# The problem of coherence from different sights

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### 1. MAXWELL'S EQUATIONS

The notion of coherence arises each time when one needs to summarize different wave fields of different nature. As it is well known, the X-rays being electromagnetic waves are the solutions of the set of Maxwell's equations for the amplitudes of electric field  $\mathbf{E}(\mathbf{r}, t)$ and magnetic field  $\mathbf{H}(\mathbf{r}, t)$ . Inside a matter without sources of the radiation the equation may be written as follow:

$$-\operatorname{rot} \mathbf{E} = \frac{1}{c} \frac{\partial \mathbf{H}}{\partial t}, \quad \operatorname{rot} \mathbf{H} = \frac{1}{c} \left( \frac{\partial \mathbf{E}}{\partial t} + 4\pi \mathbf{j} \right),$$
$$\operatorname{div} \mathbf{E} = 4\pi\rho, \qquad \operatorname{div} \mathbf{H} = 0, \tag{1}$$

where c is a light velocity,  $\mathbf{j}(\mathbf{r}, t)$  is the induced current density and  $\rho$  is the induced charge density. Since the electric and magnetic fields relate closely to each other one can consider the equation only for electric field  $\mathbf{E}(\mathbf{r}, t)$ .

Such an equation is obtained making a use of the relation

$$rot rot \mathbf{E} = grad \operatorname{div} \mathbf{E} - grad^2 \mathbf{E}$$
(2)

and may be written in the form:

$$\left(\operatorname{grad}^{2}-\frac{1}{c^{2}}\frac{\partial^{2}}{\partial t^{2}}\right)\mathbf{E} = \frac{4\pi}{c^{2}}\frac{\partial\mathbf{j}}{\partial t} + 4\pi\operatorname{grad}\rho \tag{3}$$

where  $\mathbf{j}(\mathbf{r}, t)$  is, in general, a linear function of  $\mathbf{E}(\mathbf{r}, t)$ . The high energy X-Rays have:

 $E = \hbar \omega$ , an energy of photons from 5 to 50 keV,

 $\lambda = hc/E = 12.397/E$  Å, a wavelength where E is in keV.

In case of elastic scattering it is enough to keep the approximation when

$$\mathbf{j}(\mathbf{r},t) = \int dt' \sigma(\mathbf{r},t-t') \mathbf{E}(\mathbf{r},t')$$
(4)

for many simple samples, where  $\sigma(\mathbf{r}, t)$  is the inhomogeneous in space scalar conductivity of the matter. As for the induced charge density  $\rho$ , it influences the field weakly and, usually, it is neglected.

The solution of Maxwell's equation inside the volume of space without radiators is always the coherent wave. It is convenient to represent the electric field  $\mathbf{E}(\mathbf{r}, t)$  as the complex value having the modulus and the phase  $\mathbf{E}(\mathbf{r}, t) = \mathbf{A}(\mathbf{r}, t) \exp(i\varphi(\mathbf{r}, t))$ . Both the modulus  $\mathbf{A}(\mathbf{r}, t)$  and the phase  $\varphi(\mathbf{r}, t)$  of the solution are continuous in space and in time values. They are defined to a great extent by the boundary conditions, i.e. the known values at the boundary of the volume under consideration (usually the boundaries of the matter, for example, the crystalline plate). It is known that the energy density of the radiation averaged over the period of oscillation in time is proportional to the square modulus  $|\mathbf{A}(\mathbf{r}, t)|^2$  of the wave field. Just this value is measured by detector.

The wave field at the boundary of the volume under consideration is defined by the source of radiation. The coherent wave field may be defined as the solution of the Maxwell's equation with one photon. However, the problem of coherence arises owing to the fact that the real wave field is produced by many sources in time and in space which radiate together. Usually, different photons have no correlation in their position in space as well as in time moments when they begin to radiate. It is often convenientin in usual optics, even if rather artificial, to divide coherence effects into two classifications, temporal and spatial. The former relates directly to the finite bandwidth of the source, the latter to its finite extent in space. In X-ray crystal optics we may introduce additionally the notion of angular coherence.

### 2. TEMPORAL COHERENCE

Let us consider, first of all, the origin of the temporal coherence in case where the source is the X-ray tube. Below we will follow the approach given in:

• A. M. Afanasev, V. G. Kohn, Sov. Phys. Crystallogr., 1977, vol. 22, No. 3., p.355. In this case the radiators are the atoms of the anode which radiate characteristic fluorescent quanta. Let the atom at the moment  $t_0$  radiate the wave with the middle frequency  $\omega_0$  and the intensity of this wave decreases essentially for the time interval  $\tau$ , then this field may be represented as follows

$$E(t) = \theta(t - t_0) \exp(i\omega_0 t) f\left[(t - t_0)/2\tau\right]$$
(5)

We can expand the time dependence over the monochromatic waves as the Fourier integral

$$E(t,t_0) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \exp(i\omega t) F(\omega - \omega_0, t_0)$$
(6)

where

$$F(\omega, t_0) = \exp(-i\omega t_0) \int_0^\infty dt \, \exp(-i\omega t) f\left(\frac{t}{2\tau}\right) \tag{7}$$

The function f(t) is exponential, for example, in case of isolated transition of 'free' atom, therefore the function  $F(\omega, t_0)$  is defined as follows

$$f(t) = \exp(-t), \qquad F(\omega) = \frac{\exp(-i\omega t_0)}{i\omega + 1/2\tau}$$
(8)

The intensity of such waves in time (at left) and frequency (at right) domains are shown in Fig.1. For many photons these are described by the formulas

$$I(t) = \sum_{k} \exp\left(-\frac{t-t_k}{\tau}\right) \theta(t-t_k), \qquad I(\omega) = \frac{1}{(2\omega\tau)^2 + 1}.$$
(9)

where  $\theta(t - t_k)$  is the teta-function which equals zero for negative arguments.

Each monochromatic component in the superposition of Eq.(6) is a coherent wave completely. As a result of subsequent elastic scattering (without a change of the frequency) the wave can be divided on two parts which will pass by different trajectories, will change the amplitude and will obtain the phase difference. Afterwards these can go at the same place in space once again. This process takes place in each interferometric device and it can be represented mathematically as

$$\exp(i\omega t) \to \exp(i\omega t) \{ R_1(\omega) + R_2(\omega) \exp[i\varphi(\omega)] \}$$
(10)

The detector measures the intensity of X-rays. Let us substitute the righthand part of the Eq.(10) instead of the lefthand part to the Eq.(6) and calculate the square modulus. As a result we obtain



FIG. 1. The intensity of resonant photons in time and frequency domains

$$I(t,t_0) = |E(t)|^2 = \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \frac{\exp[i(\omega-\omega')(t-t_0)]}{[i(\omega-\omega_0)+1/2\tau][i(\omega_0-\omega')+1/2\tau]} \times \{R_1(\omega)+R_2(\omega)\exp[i\varphi(\omega)]\}\{R_1^*(\omega')+R_2^*(\omega')\exp[-i\varphi(\omega')]\}$$
(11)

Now we have to take into account that it is impossible to measure the result of interference produced by one photon for two reasons.

(a) the intensity of one photon is very small,

(b) it is very difficult to distinguish the radiation between different photons which are radiated at very close time moments.

In the real experiment with high energy X-rays the time of observation is much longer than the duration of each photon and a huge number of photons are measured simultaneously. Therefore we can average the intensity over  $t_0$  in infinite limits. This prosedure leads to a formula

$$I = \int dt_0 I(t, t_0) = \int \frac{d\omega}{2\pi} \frac{|R_1(\omega)|^2 + |R_2(\omega)|^2 + 2\operatorname{Re}\left(R_1^*(\omega)R_2(\omega)\exp[i\varphi(\omega)]\right)}{[(\omega - \omega_0)^2 + 1/4\tau^2]}$$
(12)

Such a simple calculation, performed above, allows us to find a general recipe how to take into account the temporal coherence of the source.

(a) The photon arised in each act of radiation must be represented as the Fourier integral over frequency. The full width at half of maximum (FWHM) of the Fourier spectrum just describes the bandwidth of the radiation.

(b) The intensity of radiation which is measured by detector may be obtain from the two assumptions:

1) each monochromatic wave having the frequency inside the bandwidth is coherent completely,

2) different frequencies inside the bandwidth of the source are completely incoherent. Let the path difference between two trajectories be l. Then the phase difference for separate frequency will be  $\varphi(\omega) = \omega l/c$ . However, for finite bandwidth of the radiation  $\Delta \omega$  the phase different will have different values inside the interval  $\Delta \varphi = \Delta \omega l/c$ . The integral (12) cannot destroy the interference term in the intensity when the phase difference  $\Delta \varphi$  corresponding to the essential area of the integration in Eq.(12)  $\Delta \omega$  is less than  $2\pi$ , namely, when  $l \ll l_{lc} = 2\pi c/\Delta \omega$ .

The value  $l_{lc}$  is called the *longitudinal coherence length*.

Taking into account the relation  $\omega/c = 2\pi/\lambda$  where  $\lambda$  is a wavelength of the radiation and the fact that  $\Delta \omega \ll \omega$  we can write the longitudinal coherence length in terms of wavelength as

$$l_{lc} = \lambda^2 / \Delta \lambda. \tag{13}$$

This property is illustrated by the Fig.2. In the figure  $\lambda = 1$ ,  $\Delta \lambda = 0.05$ . One can see that at the length  $\lambda^2/2\Delta\lambda = 10$  the phase difference equals  $\pi$ . When the elastic scattering of X-rays by the sample is frequency insensitive the value  $\Delta \omega/\omega = \Delta \lambda/\lambda =$  $1/\omega\tau$  is determined by the life time of the fluorescent quanta. Usually this value is about  $1/\omega\tau \approx 2 \cdot 10^{-4}$ . In this case the longitudinal coherence length can be estimated as  $l_{lc} = 5 \cdot 10^3 \lambda = 0.5 \ \mu \text{m}$  for the typical wavelength value  $\lambda = 1\text{Å}$ . This is rather small value which shows that the initial X-rays from the source are coherent only partially and at rather small level.

However, if the elastic scattering in the samples becomes frequency sensitive, namely, the frequency dependence of the amplitude  $R_1(\omega)$  or  $R_2(\omega)$  has a sharp peak inside the bandwith of the source, then the coherence length may be rather increased. Such a procedure is called a monochromatization while the special devices which do it are called monochromators. The general way to reduce the effective bandwidth of the radiation is a usage of Bragg diffraction of X-rays in single crystals.

The problem becomes much more essential in using the synchrotron radiation which has in case of bending magnet a huge bandwidth having all frequencies of electromagnetic spectrum from visible light to very hard X-rays (the energy of photons from 1 eV to 100 keV for SR source of third generation). One of the best result of filtration of X-rays of 14.41 keV (the energy of nuclear resonance in <sup>57</sup>Fe which shows the Mössbauer effect) is achived by means of Bragg diffraction monochromator with (579) asymmetric reflections in Si and (333) symmetric reflection in Ge to conserve the initial direction of beam, the result was reported in:

- A. I. Chumakov, R. Rüffer, A. Q. R. Baron, J. Metge, H. Grünsteudel,
- H. Grünsteudel, X-ray optics for nuclear inelastic scattering.
- Proc. SPIE, 1997, vol. 3151, p.262-270.

The energy bandwidth was as narrow as 1 meV with  $\Delta\omega/\omega \approx 10^{-7}$  with the coherence length  $l_{lc} = 1.2$  mm. Usually the monochromatization up to  $\Delta\omega/\omega \approx 10^{-5}$  is enough for many experiments with X-ray diffraction.

As examples of the interference devices where the longitudinal coherence length is essential to obtain the interference pattern of high quality one may consider:

(1) Fabri-Perot interferometer where different rays interfere after reflections by semitransparent mirrors. Let d be a distance between the mirrors, then the direct wave and



FIG. 2. Two waves with slightly different frequencies. The phase difference equals  $\pi$  at the length  $\lambda^2/2\Delta\lambda = 10$  with  $\lambda = 1$ ,  $\Delta\lambda = 0.05$ 

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double reflected wave will have the phase difference  $(2\pi/\lambda)2d = (4\pi/hc)Ed$  where E is a photon energy. The transmitted radiation will have maximums when this difference equals  $2\pi n$ . Therefore in energy scale the maximums will appear through the distance  $\Delta E = hc/2d$  which depends only on the distance between mirrors. In coherent (monochromatic) radiation the peaks will be very sharp. However, if the bandwidth of the radiation is comparable with the distance between peaks these become smoothed in a great extent.

(2) Fresnel zone plate where the focusing becomes good only if the path different for different zones exceeds the longitudinal coherence length. For far zones where this condition is not met the interference disappears and the aperture of the lens becomes smaller.

(3) Bragg-Fresnel lens where the Bragg diffraction plays the role of rays reflector with changing of phase in different Fresnel zones. The lens can work with white beam because the Bragg diffraction plays the role of monochromator simultaneously with making a phase shift .

## 3. SPATIAL COHERENCE. VIEW OF THE MUTUAL COHERENCE THEORY.

Spatial coherence relates to a possibility of observing the interference fringes in space. The radiators of X-rays are atoms or electrons. These have very snall size and may be treated as point sources. Each point of the macroscopic source produces the independent coherent wave which is in fact as a spherical wave. The spherical wave is a real coherent wave in space in case where it is a monochromatic wave in time. It is a solution of the Maxwell's equation

$$(\operatorname{grad}^2 + K^2)E(\mathbf{r},\omega) = 4\pi\delta(\mathbf{r}), \qquad K = \frac{\omega}{c}$$
 (14)

Making the Fourier transformation

$$E(\mathbf{r},\omega) = \int \frac{d\mathbf{k}}{(2\pi)^3} \exp(i\mathbf{k}\mathbf{r}) E(\mathbf{k},\omega), \qquad \delta(\mathbf{k}) = 1$$
(15)

we find easily

$$E(\mathbf{k},\omega) = \frac{4\pi}{(k^2 - K^2)}.$$
(16)

Now substituting the expression in the Fourier integral and making the calculations in spherical coordinates we obtain

$$E(r,\omega) = \frac{1}{\pi i r} \int_{-\infty}^{\infty} dk \frac{k}{(k^2 - K^2)} \exp(ikr) = \frac{\exp(iKr)}{r}$$
(17)

To understand the origin of spatial coherence let us consider a simple experimental setup of in-line holography (see Fig.3) which is used for recent years in experiments on phase contrast imaging of transparent objects. Since the distance from the source to the object is rather long we can select the optical axis as the z-axis of cartesian coordinate system and use the **small angle approxima**tion, when the transverse coordinates x and y are much shorter compared to z coordinate. In this section we will suppose the monochromatic wave with the wavelength  $\lambda$  and wave number  $K = 2\pi/\lambda$ . In the plane z = const. we have

$$E(x, y, z) = E_S(x - x_s, y - y_s, z - z_s)$$
(18)

where  $x_s$ ,  $y_s$  and  $z_s$  are the coordinates of the point on the source (for example, the atom on the anode of X-ray tube or electron in the storage ring) and

$$E_S(x, y, z) = \frac{1}{r} \exp(iKr) \approx \frac{1}{z} \exp\left(iKz + iK\frac{x^2 + y^2}{2z}\right),\tag{19}$$

where

$$r = \left(x^2 + y^2 + z^2\right)^{1/2} \tag{20}$$

The formula (19) describes the wave field inside the empty space between the source and the object. When passing through the thin object the wave field can change its amplitude and phase locally. Let us consider the object which is homogeneous along the y-axis. It allows us to approximate the wave field just after the object as

$$E(x, y, z_o) = E_S(x - x_s, y - y_s, z_o - z_s)F(x),$$
  

$$F(x) = \exp\left(i\varphi'(x) - \varphi''(x)\right)$$
(21)

where we introduced the complex phase shift  $\varphi = \varphi' + i\varphi''$ 

The value of the phase shift produced by the object can be calculated under the assumption that the object is very small compared to the long distance from the source



FIG. 3. Experimental set-up of in-line holography

to the object and the rays which go through the object are approximately parallel. This allows us to consider the equation for the envelope of the wave in the form

$$\frac{dE(z)}{dz} = i\frac{2\pi}{\lambda}\chi E(z) \tag{22}$$

where E(z) = 1 at the incoming boundary of the object. It is easy to understand that if the object is homogeneous with the constant value of complex susceptibility  $\chi$  then the solution on the outgoing boundary equals

$$E(x) = \exp(i\varphi(x)), \qquad \varphi(x) = \frac{2\pi}{\lambda}\chi t(x)$$
 (23)

where t(x) is a variable thickness of the object along the ray at x-coordinate. When the object has a complicated structure the phase shift may be more complex

$$\varphi(x) = \frac{2\pi}{\lambda} \int_0^{t(x)} \chi(x, z) dz$$
(24)

To obtain the wave field of the radiation at the detector plane we need to solve the Maxwell's equation in empty space with the boundary condition (21). The solution may be written by means of using the Fresnel-Kirchhoff integral relation

$$E(x_d, y_d, z_d) = \int dx \int dy P_t(x_d - x, y_d - y, z_d - z_o) E_S(x - x_s, y - y_s, z_o - z_s) F(x)$$
(25)

where  $P_t(x, y, z)$  is the propagator of x, y-distribution of the field along the z-axis. The exact propagator is proportional to the spherical wave once again. In a frame of small angle approximation it can be expressed separately for x and y axes and x-part looks as follows

$$P_t(x, y, z) = \exp(iKz)P(x, z)P(y, z), \quad P(x, z) = \frac{1}{\sqrt{i\lambda z}}\exp\left(iK\frac{x^2}{2z}\right)$$
(26)

Since the object changes the wave field only in the x-direction we can calculate the integral over y directly. The result looks as a convolution of two propagators which equals the propagator once again but on the total distance

$$\sqrt{i\lambda} \int dy P(y_d - y, z_{do}) P(y - y_s, z_{os}) = \sqrt{i\lambda} P(y_d - y_s, z_{ds})$$
(27)

where  $z_{do} = z_d - z_o$  is the object-to-detector distance,  $z_{os} = z_o - z_s$  is the source-toobject distance,  $z_{ds} = z_{do} + z_{os} = z_d - z_s$  is the source-to-detector distance. This result is well known and it has a clear physical sense from the point of view of Fresnel-Kirchhoff principle. Thus we obtain the expression

$$E(x_d, y_d, z_d) = \exp(iKz_{ds})S(y_d - y_s, z_{ds}) \int dx P(x_d - x, z_{do})F(x)S(x - x_s, z_{os})$$
(28)

where

$$S(x,z) = \sqrt{i\lambda}P(x,z) = \frac{1}{\sqrt{z}}\exp\left(iK\frac{x^2}{2z}\right)$$
(29)

is a one-dimensional part of the spherical wave. The position sensitive detector can measure the intensity of radiation at each point  $x_d$  therefore we are interested in the value

$$J(x_d, x_s) = |E(x_d, y_d, z_d)|^2 = \frac{1}{z_{ds}} \int dx \int dx' F(x) F^*(x') \times P(x_d - x, z_{do}) P^*(x_d - x', z_{do}) S(x - x_s, z_{os}) S^*(x' - x_s, z_{os})$$
(30)

At this point of our analysis we must remember once again that each point of the source is an individual photon producer and different photons have no a correlation in their phases. Therefore we need to integrate just the intensity over all points of the source rather than the amplitude. The signal which will be really registered by detector equals

$$I(x_d) = \int dx_s J(x_d, x_s) B(x_s)$$
(31)

where B(x) is the function which describes the brightness of different points on the source. In a description of the synchrotron radiation source this function is accepted, usually, as the Gaussian with a random mean value (rms)  $\sigma$ , namely,

$$B(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right).$$
(32)

The source size in this case can be estimated as  $w_s = \sigma \sqrt{8}$ .

Substituting Eq.(30) to Eq.(31) we need to integrate only spherical waves from the source to object which leads to the function

$$\alpha(x, x') = \int dx_s B(x_s) S(x - x_s, z_{os}) S^*(x' - x_s, z_{os})$$
(33)

The integral can be calculated analytically with a help of the table integral

$$\int_{-\infty}^{\infty} dx \exp(-i\beta x + i\gamma x^2) = \left(\frac{i\pi}{\gamma}\right)^{1/2} \exp\left(-i\frac{\beta^2}{4\gamma}\right)$$
(34)

where  $\beta$  and  $\gamma$  are arbitrary complex values. As a result, we obtain

$$\alpha(x, x') = \frac{1}{z_{os}} \exp\left(iK \frac{[x^2 - x'^2]}{2z_{os}}\right) \mu(x - x')$$
(35)

where

$$\mu(x) = \exp\left(-\frac{x^2}{2l_{tc}^2}\right) \tag{36}$$

and

$$l_{tc} = \frac{\lambda z_{os}}{2\pi\sigma} = \frac{\sqrt{2}}{\pi} \frac{\lambda z_{os}}{w_s}.$$
(37)

Now we can calculate the total expression

$$I(x_d) = \frac{1}{\lambda z_{ds} z_{do} z_{os}} \int dx \int dx' \exp\left(\frac{2\pi i}{\lambda z_{do}} x_d[x'-x]\right) \times \\ \times \exp\left(\frac{i\pi z_{ds}}{\lambda z_{do} z_{os}} [x^2 - x'^2]\right) F(x) F^*(x') \mu(x - x')$$
(38)

Here the source properties are represented by the function  $\mu(x - x')$  which is called the **mutual coherence function** in the theory of partial coherence. When source size tends to zero this function equals unity. In general case it describes the possible correlation between two points in the object plane.

Let us consider a simple example of the object: a fully opaque screen with two narrow slits at the position  $x_1 = -a/2$  and  $x_2 = a/2$ . having a small width d (Fig.4) In this case the function F(x) can be approximated as  $F(x) = d[\delta(x + a/2) + \delta(x - a/2)]$  where  $\delta(x)$ is a Dirac delta-function. The intensity distribution at the detector plane is described by simple expression

$$I(x_d) = \frac{2d^2}{\lambda z_{ds} z_{do} z_{os}} \left[ 1 + \mu(a) \cos\left(2\pi \frac{ax_d}{\lambda z_{do}}\right) \right].$$
(39)

It shows that the interference pattern consists of the intensity oscillations (fringes) with the constant period  $p = \lambda z_{do}/a$ . The quality of the fringes produced by an interferometric system can be described quantitatively using the visibility V, which, as first formulated by Michelson, is given by

$$V(x) = \frac{I_{\max}(x) - I_{\min}(x)}{I_{\max}(x) + I_{\min}(x)}$$
(40)

where  $I_{\max}(x)$  and  $I_{\min}(x)$  are proportional to the maximum and minimum value of the irradiance in a vicinity of the point x. The substitution of Eq.(39) to the Eq.(40) gives



FIG. 4. The experiments with two slits separated by distance a

us that  $V(x) = \text{const} = \mu(a)$ . Now we see that the parameter  $l_{tc}$  has a physical meaning of the distance between the slits giving the value 0.6 for the fringes visibility. Usually it is called the *transverse coherent length*.

### 4. SPATIAL COHERENCE. A MAGNIFICATION FACTOR.

The approach presented above follows the corresponding chapters of the books on optics. However, in practical calculations of the complicated objects it is inconvenient to calculate a double-dimensional integral in Eq.(38) with a use of the mutual coherence function of Eq.(36). Instead of this one may calculate directly the integral of Eq.(28) for all source coordinates and then apply the Eq.(31) for averaging the intensity. In doing this one may find the useful property of the integral of Eq.(28). Namely, the kernel of the integral, i.e. the function

$$P(x_d - x, z_{do})S(x - x_s, z_{os}) = S(x_d - x_s, z_{ds})G(x, x_{ds}, z_{do}, z_{os})$$
(41)

where

$$G(x, x_{ds}, z_{do}, z_{os}) = \left(\frac{z_{ds}}{i\lambda z_{do} z_{os}}\right)^{1/2} \exp\left(-\frac{i\pi}{\lambda z_{do}} \left[2xx_{ds} - \frac{z_{ds}}{z_{os}}x^2 - \frac{z_{os}}{z_{ds}}x_{ds}^2\right]\right)$$
(42)

and

$$x_{ds} = x_d + x_s \frac{z_{do}}{z_{os}} \tag{43}$$

This property allows us to write the relative wave field as follows

$$\frac{E(x_d, y_d, z_d)}{E_S(x_d, y_d, z_d)} = \int dx \, G(x, x_{ds}, z_{do}, z_{os}) F(x)$$
(44)

Now there is no necessity to calculate the total diffraction pattern for each point of source because for each point of source the diffraction pattern is the same but it becomes only to be shifted on the definite distance. According to the Eq.(43) the shift of the source point from the origin on  $x_s$  leads to a shift of the diffraction pattern as a whole on the distance  $x_s z_{do}/z_{os}$ . Therefore we can calculate the interference fringes only for the middle point of the source and afterwards we can average the resulting intensity over the area having a width  $w'_s = w_s z_{do}/z_{os}$  where  $w_s$  is the source size (see Fig. 1.3). It is obvious that the fringes with the distance between them  $p_f$  less than  $w'_s$  will disappear or become much less visible. On the other hand, the fringes with the distance  $p_f \gg w'_s$  will be practically undisturbed by the source size.

This simple analysis allows us to formulate the main recipe for increasing the spatial coherence. Together with decreasing the source size one need to increase the distance source-to-object compared to the distance object-to-detector. It is of interest to estimate the characteristics of the ESRF (European Synchrotron Radiation Facility) beam lines. The source size of the undulator  $w_s \approx 30 \ \mu\text{m}$ , the source-to-object distance  $z_{os} \approx 40 \ \text{m}$ . With these parameters we calculate that for the object-to-detector distance  $z_{do} = 1 \ \text{m}$ , the fringes having the distance  $p_f > 1 \ \mu\text{m}$  between them can be distinguished.

### 5. SPATIAL COHERENCE. VIEW OF THE ANGULAR ANALYSIS

The monochromatic spherical wave presents by itself one kind of the coherent wave field. Its characteristics are the frequency and the point of origin. However, just another coherent wave field is widely considered in the physics of high energy particles, in general, and in the physics of high energy X-rays optics, in particular. This is a plane monochromatic wave. Its characteristics are the frequency and the direction of movement while the location in space is absent. Nevertheless, since the full set of plane waves forms a complete basis, each space function can be expanded over the plane waves, in other words, it can be expressed as a superposition of plane waves. For example, the spherical wave with the origin at  $\mathbf{r} = 0$  in the half-space  $(\mathbf{s}_0 \cdot \mathbf{r}) > 0$  has a well known representation

$$E_S(x,y,z) = \frac{\exp(iKr)}{r} = 2\pi i \int \frac{d\mathbf{q}}{(2\pi)^2} \frac{\exp\left(i\mathbf{qr} + i\mathbf{s}_0\mathbf{r}\sqrt{K^2 - q^2}\right)}{\sqrt{K^2 - q^2}},\tag{45}$$

where  $\mathbf{q} = (q_x, q_y)$  is a two-dimensional vector in the plane normal to the unit vector  $\mathbf{s}_0$ .

To obtain this relation mathematically let us begin once again from the Maxwell's equation

$$(\operatorname{grad}^2 + K^2)E(\mathbf{r},\omega) = 4\pi\delta(\mathbf{r}), \qquad K = \frac{\omega}{c}$$
(46)

Making the Fourier transformation

$$E(\mathbf{r},\omega) = \int \frac{d\mathbf{k}}{(2\pi)^3} \exp(i\mathbf{k}\mathbf{r}) E(\mathbf{k},\omega), \qquad \delta(\mathbf{k}) = 1$$
(47)

we find easily

$$E(\mathbf{k},\omega) = \frac{4\pi}{(k^2 - K^2)}.$$
(48)

Substituting this expression into the Fourier integral we represent the threedimensional wave vector  $\mathbf{k}$  as  $\mathbf{k} = \mathbf{q} + p\mathbf{s}_0$  where  $\mathbf{s}_0$  is a unit vector along the z-axis so  $z = (\mathbf{s}_0 \mathbf{r})$  and separate the integral over  $\mathbf{q}$  and over p.

$$E(\mathbf{r}) = 2 \int \frac{d\mathbf{q}}{(2\pi)^3} \exp(i\mathbf{q}\mathbf{r}) \int dp \frac{\exp(ipz)}{p^2 - (K^2 - q^2)}$$
(49)

The last integral is calculated by means of Resique Theorem giving a relation (45).

In a frame of small angle approximation the Eq.(45) can be represented as

$$E_S(x, y, z) \approx \frac{2\pi i}{K} \int \frac{dq_x dq_y}{(2\pi)^2} \exp\left[i\mathbf{k}_0(\mathbf{q})(\mathbf{r} - \mathbf{r}_s)\right]$$
(50)

with

$$\mathbf{k}_0(\mathbf{q}) = \mathbf{s}_0 \left( K - \frac{q^2}{2K} \right) + \mathbf{q}.$$
 (51)

Here we introduce the radius-vector of the point on the source  $\mathbf{r}_s$ . We shall assume also that  $\mathbf{s}_0 = (0, 0, 1)$  is a unit vector along the optical axis (axis z),  $\mathbf{q} = (q_x, q_y, 0)$  is a small vector which is perpendicular to  $\mathbf{s}_0$ . It describes the angular deviation of the particular plane wave from the base direction.

The representation of Eq.(50) allows us to move the problem of calculating the perturbation of the incident wave field by the object from the spherical wave to the plane waves having different deviations from the middle direction (z-axis). It is not convenient in case of inhomogeneous object. On the contrary, it is very useful for a description of spherical wave diffraction in single crystals. Indeed, the single crystal in a form of a plane-parallel plate is homogeneous at the macro level and it does not change the spatial properties of the plane wave. The only intensity value can be changed due to an absorption.

However, owing to a crystal lattice, i.e. an inhomogeneity at an atomic level, near the Bragg angle of two-beam diffraction, for example, the plane wave of standard polarization becomes splitted on two plane waves. These obtain different phases in passing through the crystal plate owing to the different phase velocity and this phenomenon is very sensitive to the angular deviation from the Bragg angle. The "pendellözung" fringes arise in the angular dependence of intensity as a result of interference between these two waves.

Let us consider this case in more detail from the point of view of observation of this effect in an experiment. If a scattering plane is (x, z) then the transmission amplitude  $A_t$  does not depend on  $q_y$ , namely,  $A_t = A_t(q_x)$  and the wave field after the crystal plate (at the detector) can be written as

$$E(x_d, y_d, z_d) \approx \frac{2\pi i}{K} \int \frac{dq_x dq_y}{(2\pi)^2} \exp\left[i\mathbf{k}_0(\mathbf{q})(\mathbf{r}_d - \mathbf{r}_s)\right] A_t(q_x)$$
(52)

First of all we can calculate the integral over  $q_y$  by means of table integral of Eq.(34) as

$$\left(\frac{2\pi i}{K}\right)^{1/2} \int \frac{dq_y}{2\pi} \exp\left(iq_y[y_d - y_s] - iz_{ds}\frac{q_y^2}{2K}\right) = S(y_d - y_s, z_{ds})$$
(53)

This result of calculation is evident physically once again. The partial spherical wave of y-axis stays the same as without crystal.

Now the wave field is described by the following expression

$$E(x_d, y_d, z_d) = \exp(iKz_{ds})S(y_d - y_s, z_{ds}) \left(\frac{2\pi i}{K}\right)^{1/2} \times \int \frac{dq_x}{2\pi} \exp\left(iq_x[x_d - x_s] - iz_{ds}\frac{q_x^2}{2K}\right) A_t(q_x),$$
(54)

which may be compared with Eq.(28). Spatially inhomogeneous object influences the wave field in different extent for different distances source-to-object. On the contrary, the Bragg diffraction influence in different extent the plane waves with different angular deviations from the Bragg angle and this does not depend on the position of the crystal plate between the source and the detector.

In general case of arbitrary value of the source-to-detector distance  $z_{ds}$  the integral in Eq.(54) may be rather complicated and will be analysed later. Here we consider a situation where the distance  $z_{ds}$  is very large. In this case the integral can be estimated approximately by means of stationary phase method considering the function  $A_t(q_x)$  to be slow one.

The Method of Stationary Phase is a very powerful technique in theoretical optics. It is a foundation of the geometrical optics which allows to obtain a solution of many optical problems by simple consideration of ray trajectories. This method allows to estimate approximately the integral

$$I(x) = \int dq F(q) \exp\left(i\varphi(q, x)\right)$$
(55)

where both functions F(q) and  $\varphi(q, x)$  are slow functions of the variable q. However, the phase  $\varphi(q, x)$  has very large value. In this case the integrand is strongly oscillating function, therefore the contribution of all regions of integration is very small except only the regions where the phase  $\varphi(q, x)$  has zero first derivative. Let us assume, for the sake of simplicity, that we have only one such a point  $q_0(x)$  which is a solution of the equation

$$\frac{d\varphi(q,x)}{dq} = 0 \tag{56}$$

This point is just the point of stationary phase. Near this point we may expand the phase as the Taylor series

$$\varphi(q) \approx \varphi(q_0) + \frac{1}{2} \left( \frac{d^2 \varphi}{dq^2} \right)_{q=q_0} (q-q_0)^2 + \cdots$$
(57)

Now taking into account that only small region near  $q_0$  contributes to the integral we can replace a slow function F(q) by it's value at the stationary phase point  $F(q_0)$  and consider the integral with approximate expression of the phase Eq.(57). However, since other regions don't contribute to the integral we may conserve infinite limits. Then the integral can be calculated analytically using once again the Eq.(34).

$$\int dq F(q) \exp\left(i\varphi(q,x)\right) \approx (2\pi i)^{1/2} \left(\frac{d^2\varphi(q_0)}{dq^2}\right)^{-1/2} F(q_0) \exp\left[i\varphi(q_0)\right]$$
(58)

So in accordance with this method we may replace  $A_t(q_x)$  by constant value at the point inside the integration area where the argument of the exponential has a zero first derivative. This point is easy to calculate  $q_x = K(x_d - x_s)/z_{ds}$ . After that the integral becomes equal to the partial spherical wave once again and we obtain

$$\frac{E(x_d, y_d, z_d)}{E_S(x_d, y_d, z_d)} = A_t \left( K \frac{x_d - x_s}{z_{ds}} \right)$$
(59)

The geometrical parameters which enter to the argument of transmission amplitude are illustrated in Fig.5.

We obtain the result which has a simple interpretation in a frame of geometrical optics approach. We may represent the spherical wave as a set of rays which pass in different directions. The density of rays is constant. The crystal plate influence each ray in accordance with the deviation of its direction from the Bragg direction. The intensity of radiation for each point of the source equals

$$J(x_d, x_s) = |E(x_d, y_d, z_d)|^2 = \frac{1}{z_{ds}} \left| A_t \left( K \frac{x_d - x_s}{z_{ds}} \right) \right|^2$$
(60)

while the real intensity, which will registered by the detector, is obtained after integrating Eq. (60) over the source size. If the source has a small x-size  $w_s$  compared to the period of the "pendellözung" fringes  $p_f$  then these will be registered by the position sensitive detector, for example, by the film. In the opposite case the film will be illuminated homogeneously showing no coherent effect. One can see that the magnification factor is absent in this case. The period of fringes can be obtained in the theory of two-beam diffraction. It is known that in the central part of the pattern the period  $p_f \propto z_{ds} \lambda/(t_c \Lambda)^{1/2}$  where  $t_c$  is the crystal plate thickness,  $\lambda$  ia a wavelength of X-rays and  $\Lambda$  is an extinction length. Therefore the condition of visibility of the fringes depends on the total distance source-to-detector. This means that it is essential the angular size of source  $w_s/z_{ds}$  as the source is seen from the detector rather than its real size.

#### 6. ANGULAR COHERENCE. PLANE WAVES

For a long time the study of X-ray diffraction in crystals was made under rather different conditions when the detector had a large window and it registered the total intensity over large enough area of space. It is evident that under these conditions we have to integrate the square modulus of Eq.(54) over  $x_d$ ,  $y_d$  and the limits of integration over  $x_d$  can be expanded to infinity. As a result, we obtain

$$I = \int dx_d dy_d \left| E(x_d, y_d, z_d) \right|^2 = \frac{W_y}{z_{ds}} \int \frac{dq_x}{K} \left| A_t(q_x) \right|^2$$
(61)



FIG. 5. The geometrical parameters of in-line experimental spheme including the crystal. The position of the crystal is unessential. Angular width of the source influences the resolution



FIG. 6. Measurement of "rocking curve" by double crystal experimental setup

where  $W_y$  is a width of the detector window in y-direction. This result shows that the integral intensity over the position at the detector does not depend on the source size and the source-to-detector distance. On the other hand, it can be represented as the integral transmission coefficient of the crystal over the angle of incidence of different plane waves. It is a consequence of the general property of Fourier transformation

$$\int dx \left| F(x) \right|^2 = \int \frac{dq}{2\pi} \left| F(q) \right|^2, \quad \text{if} \quad F(x) = \int \frac{dq}{2\pi} F(q) \exp(iqx)$$

which is known as the Parseval's theorem. Naturally it is not possible to study the coherent phenomena by means of this experimental setup.

However, this experimental arrangement may be much enhanced by introducing the second crystal before the sample. It must be the perfect crystal under the Bragg condition in reflection or transmission geometry and the sample can be slightly rotated near the Bragg angle. The Fig.6 shows schematically the experimental set-up in transmission geometry. In this case the detector will measure

$$I(q_0) = \frac{W_y}{z_{ds}} \int \frac{dq_x}{K} \left| A_t(q_x + q_0) \right|^2 \left| B(q_x) \right|^2$$
(62)

where  $B_r(q_x)$  is the reflection amplitude of the second crystal and  $q_0$  is the additional deviation of the plane wave from the Bragg angle owing to rotating the crystal. The preceding crystal plays the role of the plane wave source for analysing the angular dependence of the sample. It is called usually a monochromator. If the width of the reflectivity maximum of the monochromator is much less compared to the angular period of the "pendellözung" fringes of the sample then one obtains the possibility to investigate this coherent phenomenon in dependence on  $q_0$ , namely,

$$I(q_0) \approx \frac{W_y}{z_{ds}} |A_t(q_0)|^2 \int \frac{dq_x}{K} |B(q_x)|^2$$
(63)

The curve of such a type is called "the rocking curve".

Thus, the rocking curve allows us to investigate the interference phenomena as a result of partially coherent plane wave superposition. This branch of X-ray optics is known as the "X-ray multicrystal diffractometry". Just in the frame of this optics the monochromatization of the radiation is performed (see above). The coherent phenomena of X-ray diffractometry is known for a long time, while the spatial coherence of new X-ray source at the synchrotron radiation beam lines is a relatively fresh branch of X-ray optics.

Another branch of coherent X-ray crystal optics is the "Diffraction topography of crystal-lattice defects". The field of displacement of atoms from their normal position near the individual crystal-lattice defect like a dislocation may be clearly seen on the film if the front of X-ray beam before the crystal is restricted by a narrow slit. The theory of this effect is rather complicated and it is based on the spatially inhomogeneous crystal lattice. In this case the Maxwell's equations are reduced to the Takagi-Taupin equations which have to be calculated numerically.