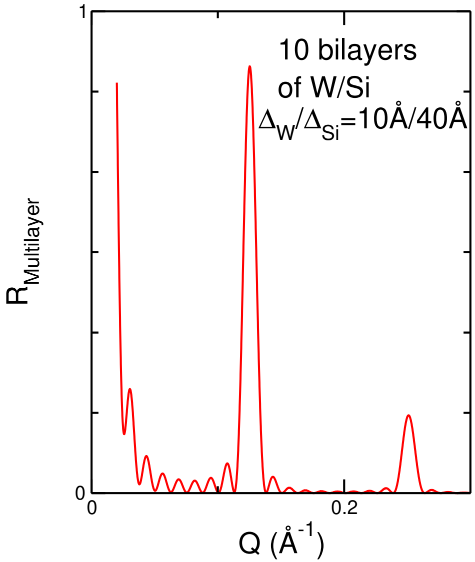
The total reflectivity for the multilayer is therefore:

$$r_N = -2ir_0\rho_{AB}\left(\frac{\Lambda^2\Gamma}{\zeta}\right)\frac{\sin(\pi\Gamma\zeta)}{\pi\Gamma\zeta}\frac{1-e^{i2\pi\zeta N}e^{-\beta N}}{1-e^{i2\pi\zeta}e^{-\beta}}$$

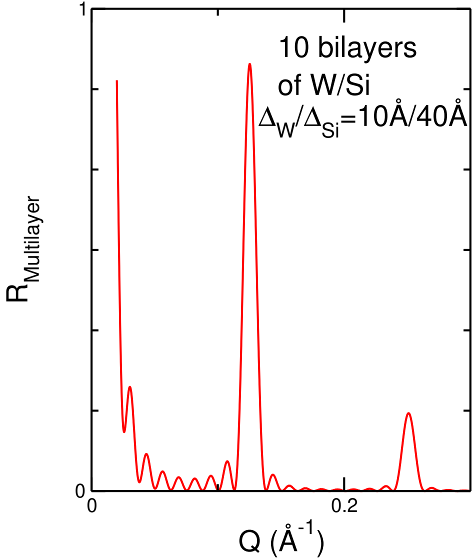
The incident x-ray has a path length $\Lambda/\sin\theta$ in a bilayer, a fraction Γ through n_A and a fraction $(1-\Gamma)$ through n_B. The amplitude absorption coefficient, β is

$$\beta = 2\left[\frac{\mu_A}{2}\frac{\Gamma\Lambda}{\sin\theta}+\frac{\mu_B}{2}\frac{(1-\Gamma)\Lambda}{\sin\theta}\right] = \frac{\Lambda}{\sin\theta}\left[\mu_A\Gamma+\mu_B(1-\Gamma)\right]$$

Reflectivity calculation

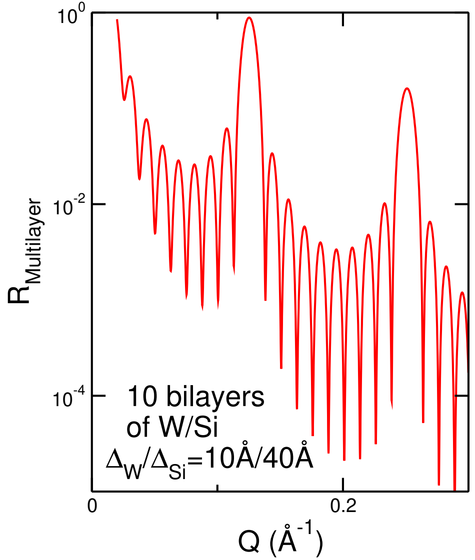


Reflectivity calculation



When $\zeta = Q\Lambda/2\pi$ is an integer, we have peaks

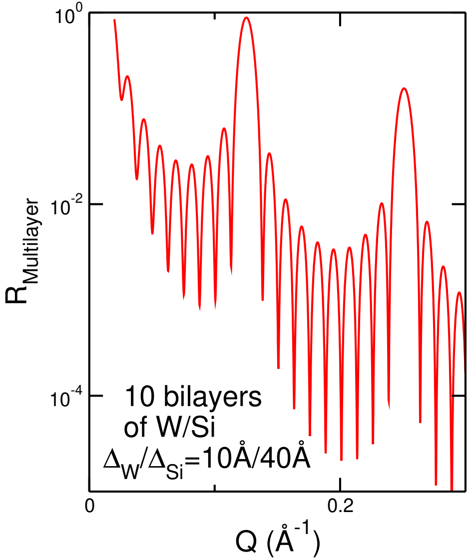
Reflectivity calculation



When $\zeta = Q\Lambda/2\pi$ is an integer, we have peaks

As N becomes larger, these peaks would become more prominent

Reflectivity calculation

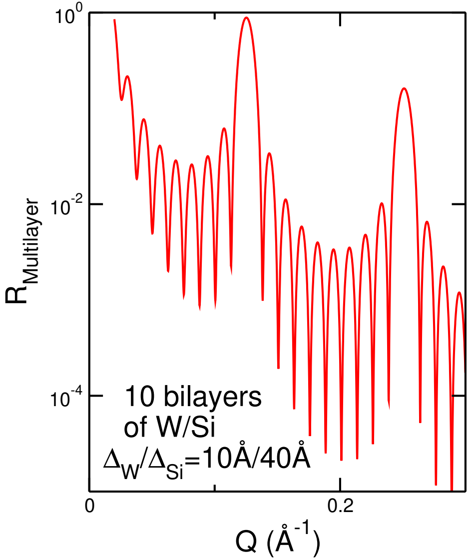


When $\zeta = Q\Lambda/2\pi$ is an integer, we have peaks

As N becomes larger, these peaks would become more prominent

This is effectively a diffraction grating for x-rays

Reflectivity calculation



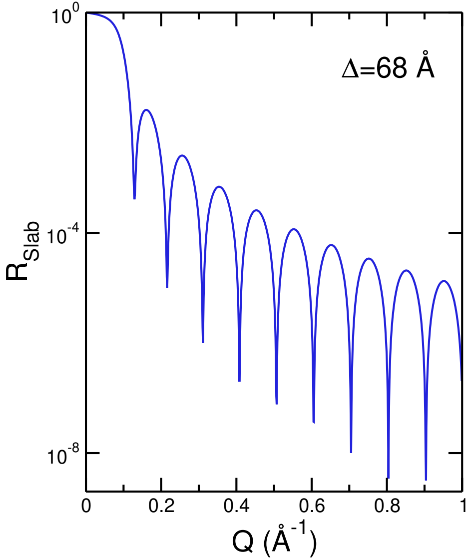
When $\zeta = Q\Lambda/2\pi$ is an integer, we have peaks

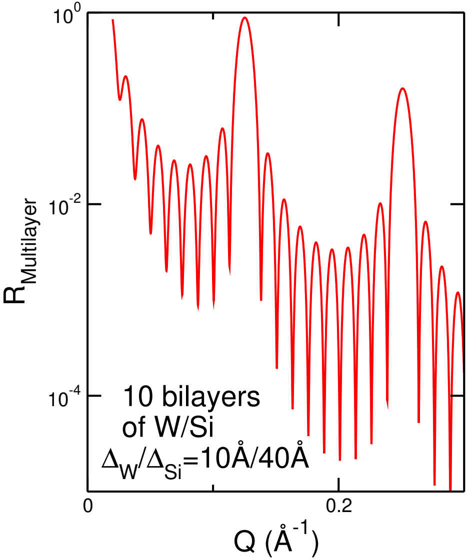
As N becomes larger, these peaks would become more prominent

This is effectively a diffraction grating for x-rays

Multilayers are used commonly on laboratory sources as well as at synchrotrons as mirrors

Slab - multilayer comparison

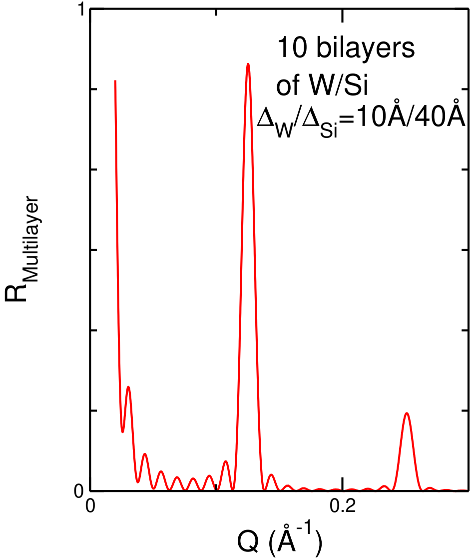




Kinematical reflectivity from a multilayer

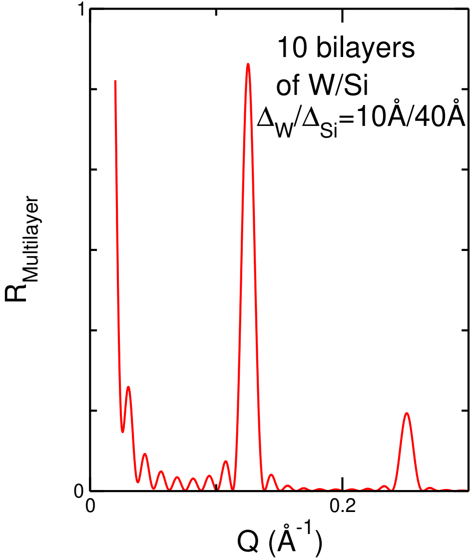
Using the kinematical approximation, we have calculated the reflectivity of a multilayer of slabs containing two contrasting elements

Kinematical reflectivity from a multilayer



Using the kinematical approximation, we have calculated the reflectivity of a multilayer of slabs containing two contrasting elements

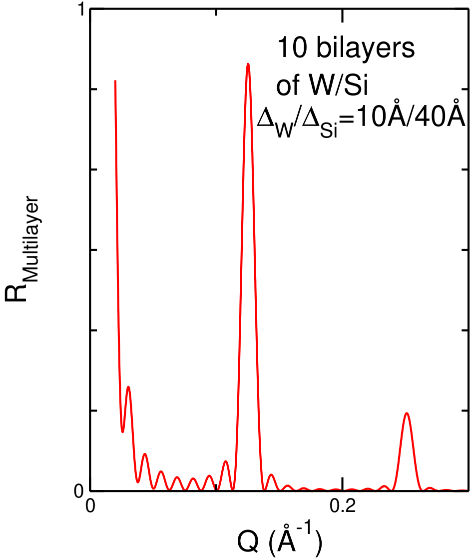
Kinematical reflectivity from a multilayer



Using the kinematical approximation, we have calculated the reflectivity of a multilayer of slabs containing two contrasting elements

This combines the Kiessig fringes from the entire multilayer and the interference obtained because of the bilayer repetition

Kinematical reflectivity from a multilayer

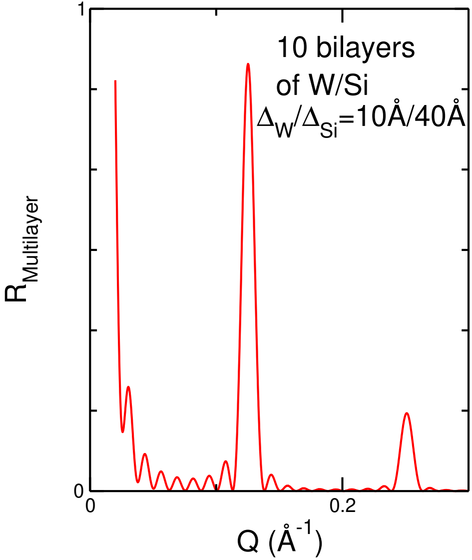


Using the kinematical approximation, we have calculated the reflectivity of a multilayer of slabs containing two contrasting elements

This combines the Kiessig fringes from the entire multilayer and the interference obtained because of the bilayer repetition

However, the simple kinematical approximation fails at very low values of Q as can be seen in the figure

Kinematical reflectivity from a multilayer



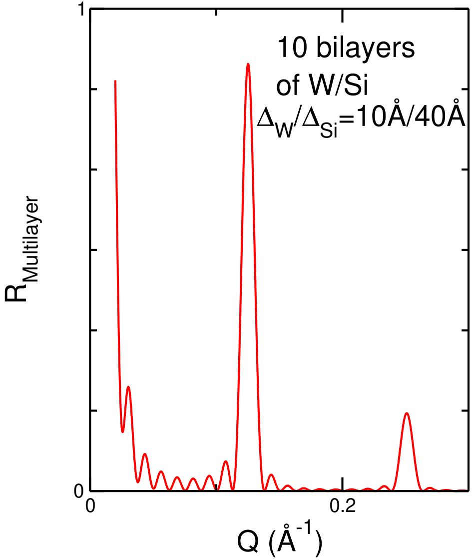
Using the kinematical approximation, we have calculated the reflectivity of a multilayer of slabs containing two contrasting elements

This combines the Kiessig fringes from the entire multilayer and the interference obtained because of the bilayer repetition

However, the simple kinematical approximation fails at very low values of Q as can be seen in the figure

An exact approach is required to give a solution which holds for all values of Q

Kinematical reflectivity from a multilayer



Using the kinematical approximation, we have calculated the reflectivity of a multilayer of slabs containing two contrasting elements

This combines the Kiessig fringes from the entire multilayer and the interference obtained because of the bilayer repetition

However, the simple kinematical approximation fails at very low values of Q as can be seen in the figure

An exact approach is required to give a solution which holds for all values of Q

This is Parratt's recursive approach and needs to be computed numerically

Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

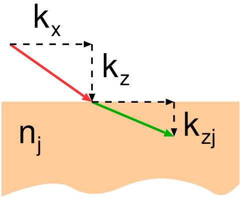
take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$



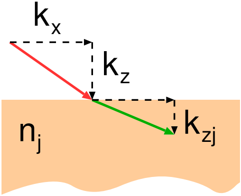
Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$

$$k_{zj}^2 = (n_j k)^2 - k_x^2$$



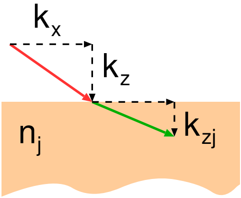
Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$

$$k_{zj}^2 = (n_j k)^2 - k_x^2 = (1 - \delta_j + i\beta_j)^2 k^2 - k_x^2$$



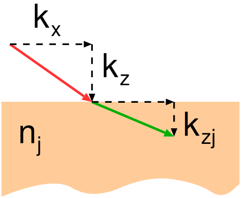
Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$

$$\begin{aligned} k_{zj}^2 &= (n_j k)^2 - k_x^2 = (1 - \delta_j + i\beta_j)^2 k^2 - k_x^2 \\ &\approx k_z^2 - 2\delta_j k^2 + 2i\beta_j k^2 \end{aligned}$$



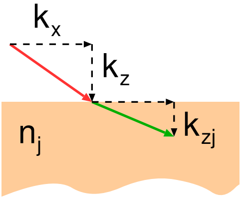
Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$

$$
\begin{aligned}
k_{zj}^2 &= (n_j k)^2 - k_x^2 = (1 - \delta_j + i\beta_j)^2 k^2 - k_x^2 \\
&\approx k_z^2 - 2\delta_j k^2 + 2i\beta_j k^2
\end{aligned}
$$



and the wavevector transfer in the j^{th} layer

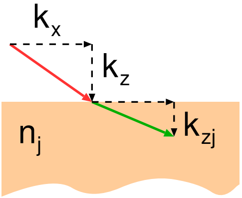
Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$

$$
\begin{aligned}
k_{zj}^2 &= (n_j k)^2 - k_x^2 = (1 - \delta_j + i\beta_j)^2 k^2 - k_x^2 \\
&\approx k_z^2 - 2\delta_j k^2 + 2i\beta_j k^2
\end{aligned}
$$



$$Q_j = 2k_j \sin\alpha_j = 2k_{zj}$$

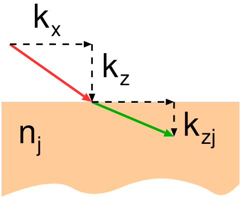
and the wavevector transfer in the jth layer

Parratt's recursive method

Treat the multilayer as a stratified medium on top of an infinitely thick substrate.

take Δ_j as the thickness of each layer and $n_j = 1 - \delta_j + i\beta_j$ as the index of refraction of each layer

because of continuity, $k_{xj} = k_x$ and therefore, we can compute the z-component of $\vec{k}_j$



$$\begin{aligned} k_{zj}^2 &= (n_j k)^2 - k_x^2 = (1 - \delta_j + i\beta_j)^2 k^2 - k_x^2 \\ &\approx k_z^2 - 2\delta_j k^2 + 2i\beta_j k^2 \end{aligned}$$

and the wavevector transfer in the jth layer

$$Q_j = 2k_j \sin\alpha_j = 2k_{zj} = \sqrt{Q^2 - 8k^2\delta_j + 8ik^2\beta_j}$$

Parratt reflectivity calculation

The reflectivity from the interface between layer j and $j+1$, not including multiple reflections is

Parratt reflectivity calculation

The reflectivity from the interface between layer j and $j+1$, not including multiple reflections is

$$r'_{j,j+1} = \frac{Q_j - Q_{j+1}}{Q_j + Q_{j+1}}$$

Parratt reflectivity calculation

The reflectivity from the interface between layer j and $j+1$, not including multiple reflections is

$$r'_{j,j+1} = \frac{Q_j - Q_{j+1}}{Q_j + Q_{j+1}}$$

Now start calculating the reflectivity from the bottom of the N^{th} layer, closest to the substrate, where multiple reflections are not present

Parratt reflectivity calculation

The reflectivity from the interface between layer j and $j+1$, not including multiple reflections is

$$r'_{j,j+1} = \frac{Q_j - Q_{j+1}}{Q_j + Q_{j+1}}$$

Now start calculating the reflectivity from the bottom of the N^{th} layer, closest to the substrate, where multiple reflections are not present

$$r'_{N,\infty} = \frac{Q_N - Q_\infty}{Q_N + Q_\infty}$$

Parratt reflectivity calculation

The reflectivity from the interface between layer j and $j+1$, not including multiple reflections is

$$r'_{j,j+1} = \frac{Q_j - Q_{j+1}}{Q_j + Q_{j+1}}$$

Now start calculating the reflectivity from the bottom of the N^{th} layer, closest to the substrate, where multiple reflections are not present

$$r'_{N,\infty} = \frac{Q_N - Q_\infty}{Q_N + Q_\infty}$$

The reflectivity from the top of the N^{th} layer, including multiple reflections is now calculated (note no prime!)

Parratt reflectivity calculation

The reflectivity from the interface between layer j and $j+1$, not including multiple reflections is

$$r'_{j,j+1} = \frac{Q_j - Q_{j+1}}{Q_j + Q_{j+1}}$$

Now start calculating the reflectivity from the bottom of the N^{th} layer, closest to the substrate, where multiple reflections are not present

$$r'_{N,\infty} = \frac{Q_N - Q_\infty}{Q_N + Q_\infty}$$

The reflectivity from the top of the N^{th} layer, including multiple reflections is now calculated (note no prime!)

$$r_{N-1,N} = \frac{r'_{N-1,N} + r'_{N,\infty} p_N^2}{1 + r'_{N-1,N} r'_{N,\infty} p_N^2}$$

Parratt reflectivity calculation

The reflectivity from the interface between layer j and $j+1$, not including multiple reflections is

$$r'_{j,j+1} = \frac{Q_j - Q_{j+1}}{Q_j + Q_{j+1}}$$

Now start calculating the reflectivity from the bottom of the N^{th} layer, closest to the substrate, where multiple reflections are not present

$$r'_{N,\infty} = \frac{Q_N - Q_\infty}{Q_N + Q_\infty}$$

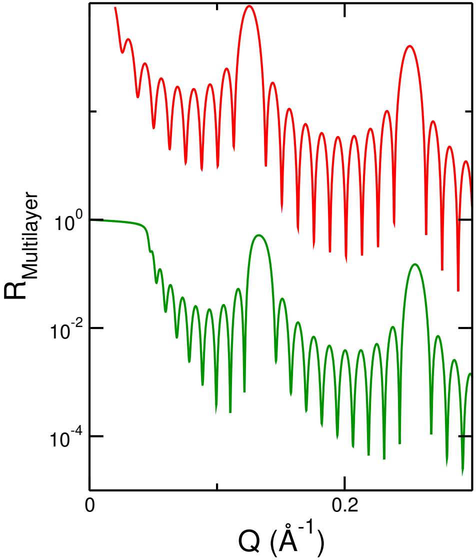
The reflectivity from the top of the N^{th} layer, including multiple reflections is now calculated (note no prime!)

$$r_{N-1,N} = \frac{r'_{N-1,N} + r'_{N,\infty} p_N^2}{1 + r'_{N-1,N} r'_{N,\infty} p_N^2}$$

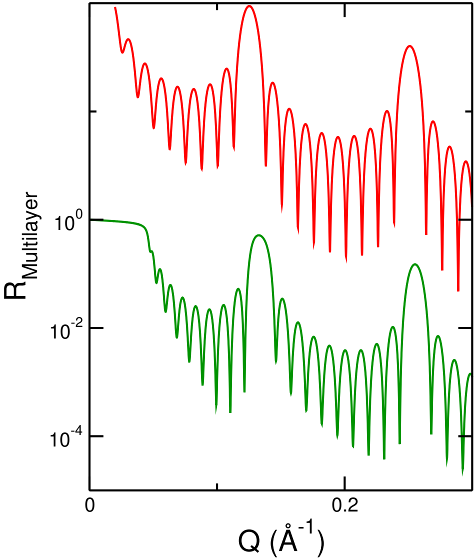
The recursive relation can be seen from the calculation of reflectivity of the next layer up

$$r_{N-2,N-1} = \frac{r'_{N-2,N-1} + r_{N-1,N} p_{N-1}^2}{1 + r'_{N-2,N-1} r_{N-1,N} p_{N-1}^2}$$

Kinematical - Parratt comparison

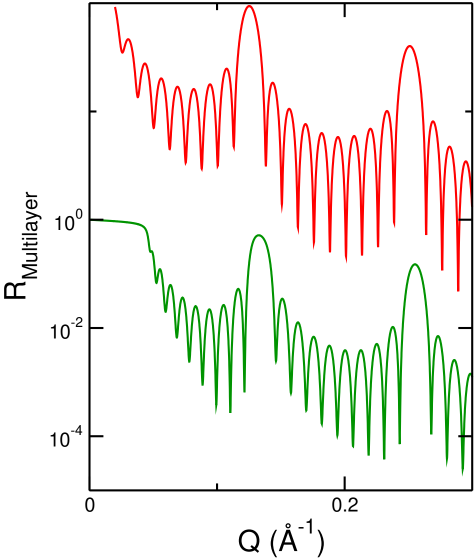


Kinematical - Parratt comparison



Kinematical approximation gives a reasonably good approximation to the correct calculation, with a few exceptions.

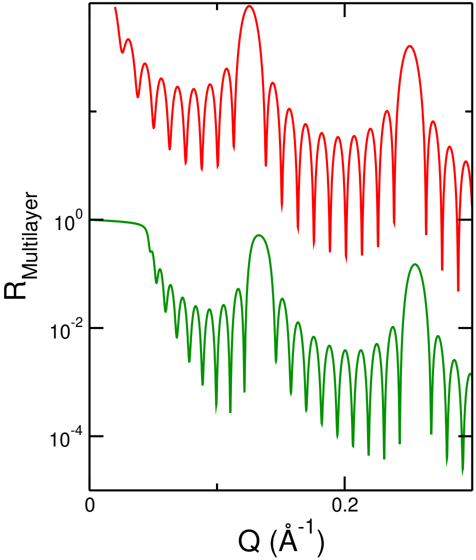
Kinematical - Parratt comparison



Kinematical approximation gives a reasonably good approximation to the correct calculation, with a few exceptions.

Parratt calculation gives $R_{Par} = 1$ as $Q \to 0$ while kinematical diverges ($R_{Kin} \to \infty$).

Kinematical - Parratt comparison

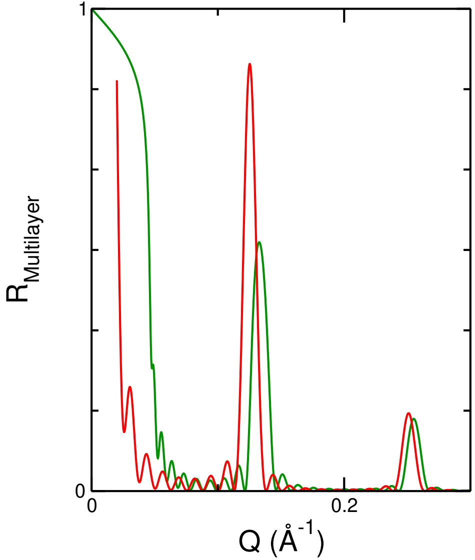


Kinematical approximation gives a reasonably good approximation to the correct calculation, with a few exceptions.

Parratt calculation gives $R_{Par} = 1$ as $Q \to 0$ while kinematical diverges ($R_{Kin} \to \infty$).

Parratt peaks shifted to slightly higher values of Q

Kinematical - Parratt comparison



Kinematical approximation gives a reasonably good approximation to the correct calculation, with a few exceptions.

Parratt calculation gives $R_{Par} = 1$ as $Q \to 0$ while kinematical diverges ($R_{Kin} \to \infty$).

Parratt peaks shifted to slightly higher values of Q

Peaks in kinematical calculation are somewhat higher reflectivity than true value.

Multilayer design

Materials for multilayer monochromator chosen to reflect 12 keV x-rays at ~ 2 degrees with 0.5% and 1.0% bandwidth

A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

Multilayer design

Materials for multilayer monochromator chosen to reflect 12 keV x-rays at ~ 2 degrees with 0.5% and 1.0% bandwidth

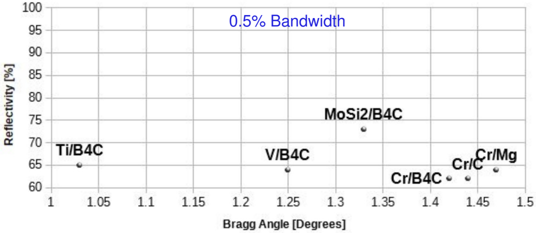
Common design parameters include bilayer filler fraction $\Gamma = 0.5$, roughness $\sigma = 0.35$ nm, and number of bilayers $N = 300$

A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

Multilayer design

Materials for multilayer monochromator chosen to reflect 12 keV x-rays at ~ 2 degrees with 0.5% and 1.0% bandwidth

Common design parameters include bilayer filler fraction $\Gamma = 0.5$, roughness $\sigma = 0.35$ nm, and number of bilayers $N = 300$

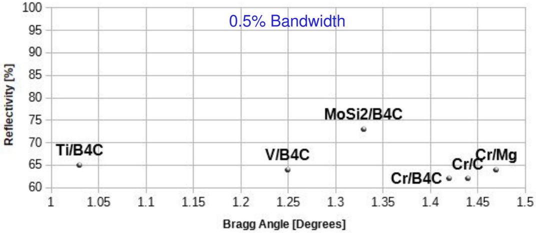


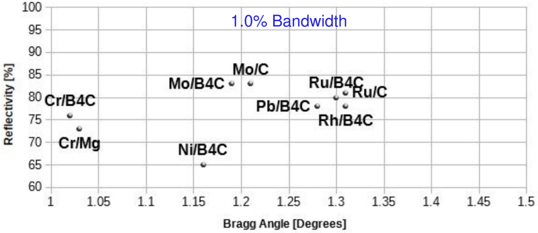
A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

Multilayer design

Materials for multilayer monochromator chosen to reflect 12 keV x-rays at ~ 2 degrees with 0.5% and 1.0% bandwidth

Common design parameters include bilayer filler fraction $\Gamma = 0.5$, roughness $\sigma = 0.35$ nm, and number of bilayers $N = 300$





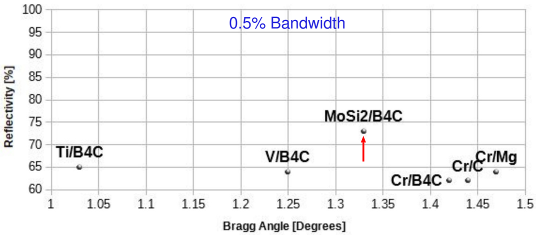
A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

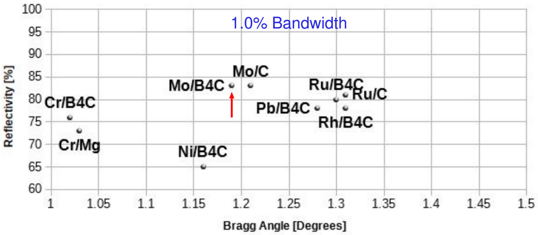
Multilayer design

Materials for multilayer monochromator chosen to reflect 12 keV x-rays at ~ 2 degrees with 0.5% and 1.0% bandwidth

Common design parameters include bilayer filler fraction $\Gamma = 0.5$, roughness $\sigma = 0.35$ nm, and number of bilayers $N = 300$

$MoSi_2/B_4C$ and Mo/B_4C were selected for the 0.5% and 1.0% bandwidth coatings, respectively

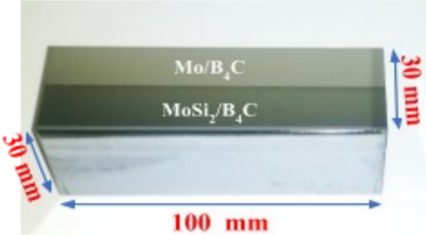




A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

Multilayer fabrication & testing

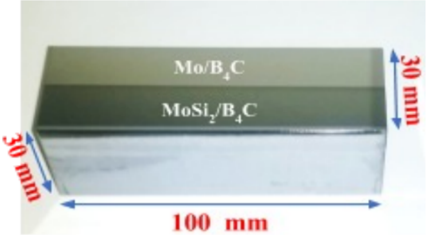
The 0.5% and 1.0% bandwidth layers were deposited side-by-side on a monolithic 20 mm × 30 mm × 100 mm polished silicon block

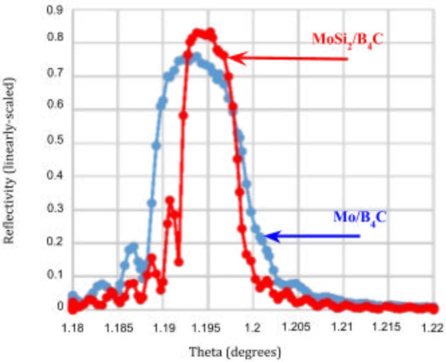


A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

Multilayer fabrication & testing

The 0.5% and 1.0% bandwidth layers were deposited side-by-side on a monolithic 20 mm $\times$ 30 mm $\times$ 100 mm polished silicon block

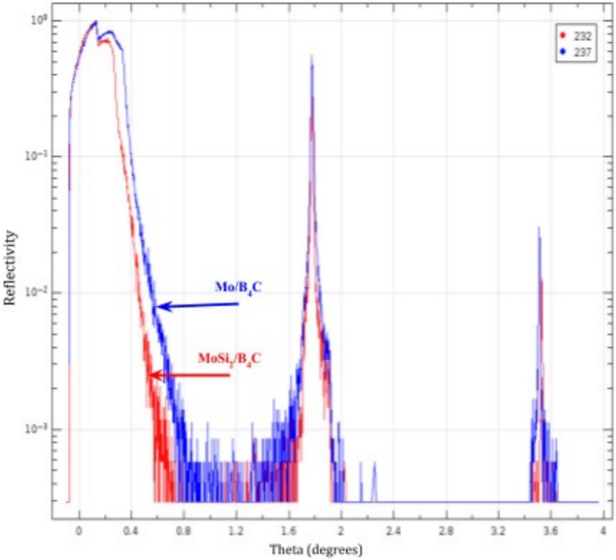




When illuminated with 12 keV x-rays the two multilayers showed diffraction peaks at nearly the same angle. The reflectivities were both over 75% and the bandwidths were 0.52% and 0.86%, respectively.

A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

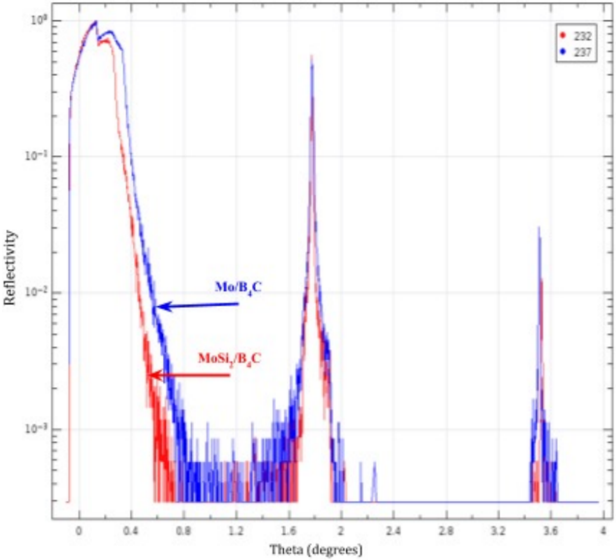
Multilayer spectrum



The reflectivity over a wide range of angles at 8 keV shows total external reflection at low angles with cutoff at zero degrees

A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

Multilayer spectrum



The reflectivity over a wide range of angles at 8 keV shows total external reflection at low angles with cutoff at zero degrees

First and second order multilayer diffraction peaks appear at higher angles

A. Khounsary et al., "A dual-bandwidth multilayer monochromator system," *Proc. SPIE* **10760**, 107600j (2018).

Graded interfaces

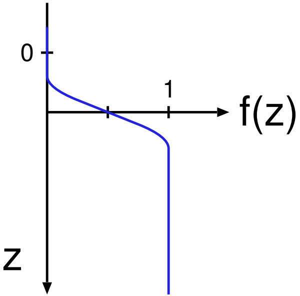
Since most interfaces are not sharp, it is important to be able to model a graded interface, where the density, and therefore the index of refraction varies near the interface itself.

Graded interfaces

Since most interfaces are not sharp, it is important to be able to model a graded interface, where the density, and therefore the index of refraction varies near the interface itself.

The reflectivity of this kind of interface can be calculated best in the kinematical limit ($Q > Q_c$).

Graded interfaces

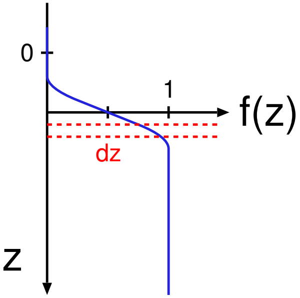


Since most interfaces are not sharp, it is important to be able to model a graded interface, where the density, and therefore the index of refraction varies near the interface itself.

The reflectivity of this kind of interface can be calculated best in the kinematical limit ($Q > Q_c$).

The density profile of the interface can be described by the function $f(z)$ which approaches 1 as $z \to \infty$.

Graded interfaces



Since most interfaces are not sharp, it is important to be able to model a graded interface, where the density, and therefore the index of refraction varies near the interface itself.

The reflectivity of this kind of interface can be calculated best in the kinematical limit ($Q > Q_c$).

The density profile of the interface can be described by the function $f(z)$ which approaches 1 as $z \to \infty$.

The reflectivity can be computed as the superposition of the reflectivity of a series of infinitesmal slabs of thickness dz at a depth z.

Reflectivity of a graded interface

The differential reflectivity from a slab of thickness dz at depth z is:

Reflectivity of a graded interface

$$\delta r(Q) = -i\frac{Q_c^2}{4Q}f(z)dz$$

The differential reflectivity from a slab of thickness dz at depth z is:

Reflectivity of a graded interface

$$\delta r(Q) = -i\frac{Q_c^2}{4Q}f(z)dz$$

The differential reflectivity from a slab of thickness dz at depth z is:

integrating, to get the entire reflectivity

Reflectivity of a graded interface

$$\delta r(Q) = -i\frac{Q_c^2}{4Q} f(z) dz$$

The differential reflectivity from a slab of thickness dz at depth z is:

integrating, to get the entire reflectivity

$$r(Q) = -i\frac{Q_c^2}{4Q} \int_{-\infty}^{\infty} f(z) e^{iQz} dz$$

Reflectivity of a graded interface

$$\delta r(Q) = -i\frac{Q_c^2}{4Q} f(z) dz$$

The differential reflectivity from a slab of thickness dz at depth z is:

$$r(Q) = -i\frac{Q_c^2}{4Q} \int_{-\infty}^{\infty} f(z) e^{iQz} dz$$

integrating, to get the entire reflectivity

integrating by parts simplifies

Reflectivity of a graded interface

The differential reflectivity from a slab of thickness dz at depth z is:

$$\delta r(Q) = -i\frac{Q_c^2}{4Q}f(z)dz$$

integrating, to get the entire reflectivity

$$r(Q) = -i\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f(z)e^{iQz}dz$$

integrating by parts simplifies

$$= i\frac{1}{iQ}\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f'(z)e^{iQz}dz$$

Reflectivity of a graded interface

The differential reflectivity from a slab of thickness dz at depth z is:

$$\delta r(Q) = -i\frac{Q_c^2}{4Q} f(z) dz$$

integrating, to get the entire reflectivity

$$r(Q) = -i\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f(z) e^{iQz} dz$$

integrating by parts simplifies

$$= i\frac{1}{iQ}\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f'(z) e^{iQz} dz$$

$$= \frac{Q_c^2}{4Q^2}\int_{-\infty}^{\infty} f'(z) e^{iQz} dz$$

Reflectivity of a graded interface

$$\delta r(Q) = -i\frac{Q_c^2}{4Q}f(z)dz$$

The differential reflectivity from a slab of thickness dz at depth z is:

integrating, to get the entire reflectivity

$$r(Q) = -i\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f(z)e^{iQz}dz$$

integrating by parts simplifies

$$= i\frac{1}{iQ}\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f'(z)e^{iQz}dz$$

$$= \frac{Q_c^2}{4Q^2}\int_{-\infty}^{\infty} f'(z)e^{iQz}dz$$

the term in front is simply the Fresnel reflectivity for an interface, $r_F(Q)$ when $q \gg 1$

Reflectivity of a graded interface

$$\delta r(Q) = -i\frac{Q_c^2}{4Q} f(z)dz$$

The differential reflectivity from a slab of thickness dz at depth z is:

integrating, to get the entire reflectivity

$$r(Q) = -i\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f(z)e^{iQz}dz$$

integrating by parts simplifies

$$= i\frac{1}{iQ}\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f'(z)e^{iQz}dz$$

$$= \frac{Q_c^2}{4Q^2}\int_{-\infty}^{\infty} f'(z)e^{iQz}dz$$

the term in front is simply the Fresnel reflectivity for an interface, $r_F(Q)$ when $q \gg 1$, the integral is the Fourier transform of the density gradient, $\phi(Q)$

Reflectivity of a graded interface

The differential reflectivity from a slab of thickness dz at depth z is:

$$\delta r(Q) = -i\frac{Q_c^2}{4Q}f(z)dz$$

integrating, to get the entire reflectivity

$$r(Q) = -i\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f(z)e^{iQz}dz$$

integrating by parts simplifies

$$= i\frac{1}{iQ}\frac{Q_c^2}{4Q}\int_{-\infty}^{\infty} f'(z)e^{iQz}dz$$

$$= \frac{Q_c^2}{4Q^2}\int_{-\infty}^{\infty} f'(z)e^{iQz}dz$$

the term in front is simply the Fresnel reflectivity for an interface, $r_F(Q)$ when $q \gg 1$, the integral is the Fourier transform of the density gradient, $\phi(Q)$

Calculating the full reflection coefficient relative to the Fresnel reflection coefficient

$$\frac{R(Q)}{R_F(Q)} = \left|\int_{-\infty}^{\infty}\left(\frac{df}{dz}\right)e^{iQz}dz\right|^2$$

The error function - a specific case

The error function is often chosen as a model for the density gradient

$$f(z) = erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{\pi}} \int_0^{z/\sqrt{2}\sigma} e^{-t^2} dt$$

The error function - a specific case

The error function is often chosen as a model for the density gradient

$$f(z) = erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{\pi}} \int_0^{z/\sqrt{2}\sigma} e^{-t^2} dt$$

the gradient of the error function is simply a Gaussian

$$\frac{df(z)}{dz} = \frac{d}{dz} erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{z^2}{\sigma^2}}$$

The error function - a specific case

The error function is often chosen as a model for the density gradient

$$f(z) = erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{\pi}} \int_0^{z/\sqrt{2}\sigma} e^{-t^2} dt$$

the gradient of the error function is simply a Gaussian

$$\frac{df(z)}{dz} = \frac{d}{dz} erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{z^2}{\sigma^2}}$$

whose Fourier transform is also a Gaussian, which when squared to obtain the reflection coefficient, gives.

$$R(Q) = R_F(Q) e^{-Q^2\sigma^2}$$

The error function - a specific case

The error function is often chosen as a model for the density gradient

$$f(z) = erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{\pi}}\int_0^{z/\sqrt{2}\sigma} e^{-t^2}dt$$

the gradient of the error function is simply a Gaussian

$$\frac{df(z)}{dz} = \frac{d}{dz}erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}\frac{z^2}{\sigma^2}}$$

whose Fourier transform is also a Gaussian, which when squared to obtain the reflection coefficient, gives. Or more accurately.

$$R(Q) = R_F(Q)e^{-Q^2\sigma^2} = R_F(Q)e^{-QQ'\sigma^2}$$

The error function - a specific case

The error function is often chosen as a model for the density gradient

$$f(z) = erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{\pi}} \int_0^{z/\sqrt{2}\sigma} e^{-t^2} dt$$

the gradient of the error function is simply a Gaussian

$$\frac{df(z)}{dz} = \frac{d}{dz} erf(\frac{z}{\sqrt{2}\sigma}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\frac{z^2}{\sigma^2}}$$

whose Fourier transform is also a Gaussian, which when squared to obtain the reflection coefficient, gives. Or more accurately.

$$R(Q) = R_F(Q) e^{-Q^2\sigma^2} = R_F(Q) e^{-QQ'\sigma^2}$$

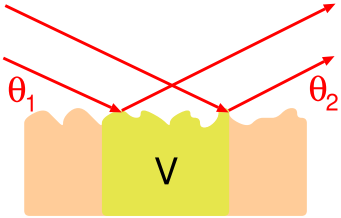
$$Q = k \sin\theta, \qquad Q' = k' \sin\theta'$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.

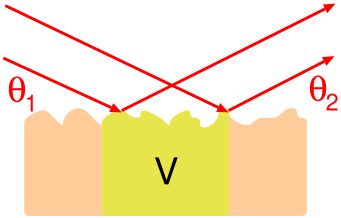
Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



Rough surfaces

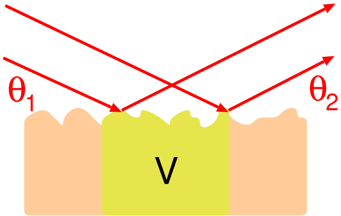
When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V.

Rough surfaces

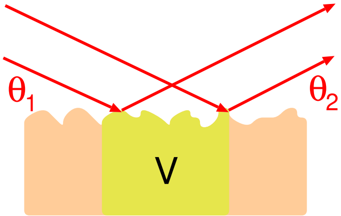
When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral,

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.

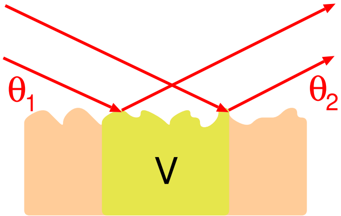


The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral,

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}},$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.

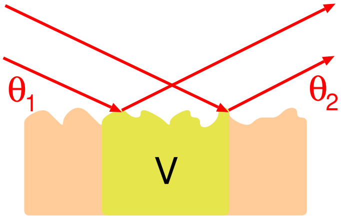


The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}},$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.

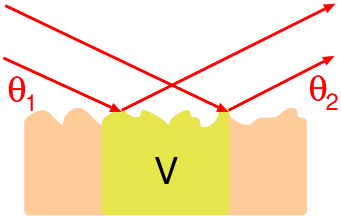


The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



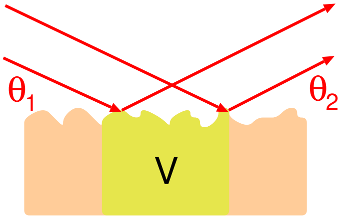
The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

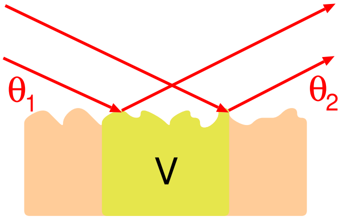
$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

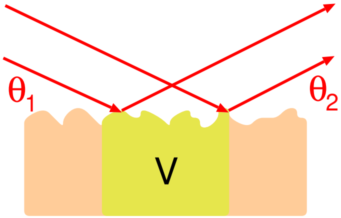
Taking C to be

$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

its divergence is

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

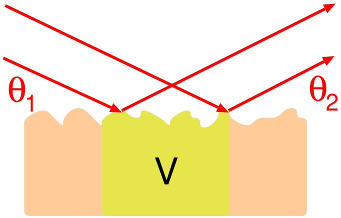
$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

its divergence is

$$\vec{\nabla}\cdot\vec{C} = \frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z} iQ_z$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

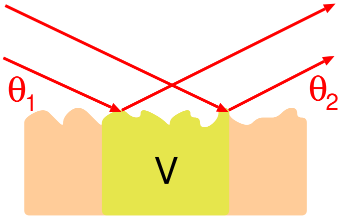
$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

its divergence is

$$\vec{\nabla}\cdot\vec{C} = \frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z} iQ_z = e^{i\vec{Q}\cdot\vec{r}}$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

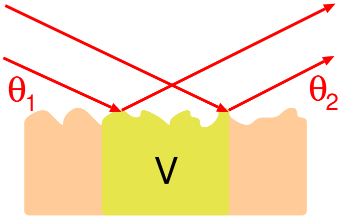
$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

its divergence is

$$\vec{\nabla}\cdot\vec{C} = \frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z} iQ_z = e^{i\vec{Q}\cdot\vec{r}}$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

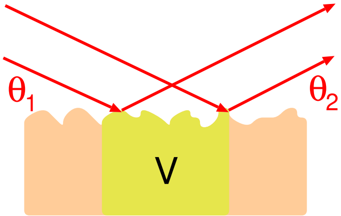
its divergence is

$$\vec{\nabla}\cdot\vec{C} = \frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z} iQ_z = e^{i\vec{Q}\cdot\vec{r}}$$

$$r_V = -r_0\rho \int_V \vec{\nabla}\cdot\left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z}\right) d\vec{r}$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

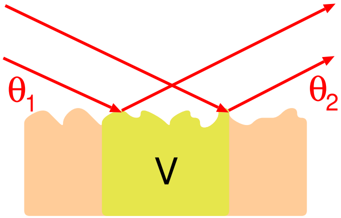
its divergence is

$$\vec{\nabla}\cdot\vec{C} = \frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z} iQ_z = e^{i\vec{Q}\cdot\vec{r}}$$

$$r_V = -r_0\rho \int_V \vec{\nabla}\cdot\left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z}\right) d\vec{r} = -r_0\rho \int_S \left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z}\right)\cdot d\vec{S}$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

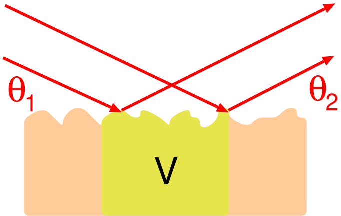
its divergence is

$$\vec{\nabla}\cdot\vec{C} = \frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z} iQ_z = e^{i\vec{Q}\cdot\vec{r}}$$

$$r_V = -r_0\rho \int_V \vec{\nabla}\cdot\left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z}\right) d\vec{r} = -r_0\rho \int_S \left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z}\right)\cdot d\vec{S} = -r_0\rho\frac{1}{iQ_z}\int_S e^{i\vec{Q}\cdot\vec{r}} dxdy$$

Rough surfaces

When a surface or interface is not perfectly smooth but has some roughness the reflectivity is no longer simply specular but has a non-zero diffuse component which we must include in the model.



The incident and scattered angles are no longer the same, the x-rays illuminate the volume V. The scattering from the entire, illuminated volume is given by an integral, which can be solved using Gauss' theorem.

$$r_V = -r_0 \int_V (\rho d\vec{r}) e^{i\vec{Q}\cdot\vec{r}}, \qquad \int_V \left(\vec{\nabla}\cdot\vec{C}\right) d\vec{r} = \int_S \vec{C}\cdot d\vec{S}$$

Taking C to be

$$\vec{C} = \hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z},$$

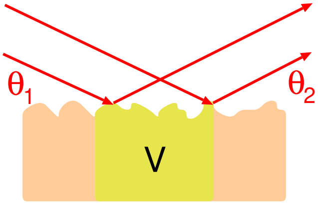
its divergence is

$$\vec{\nabla}\cdot\vec{C} = \frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z} iQ_z = e^{i\vec{Q}\cdot\vec{r}}$$

$$r_V = -r_0\rho \int_V \vec{\nabla}\cdot\left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z}\right) d\vec{r} = -r_0\rho \int_S \left(\hat{z}\frac{e^{i\vec{Q}\cdot\vec{r}}}{iQ_z}\right)\cdot d\vec{S} = -r_0\rho\frac{1}{iQ_z}\int_S e^{i\vec{Q}\cdot\vec{r}} dxdy = r_S$$

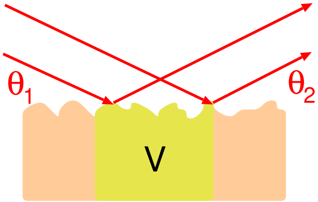
Rough surfaces

Reflection from a rough surface leads to some amount of diffuse scattering on top of the specular reflection from a flat surface. The scattering from an illuminated volume is given by V.



Rough surfaces

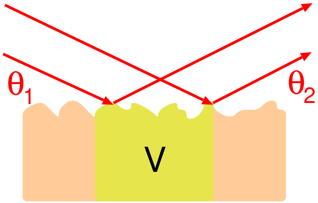
Reflection from a rough surface leads to some amount of diffuse scattering on top of the specular reflection from a flat surface. The scattering from an illuminated volume is given by V.



$$r_V = -r_0 \rho \int_V e^{i\vec{Q}\cdot\vec{r}}\, d^3 r$$

Rough surfaces

Reflection from a rough surface leads to some amount of diffuse scattering on top of the specular reflection from a flat surface. The scattering from an illuminated volume is given by V.

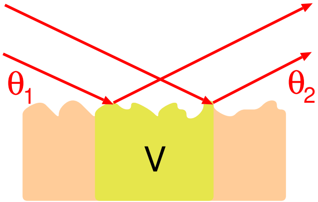


Using Gauss' theorem, this volume integral can be converted to an integral over the surface of the illuminated volume.

$$r_V = -r_0 \rho \int_V e^{i\vec{Q}\cdot\vec{r}}\, d^3 r$$

Rough surfaces

Reflection from a rough surface leads to some amount of diffuse scattering on top of the specular reflection from a flat surface. The scattering from an illuminated volume is given by V.



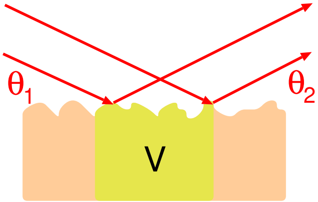
Using Gauss' theorem, this volume integral can be converted to an integral over the surface of the illuminated volume.

$$r_V = -r_0\rho \int_V e^{i\vec{Q}\cdot\vec{r}}\, d^3r$$

$$r_S = -r_0\rho \frac{1}{iQ_z} \int_S e^{i\vec{Q}\cdot\vec{r}} dxdy$$

Rough surfaces

Reflection from a rough surface leads to some amount of diffuse scattering on top of the specular reflection from a flat surface. The scattering from an illuminated volume is given by V.



$$r_V = -r_0\rho \int_V e^{i\vec{Q}\cdot\vec{r}}\, d^3r$$

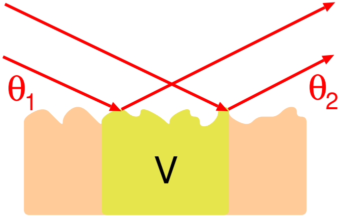
$$r_S = -r_0\rho \frac{1}{iQ_z} \int_S e^{i\vec{Q}\cdot\vec{r}} dxdy$$

Using Gauss' theorem, this volume integral can be converted to an integral over the surface of the illuminated volume.

This integral is highly model dependent and can now be evaluated for a number of different cases.

Evaluation of surface integral

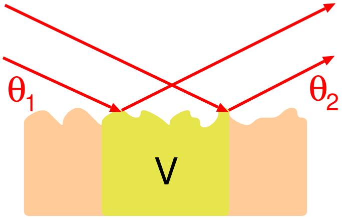
The side surfaces of the volume do not contribute to this integral as they are along the $\hat{z}$ direction, and we can also choose the thickness of the slab sufficiently large such that the lower surface will not contribute.



$$r_S = -r_0 \rho \frac{1}{iQ_z} \int_S e^{i\vec{Q}\cdot\vec{r}} dxdy$$

Evaluation of surface integral

The side surfaces of the volume do not contribute to this integral as they are along the $\hat{z}$ direction, and we can also choose the thickness of the slab sufficiently large such that the lower surface will not contribute.

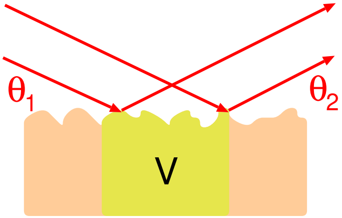


Thus, the integral need only be evaluated over the top, rough surface whose variation we characterize by the function $h(x,y)$

$$r_S = -r_0 \rho \frac{1}{iQ_z} \int_S e^{i\vec{Q}\cdot\vec{r}} dxdy$$

Evaluation of surface integral

The side surfaces of the volume do not contribute to this integral as they are along the $\hat{z}$ direction, and we can also choose the thickness of the slab sufficiently large such that the lower surface will not contribute.



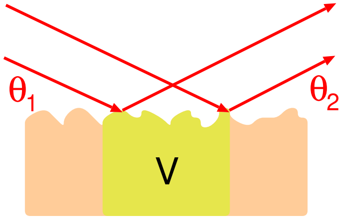
Thus, the integral need only be evaluated over the top, rough surface whose variation we characterize by the function $h(x,y)$

$$\vec{Q}\cdot\vec{r} = Q_z h(x,y) + Q_x x + Q_y y$$

$$r_S = -r_0\rho\frac{1}{iQ_z}\int_S e^{i\vec{Q}\cdot\vec{r}}dxdy$$

Evaluation of surface integral

The side surfaces of the volume do not contribute to this integral as they are along the $\hat{z}$ direction, and we can also choose the thickness of the slab sufficiently large such that the lower surface will not contribute.



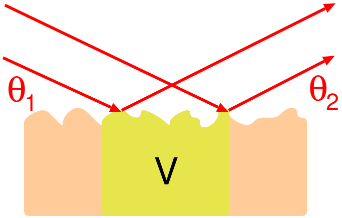
Thus, the integral need only be evaluated over the top, rough surface whose variation we characterize by the function $h(x, y)$

$$\vec{Q} \cdot \vec{r} = Q_z h(x, y) + Q_x x + Q_y y$$

$$r_S = -r_0 \rho \frac{1}{iQ_z} \int_S e^{i\vec{Q}\cdot\vec{r}} dxdy = -\frac{r_0 \rho}{iQ_z} \int_S e^{iQ_z h(x,y)} e^{i(Q_x x + Q_y y)} dxdy$$

Evaluation of surface integral

The side surfaces of the volume do not contribute to this integral as they are along the $\hat{z}$ direction, and we can also choose the thickness of the slab sufficiently large such that the lower surface will not contribute.



Thus, the integral need only be evaluated over the top, rough surface whose variation we characterize by the function $h(x, y)$

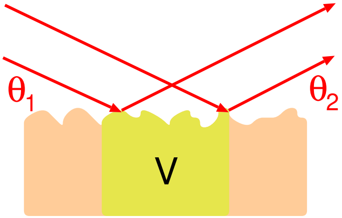
$$\vec{Q} \cdot \vec{r} = Q_z h(x, y) + Q_x x + Q_y y$$

$$r_S = -r_0 \rho \frac{1}{iQ_z} \int_S e^{i\vec{Q}\cdot\vec{r}} dxdy = -\frac{r_0 \rho}{iQ_z} \int_S e^{iQ_z h(x,y)} e^{i(Q_x x + Q_y y)} dxdy$$

$$\frac{d\sigma}{d\Omega} = r_S^2$$

Evaluation of surface integral

The side surfaces of the volume do not contribute to this integral as they are along the $\hat{z}$ direction, and we can also choose the thickness of the slab sufficiently large such that the lower surface will not contribute.



Thus, the integral need only be evaluated over the top, rough surface whose variation we characterize by the function $h(x, y)$

$$\vec{Q} \cdot \vec{r} = Q_z h(x, y) + Q_x x + Q_y y$$

$$r_S = -r_0 \rho \frac{1}{iQ_z} \int_S e^{i\vec{Q}\cdot\vec{r}} dxdy = -\frac{r_0 \rho}{iQ_z} \int_S e^{iQ_z h(x,y)} e^{i(Q_x x + Q_y y)} dxdy$$

$$\frac{d\sigma}{d\Omega} = r_S^2 = \left(\frac{r_0 \rho}{Q_z}\right)^2 \int_S \int_{S'} e^{iQ_z(h(x,y) - h(x',y'))} e^{iQ_x(x-x')} e^{iQ_y(y-y')} dxdydx'dy'$$

Scattering cross section

If we assume that $h(x, y) - h(x', y')$ depends only on the relative difference in position, $x - x'$ and $y - y'$ the four dimensional integral collapses to the product of two two dimensional integrals

Scattering cross section

If we assume that $h(x, y) - h(x', y')$ depends only on the relative difference in position, $x - x'$ and $y - y'$ the four dimensional integral collapses to the product of two two dimensional integrals

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \int_{S'} dx'dy' \int_S \left\langle e^{iQ_z(h(0,0)-h(x,y))} \right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

Scattering cross section

If we assume that $h(x,y) - h(x',y')$ depends only on the relative difference in position, $x - x'$ and $y - y'$ the four dimensional integral collapses to the product of two two dimensional integrals

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \int_{S'} dx'dy' \int_S \left\langle e^{iQ_z(h(0,0)-h(x,y))}\right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int \left\langle e^{iQ_z(h(0,0)-h(x,y))}\right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

Scattering cross section

If we assume that $h(x, y) - h(x', y')$ depends only on the relative difference in position, $x - x'$ and $y - y'$ the four dimensional integral collapses to the product of two two dimensional integrals

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \int_{S'} dx'dy' \int_S \left\langle e^{iQ_z(h(0,0)-h(x,y))} \right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int \left\langle e^{iQ_z(h(0,0)-h(x,y))} \right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

where $A_0/\sin\theta_1$ is just the illuminated surface area

Scattering cross section

If we assume that $h(x,y) - h(x',y')$ depends only on the relative difference in position, $x - x'$ and $y - y'$ the four dimensional integral collapses to the product of two two dimensional integrals

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \int_{S'} dx'dy' \int_S \left\langle e^{iQ_z(h(0,0)-h(x,y))} \right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int \left\langle e^{iQ_z(h(0,0)-h(x,y))} \right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

where $A_0/\sin\theta_1$ is just the illuminated surface area and the term in the angled brackets is an ensemble average over all possible choices of the origin within the illuminated area.

Scattering cross section

If we assume that $h(x, y) - h(x', y')$ depends only on the relative difference in position, $x - x'$ and $y - y'$ the four dimensional integral collapses to the product of two two dimensional integrals

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \int_{S'} dx'dy' \int_S \left\langle e^{iQ_z(h(0,0)-h(x,y))} \right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int \left\langle e^{iQ_z(h(0,0)-h(x,y))} \right\rangle e^{iQ_x x} e^{iQ_y y} dxdy$$

where $A_0/\sin\theta_1$ is just the illuminated surface area and the term in the angled brackets is an ensemble average over all possible choices of the origin within the illuminated area.
Finally, it is assumed that the statistics of the height variation are Gaussian and

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2 \right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Define a function $g(x,y) = \left\langle [h(0,0) - h(x,y)]^2 \right\rangle$ which can be modeled in various ways.

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Define a function $g(x,y) = \left\langle [h(0,0) - h(x,y)]^2 \right\rangle$ which can be modeled in various ways.

For a perfectly flat surface, $h(x,y) = 0$ for all x and y.

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{iQ_x x} e^{iQ_y y} dxdy$$

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Define a function $g(x, y) = \left\langle [h(0, 0) - h(x, y)]^2 \right\rangle$ which can be modeled in various ways. For a perfectly flat surface, $h(x, y) = 0$ for all x and y.

by the definition of a delta function

$$2\pi\delta(q) = \int e^{iqx} dx$$

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{iQ_x x} e^{iQ_y y} dxdy$$

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Define a function $g(x,y) = \left\langle [h(0,0) - h(x,y)]^2 \right\rangle$ which can be modeled in various ways.

For a perfectly flat surface, $h(x,y) = 0$ for all x and y.

by the definition of a delta function

$$2\pi\delta(q) = \int e^{iqx} dx$$

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{iQ_x x} e^{iQ_y y} dxdy$$

$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \delta(Q_x)\delta(Q_y)$$

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Define a function $g(x,y) = \left\langle [h(0,0) - h(x,y)]^2 \right\rangle$ which can be modeled in various ways.

For a perfectly flat surface, $h(x,y) = 0$ for all x and y.

by the definition of a delta function

$$2\pi\delta(q) = \int e^{iqx} dx$$

the expression for the scattered intensity in terms of the momentum transfer wave vectors is

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{iQ_x x} e^{iQ_y y} dxdy$$

$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \delta(Q_x)\delta(Q_y)$$

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Define a function $g(x,y) = \left\langle [h(0,0) - h(x,y)]^2 \right\rangle$ which can be modeled in various ways.

For a perfectly flat surface, $h(x,y) = 0$ for all x and y.

by the definition of a delta function

$$2\pi\delta(q) = \int e^{iqx} dx$$

the expression for the scattered intensity in terms of the momentum transfer wave vectors is

$$I_{sc} = \left(\frac{I_0}{A_0}\right)\left(\frac{d\sigma}{d\Omega}\right)\frac{\Delta Q_x \Delta Q_y}{k^2 \sin\theta_2}$$

$$\begin{aligned}\left(\frac{d\sigma}{d\Omega}\right) &= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{iQ_x x} e^{iQ_y y} dxdy \\ &= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \delta(Q_x)\delta(Q_y)\end{aligned}$$

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y}\, dxdy$$

Define a function $g(x,y) = \left\langle [h(0,0) - h(x,y)]^2 \right\rangle$ which can be modeled in various ways.

For a perfectly flat surface, $h(x,y) = 0$ for all x and y.

by the definition of a delta function

$$2\pi\delta(q) = \int e^{iqx}\, dx$$

the expression for the scattered intensity in terms of the momentum transfer wave vectors is

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{iQ_x x} e^{iQ_y y}\, dxdy$$

$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \delta(Q_x)\delta(Q_y)$$

$$I_{sc} = \left(\frac{I_0}{A_0}\right)\left(\frac{d\sigma}{d\Omega}\right)\frac{\Delta Q_x \Delta Q_y}{k^2 \sin\theta_2} \quad \longrightarrow \quad R(Q_z) = \frac{I_{sc}}{I_0} = \left(\frac{Q_c^2/8}{Q_z}\right)^2 \left(\frac{1}{Q_z/2}\right)^2$$

Limiting Case - Flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Define a function $g(x,y) = \left\langle [h(0,0) - h(x,y)]^2 \right\rangle$ which can be modeled in various ways.

For a perfectly flat surface, $h(x,y) = 0$ for all x and y.

by the definition of a delta function

$$2\pi\delta(q) = \int e^{iqx} dx$$

the expression for the scattered intensity in terms of the momentum transfer wave vectors is

$$\begin{aligned}\left(\frac{d\sigma}{d\Omega}\right) &= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{iQ_x x} e^{iQ_y y} dxdy \\ &= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \delta(Q_x)\delta(Q_y)\end{aligned}$$

$$I_{sc} = \left(\frac{I_0}{A_0}\right)\left(\frac{d\sigma}{d\Omega}\right)\frac{\Delta Q_x \Delta Q_y}{k^2 \sin\theta_2} \quad \longrightarrow \quad R(Q_z) = \frac{I_{sc}}{I_0} = \left(\frac{Q_c^2/8}{Q_z}\right)^2 \left(\frac{1}{Q_z/2}\right)^2 = \left(\frac{Q_c}{2Q_z}\right)^4$$

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

For a totally uncorrelated surface, $h(x, y)$ is independent from $h(x', y')$ and

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

For a totally uncorrelated surface, $h(x,y)$ is independent from $h(x',y')$ and

$$\left\langle [h(0,0)-h(x,y)]^2 \right\rangle = \langle h(0,0)\rangle^2 - 2\,\langle h(0,0)\rangle\,\langle h(x,y)\rangle + \langle h(x,y)\rangle^2$$

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

For a totally uncorrelated surface, $h(x,y)$ is independent from $h(x',y')$ and

$$\left\langle[h(0,0)-h(x,y)]^2\right\rangle = \langle h(0,0)\rangle^2 - 2\,\langle h(0,0)\rangle\,\langle h(x,y)\rangle + \langle h(x,y)\rangle^2 \;= 2\left\langle h^2\right\rangle$$

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

For a totally uncorrelated surface, $h(x,y)$ is independent from $h(x',y')$ and

$$\left\langle [h(0,0) - h(x,y)]^2 \right\rangle = \langle h(0,0)\rangle^2 - 2\,\langle h(0,0)\rangle\,\langle h(x,y)\rangle + \langle h(x,y)\rangle^2 = 2\left\langle h^2 \right\rangle$$

This quantity is related to the rms roughness, σ by $\sigma^2 = \left\langle h^2 \right\rangle$ and the cross-section is

$$\left(\frac{d\sigma}{d\Omega}\right) =$$

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

For a totally uncorrelated surface, $h(x,y)$ is independent from $h(x',y')$ and

$$\left\langle [h(0,0)-h(x,y)]^2 \right\rangle = \langle h(0,0)\rangle^2 - 2\langle h(0,0)\rangle \langle h(x,y)\rangle + \langle h(x,y)\rangle^2 = 2\left\langle h^2 \right\rangle$$

This quantity is related to the rms roughness, σ by $\sigma^2 = \left\langle h^2 \right\rangle$ and the cross-section is

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle h^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

For a totally uncorrelated surface, $h(x,y)$ is independent from $h(x',y')$ and

$$\left\langle [h(0,0)-h(x,y)]^2 \right\rangle = \langle h(0,0)\rangle^2 - 2\,\langle h(0,0)\rangle \langle h(x,y)\rangle + \langle h(x,y)\rangle^2 = 2\left\langle h^2 \right\rangle$$

This quantity is related to the rms roughness, σ by $\sigma^2 = \left\langle h^2 \right\rangle$ and the cross-section is

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle h^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int e^{iQ_x x} e^{iQ_y y} dxdy$$

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

For a totally uncorrelated surface, $h(x,y)$ is independent from $h(x',y')$ and

$$\left\langle [h(0,0) - h(x,y)]^2 \right\rangle = \langle h(0,0)\rangle^2 - 2\,\langle h(0,0)\rangle\,\langle h(x,y)\rangle + \langle h(x,y)\rangle^2 = 2\left\langle h^2\right\rangle$$

This quantity is related to the rms roughness, σ by $\sigma^2 = \left\langle h^2 \right\rangle$ and the cross-section is

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle h^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int e^{iQ_x x} e^{iQ_y y} dxdy$$

Which, apart from the term containing σ is simply the Fresnel cross-section for a flat surface

Uncorrelated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

For a totally uncorrelated surface, $h(x,y)$ is independent from $h(x',y')$ and

$$\left\langle [h(0,0)-h(x,y)]^2\right\rangle = \langle h(0,0)\rangle^2 - 2\langle h(0,0)\rangle\langle h(x,y)\rangle + \langle h(x,y)\rangle^2 = 2\left\langle h^2\right\rangle$$

This quantity is related to the rms roughness, σ by $\sigma^2 = \left\langle h^2\right\rangle$ and the cross-section is

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle h^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int e^{iQ_x x} e^{iQ_y y} dxdy$$

Which, apart from the term containing σ is simply the Fresnel cross-section for a flat surface

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-Q_z^2\sigma^2}$$

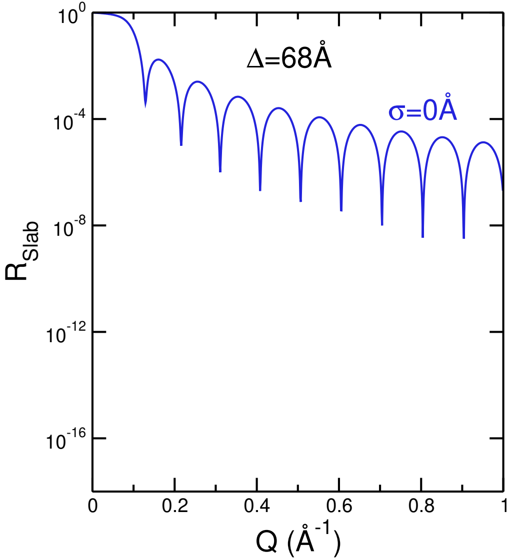
Surface roughness effect

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-Q_z^2\sigma^2}$$

Surface roughness effect

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-Q_z^2\sigma^2}$$

for a perfectly flat surface, we get the Fresnel reflectivity derived for a thin slab

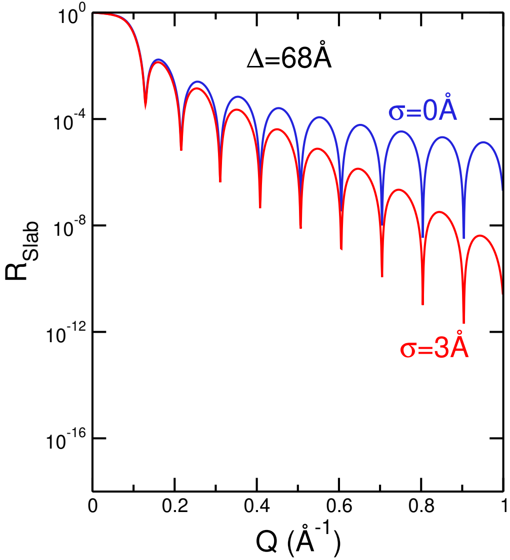


Surface roughness effect

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-Q_z^2\sigma^2}$$

for a perfectly flat surface, we get the Fresnel reflectivity derived for a thin slab

for an uncorrelated rough surface, the reflectivity is reduced by an exponential factor controlled by the rms surface roughness σ



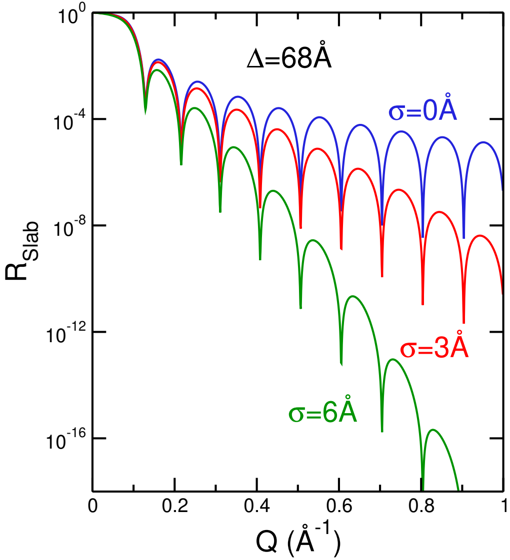
Surface roughness effect

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-Q_z^2\sigma^2}$$

for a perfectly flat surface, we get the Fresnel reflectivity derived for a thin slab

for an uncorrelated rough surface, the reflectivity is reduced by an exponential factor controlled by the rms surface roughness σ

this leads to a rapid drop in reflectivity as the surface roughness increases



Correlated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Correlated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Assume that height fluctuations are isotropically correlated in the x-y plane. Therefore,

$$g(x,y) = g(r) = g(\sqrt{x^2+y^2})$$

Correlated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Assume that height fluctuations are isotropically correlated in the x-y plane. Therefore,

$$g(x,y) = g(r) = g(\sqrt{x^2+y^2})$$

In the limit that the correlations are unbounded as $r \to \infty$, $g(x,y)$ is given by $g(x,y) = \mathcal{A}r^{2h}$

Correlated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2 \right\rangle /2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Assume that height fluctuations are isotropically correlated in the x-y plane. Therefore,

$$g(x,y) = g(r) = g(\sqrt{x^2+y^2})$$

In the limit that the correlations are unbounded as $r \to \infty$, $g(x,y)$ is given by $g(x,y) = \mathcal{A}r^{2h}$ where h is a fractal parameter which defines the shape of the surface.

Correlated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Assume that height fluctuations are isotropically correlated in the x-y plane. Therefore,

$$g(x,y) = g(r) = g(\sqrt{x^2+y^2})$$

In the limit that the correlations are unbounded as $r \to \infty$, $g(x,y)$ is given by $g(x,y) = \mathcal{A}r^{2h}$ where h is a fractal parameter which defines the shape of the surface.

jagged surface for $h \ll 1$

Correlated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Assume that height fluctuations are isotropically correlated in the x-y plane. Therefore,

$$g(x,y) = g(r) = g(\sqrt{x^2+y^2})$$

In the limit that the correlations are unbounded as $r \to \infty$, $g(x,y)$ is given by $g(x,y) = \mathcal{A}r^{2h}$ where h is a fractal parameter which defines the shape of the surface.

jagged surface for $h \ll 1$ smoother surface for $h \to 1$

Correlated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\langle[h(0,0)-h(x,y)]^2\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Assume that height fluctuations are isotropically correlated in the x-y plane. Therefore,

$$g(x,y) = g(r) = g(\sqrt{x^2+y^2})$$

In the limit that the correlations are unbounded as $r \to \infty$, $g(x,y)$ is given by $g(x,y) = \mathcal{A}r^{2h}$ where h is a fractal parameter which defines the shape of the surface.

jagged surface for $h \ll 1$ smoother surface for $h \to 1$

If the resolution in the y direction is very broad (typical for a synchrotron), we can eliminate the y-integral and have

Correlated surfaces

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Assume that height fluctuations are isotropically correlated in the x-y plane. Therefore,

$$g(x,y) = g(r) = g(\sqrt{x^2+y^2})$$

In the limit that the correlations are unbounded as $r \to \infty$, $g(x,y)$ is given by $g(x,y) = \mathcal{A}r^{2h}$ where h is a fractal parameter which defines the shape of the surface.

jagged surface for $h \ll 1$ smoother surface for $h \to 1$

If the resolution in the y direction is very broad (typical for a synchrotron), we can eliminate the y-integral and have

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-\mathcal{A}Q_z^2|x|^{2h}/2} \cos(Q_x x) dx$$

Unbounded correlations - limiting cases

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-\mathcal{A}Q_z^2|x|^{2h}/2} \cos(Q_x x)dx$$

Unbounded correlations - limiting cases

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-\mathcal{A}Q_z^2|x|^{2h}/2} \cos(Q_x x)dx$$

This integral can be evaluated in closed form for two special cases, both having a broad diffuse scattering and no specular peak.

Unbounded correlations - limiting cases

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-\mathcal{A}Q_z^2|x|^{2h}/2} \cos(Q_x x) dx$$

This integral can be evaluated in closed form for two special cases, both having a broad diffuse scattering and no specular peak.

$h = 1/2$:

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{A_0 r_0^2 \rho^2}{2\sin\theta_1}\right) \frac{\mathcal{A}}{(Q_x^2 + (\mathcal{A}/2)^2 Q_z^4)}$$

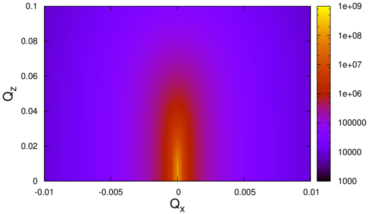
Unbounded correlations - limiting cases

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-\mathcal{A}Q_z^2|x|^{2h}/2} \cos(Q_x x)dx$$

This integral can be evaluated in closed form for two special cases, both having a broad diffuse scattering and no specular peak.

$h = 1/2$: Lorentzian with half-width $\mathcal{A}Q_z^2/2$

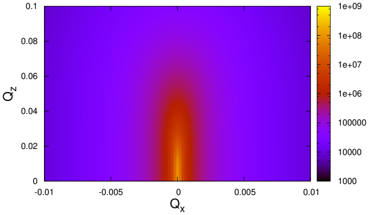
$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{A_0 r_0^2 \rho^2}{2\sin\theta_1}\right) \frac{\mathcal{A}}{(Q_x^2 + (\mathcal{A}/2)^2 Q_z^4)}$$



Unbounded correlations - limiting cases

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-\mathcal{A}Q_z^2|x|^{2h}/2} \cos(Q_x x)dx$$

This integral can be evaluated in closed form for two special cases, both having a broad diffuse scattering and no specular peak.



$h = 1/2$: Lorentzian with half-width $\mathcal{A}Q_z^2/2$

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{A_0 r_0^2 \rho^2}{2\sin\theta_1}\right) \frac{\mathcal{A}}{(Q_x^2 + (\mathcal{A}/2)^2 Q_z^4)}$$

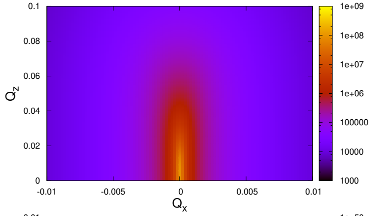
$h = 1$:

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{2\sqrt{\pi}A_0 r_0^2 \rho^2}{2\sin\theta_1}\right) \frac{1}{Q_z^4} e^{-\frac{1}{2}\left(\frac{Q_x^2}{\mathcal{A}Q_z^2}\right)}$$

Unbounded correlations - limiting cases

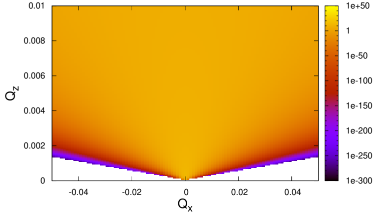
$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1}\int e^{-\mathcal{A}Q_z^2|x|^{2h}/2}\cos(Q_x x)dx$$

This integral can be evaluated in closed form for two special cases, both having a broad diffuse scattering and no specular peak.



$h = 1/2$: Lorentzian with half-width $\mathcal{A}Q_z^2/2$

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{A_0 r_0^2\rho^2}{2\sin\theta_1}\right)\frac{\mathcal{A}}{(Q_x^2 + (\mathcal{A}/2)^2 Q_z^4)}$$



$h = 1$: Gaussian with variance $\mathcal{A}Q_z^2$

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{2\sqrt{\pi}A_0 r_0^2\rho^2}{2\sin\theta_1}\right)\frac{1}{Q_z^4}e^{-\frac{1}{2}\left(\frac{Q_x^2}{\mathcal{A}Q_z^2}\right)}$$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

If the correlations remain bounded as $r \to \infty$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

If the correlations remain bounded as $r \to \infty$

$$g(x,y) = 2\left\langle h^2\right\rangle - 2\left\langle h(0,0)h(x.y)\right\rangle = 2\sigma^2 - 2C(x,y),$$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

If the correlations remain bounded as $r \to \infty$

$$g(x,y) = 2\left\langle h^2\right\rangle - 2\left\langle h(0,0)h(x.y)\right\rangle = 2\sigma^2 - 2C(x,y), \quad C(x,y) = \sigma^2 e^{-(r/\xi)^{2h}}$$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

If the correlations remain bounded as $r \to \infty$

$$g(x,y) = 2\left\langle h^2\right\rangle - 2\left\langle h(0,0)h(x.y)\right\rangle = 2\sigma^2 - 2C(x,y), \quad C(x,y) = \sigma^2 e^{-(r/\xi)^{2h}}$$

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int e^{Q_z^2 C(x,y)} e^{iQ_x x} e^{iQ_y y} dxdy$$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

If the correlations remain bounded as $r \to \infty$

$$g(x,y) = 2\left\langle h^2\right\rangle - 2\left\langle h(0,0)h(x.y)\right\rangle = 2\sigma^2 - 2C(x,y), \quad C(x,y) = \sigma^2 e^{-(r/\xi)^{2h}}$$

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int e^{Q_z^2 C(x,y)} e^{iQ_x x} e^{iQ_y y} dxdy$$

$$= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int \left[e^{Q_z^2 C(x,y)} - 1 + 1\right] e^{iQ_x x} e^{iQ_y y} dxdy$$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1}\int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

If the correlations remain bounded as $r \to \infty$

$$g(x,y) = 2\left\langle h^2\right\rangle - 2\left\langle h(0,0)h(x.y)\right\rangle = 2\sigma^2 - 2C(x,y), \quad C(x,y) = \sigma^2 e^{-(r/\xi)^{2h}}$$

$$\begin{aligned}
\left(\frac{d\sigma}{d\Omega}\right) &= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2}\int e^{Q_z^2 C(x,y)} e^{iQ_x x} e^{iQ_y y} dxdy \\
&= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2}\int \left[e^{Q_z^2 C(x,y)} - 1 + 1\right] e^{iQ_x x} e^{iQ_y y} dxdy
\end{aligned}$$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle [h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

If the correlations remain bounded as $r \to \infty$

$$g(x,y) = 2\left\langle h^2\right\rangle - 2\left\langle h(0,0)h(x.y)\right\rangle = 2\sigma^2 - 2C(x,y), \quad C(x,y) = \sigma^2 e^{-(r/\xi)^{2h}}$$

$$\begin{aligned}
\left(\frac{d\sigma}{d\Omega}\right) &= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int e^{Q_z^2 C(x,y)} e^{iQ_x x} e^{iQ_y y} dxdy \\
&= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int \left[e^{Q_z^2 C(x,y)} - 1 + 1\right] e^{iQ_x x} e^{iQ_y y} dxdy \\
&= \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-Q_z^2\sigma^2} + \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} F_{diffuse}(\vec{Q})
\end{aligned}$$

Bounded correlations

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} \int e^{-Q_z^2\left\langle[h(0,0)-h(x,y)]^2\right\rangle/2} e^{iQ_x x} e^{iQ_y y} dxdy$$

If the correlations remain bounded as $r \to \infty$

$$g(x,y) = 2\left\langle h^2\right\rangle - 2\left\langle h(0,0)h(x.y)\right\rangle = 2\sigma^2 - 2C(x,y), \quad C(x,y) = \sigma^2 e^{-(r/\xi)^{2h}}$$

$$\begin{aligned}
\left(\frac{d\sigma}{d\Omega}\right) &= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int e^{Q_z^2 C(x,y)} e^{iQ_x x} e^{iQ_y y} dxdy \\
&= \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} \int \left[e^{Q_z^2 C(x,y)} - 1 + 1\right] e^{iQ_x x} e^{iQ_y y} dxdy \\
&= \left(\frac{d\sigma}{d\Omega}\right)_{Fresnel} e^{-Q_z^2\sigma^2} + \left(\frac{r_0\rho}{Q_z}\right)^2 \frac{A_0}{\sin\theta_1} e^{-Q_z^2\sigma^2} F_{diffuse}(\vec{Q})
\end{aligned}$$

And the scattering exhibits both a specular peak, reduced by uncorrelated roughness, and diffuse scattering from the correlated portion of the surface