Phase shift of a partially coherent electron wave as it passes through a crystal

P. M. Eremeev and D. I. Piskunov
Institute of Electronic Technology, Moscow

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The phase shift of the mutual coherence function of a partially coherent electron wave transmitted through an ideal absorbing crystal depends on the distance between the points at the exit surface of the crystal.

Partially coherent wave fields are usually described by means of a mutual coherence function, defined as the time average of the correlation between the wave functions at two points,[1] x_1 and x_2:

$$\Gamma(x_1;x_2) = \langle \Psi(x_1;t)\Psi^*(x_2;t)\rangle \ . \tag{1}$$

The mutual coherence function can also be written in the normalized form

$$\gamma(x_1;x_2) \equiv \gamma_{12} = |\gamma_{12}|e^{i\beta_{12}} = \frac{\Gamma(x_1;x_2)}{[I(x_1)I(x_2)]^{1/2}} \ , \tag{2}$$

with $0 \leqslant |\gamma_{12}| \leqslant 1$. If $x_1 \neq x_2$, we have $|\gamma_{12}| = 0$ for a completely incoherent field or $|\gamma_{12}| = 1$ for a completely coherent field. Here $I(x) = \Gamma(x;x)$ is the field intensity at the point x.

The quantity β_{12} is the phase shift between the points x_1 and x_2.

The change in the mutual coherence function as an electron wave propagates through a crystal can be described by an integral equation with the help of Green's functions[2]:

$$\Gamma_h(x_1;x_2) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Gamma(y_1;y_2)G_h(y_1 - x_1;z)G_h^*(y_2 - x_2;z)\,dy_1dy_2 \ , \tag{3}$$

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where z is the thickness of the crystal, y_1 and y_2 are points on the entrance surface of the crystal, x_1 and x_2 are points on the exit surface, and $h = 0$ for the transmitted beam and $h = g$ for the diffracted beam.

Using the Takagi approximation for the case of symmetric reflection, we can write explicit expressions for the Green's function for the transmitted and diffracted beams[3]:

$$G_0(x;z) = \delta(z - x') - \frac{\pi}{2\xi_g}\sqrt{\frac{z + x'}{z - x'}}\, J_1\left[\frac{\pi}{\xi_g}\sqrt{z^2 - (x')^2}\right] S(z - |x'|), \tag{4}$$

$$G_g(x;z) = \frac{\pi i}{2\xi_g} J_0\left[\frac{\pi}{\xi_g}\sqrt{z^2 - (x')^2}\right] S(z - |x'|); \tag{5}$$

where $\delta(z)$ is the Dirac δ-function, $J_0(z)$ and $J_1(z)$ are the Bessel functions of index zero and one, $S(z)$ is the unit step function [$S(z) = 0$ at $z < 0$ and $S(z) = 1$ at $z \geqslant 0$], $x' = x \cot\theta$, θ is the Bragg angle, and ξ_g is the extinction length.

If the electron source is at a distance R from the entrance surface of the crystal and is completely incoherent, the mutual coherence function at the entrance surface is the Fourier transform of the source intensity function.[1] Assuming that the source intensity function is Gaussian,[4] we have

$$\gamma(y_1;y_2) = \exp\left[\frac{i\pi(y_1^2 - y_2^2)}{R\lambda}\right] \exp\left[-\frac{(y_1 - y_2)^2}{2 l_k^2}\right], \tag{6}$$

where $l_k = R\lambda/2\pi a$ is the size of the region of coherent illumination at the crystal surface, a is the transverse dimension of the source, and λ is the electron wavelength. If the source is far away, i.e., if $R\lambda \gg y_{1,2}^2$, and if it has finite angular dimensions a/R, we have a partially coherent illumination at the surface of the crystal, with a value $\beta_{12} \approx 0$ for points $y_{1,2} \ll \sqrt{R\lambda}$.

In calculations of the mutual coherence function for a beam transmitted through a crystal with a thickness $z < 0.5\xi_g$, we found that when the illumination is partially coherent, there is a phase shift of the mutual coherence function at the exit surface of the crystal, depending on the distance between the points on the exit surface (Fig. 1). Inelastic scattering can be determined through the replacement[5] $1/\xi_g \to 1/\xi_g + i/\xi'_g$.

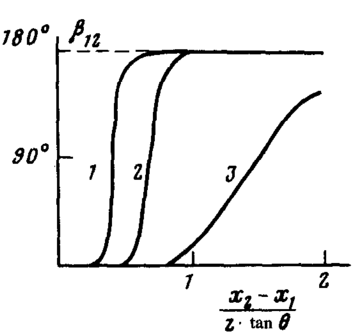

FIG. 1. Phase shift of the mutual coherence function versus the distance between points on the exit surface. $\xi_g/\xi'_g = 0.03$, $z = 0.49\xi_g$. 1—$l_k = 0.0001\xi_g$; 2—$l_k = 0.0003\xi_g$; 3—$l_k = 0.001\xi_g$.

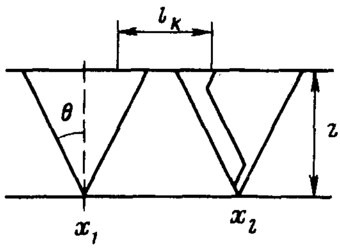

FIG. 2. Formation of the phase shift between points on the exit surface.

The phase shift β_{12} of the mutual coherence function is formed because of a correlation between the random wave functions at the points x_1 and x_2. The wave functions at the points x_1 and x_2 receive contributions from beams which arrive from regions of the entrance surface bounded by Takagi triangles (Fig. 2).

If the incident wave has a low spatial coherence, the correlation of the wave functions at the points x_1 and x_2 is determined primarily by beams which arrive from regions on the entrance surface with dimensions on the order of l_k. If a beam arrives at the point x_1 from this region as a transmitted beam, it arrives at x_2 as a doubly diffracted beam and therefore has a phase shift of 180°. Accordingly, if the region of coherent illumination is sufficiently small, $l_k \lessgtr \tan\theta \cdot z$, and if the distance between the points on the exit surface is $2\tan\theta \cdot z$, the phase shift of the mutual coherence function is approximately 180°. At $x_1 = x_2$, this phase shift is zero by definition.

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Translated by Dave Parsons