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On a phase problem of high-resolution Fourier transform X-ray spectroscopy

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A phase problem is discussed for high-resolution Fourier transform X-ray spectroscopy where the phase of the interferogram is missing. A numerical iterative method and an analytic logarithmic Hilbert transform method were tested for recovery of the missing phase information from the modulus of the interferogram. These methods were applied to measured data of the Si 14 6 0 back reflection and a calculated interferogram from an X-ray Fabry-Perot interferometer. The iterative method experienced an ambiguity of reconstruction; however, the ambiguity was relatively small and may be acceptable. The logarithmic Hilbert transform method gave a poorer reconstruction for the measured data owing to a lower signal-to-noise ratio, whereas it recovered the original spectrum from the calculated data without noise.

Keywords: X-ray optics; Fourier transform spectroscopy; phase problem.

1. Introduction

Recently an X-ray Michelson interferometer with a large path difference of 6.1 mm was realised (Tamasaku *et al.*, 2003). Such an interferometer combined with the Fourier transform technique would fill a resolution gap in X-ray spectroscopy between high-resolution crystal monochromators and time domain measurements (Gerdau *et al.*, 1986). For example, the highest-resolution crystal monochromator has an energy resolution of $\sim$120 μeV at 14.41 keV (Yabashi, Tamasaku *et al.*, 2001), whereas the time domain measurement covers energy resolutions below $\sim$10 μeV (Baron, 2000). At present, the crystal perfection limits the resolution of the crystal monochromator, while the response time limits that of the time domain measurement. On the other hand, the energy resolution of the Michelson interferometer is independent of these limitations, but is determined simply by $\lambda/2x_m$, where λ is the wavelength and x_m is the maximum path difference. With x_m = 100 mm, an energy resolution of 6.2 μeV at 14.41 keV will be realised using Fourier transform X-ray spectroscopy.

However, full determination of the spectrum requires an interferogram sampled with an interval of less than $\lambda/2$ over x_m, which consists of more than 2×10^9 data points under the above conditions. Furthermore, the path difference must be controlled with a resolution finer than $\lambda/2$. In practice the phase of the interferogram cannot be measured and must be recovered for reconstruction of the spectrum. Since a phase problem has been one of the most common problems in the optical measurements, there are many discussions about the phase recovery. In connection with the one-dimensional phase problem at present, many attempts were carried out both theoretically and experimentally, for example, using a logarithmic Hilbert transform (Bates, 1969; Burge *et al.*, 1976), an exponential filter (Kohler & Mandel, 1973), a combination of the previous two methods (Wood *et al.*, 1981) and a numerical iteration (Fienup, 1978).

In this report we will discuss the phase problem of high-resolution Fourier transform X-ray spectroscopy. We will apply the iterative and the logarithmic Hilbert transform methods to recover the missing phase and to reconstruct two spectra, a simple and a complicated spectra. We will use measured data of the Si 14 6 0 back reflection from a Michelson interferometer as the simple spectrum and a simulated spectrum from an X-ray Fabry-Perot interferometer as the complicated spectrum.

2. Phase recovery

2.1. Phase problem

The Michelson interferometer divides the incoming beam into two coherent beams, and combines them with a certain path difference, x. The output intensity is written as

$$I(x) = \int_{-\infty}^{\infty} s(\Delta k)\left[2 + 2\cos 2\pi(k_0 + \Delta k)x\right] \mathrm{d}\Delta k, \qquad (1)$$

where $s(\Delta k)$ is the spectral intensity at a wavenumber of $k_0 + \Delta k$, and Δk is the deviation from the mean wavenumber, k_0. Here we assumed that the throughput of the two branches of the Michelson interferometer is identical for simplicity. In usual Fourier transform spectroscopy, the spectrum is reproduced from $I(x)$ using (1).

After integration with Δk, the output intensity is

$$I(x) = A + 2|\gamma(x)| \cos 2\pi[k_0 x + \varphi(x)], \quad (2)$$

where

$$\gamma(x) = \mathcal{F}^{-1}[s(\Delta k)] = \int_{-\infty}^{\infty} s(\Delta k) \exp(-2\pi i \Delta k x)\, \mathrm{d}\Delta k, \quad (3)$$

$$\varphi(x) = \arg[\gamma(x)]. \quad (4)$$

Here A is a constant, $\gamma(x)$ is the inverse Fourier transform of the spectrum, and $\varphi(x)$ is the phase of $\gamma(x)$. We note that $\gamma(x)$ is not the complex coherence factor given by $\mathcal{F}^{-1}[s(k_0 + \Delta k)]$. $\gamma(x)$ does not incorporate information of the absolute wavelength. In the present case of high-resolution Fourier transform X-ray spectroscopy, measurement of k_0 is not important because it is known with sufficient accuracy. The important information to be determined is the shape of the spectrum, $s(\Delta k)$. We will refer to $\gamma(x)$ as the 'interferogram' for convenience.

For narrower band spectra, $\gamma(x)$ is considered to be a slowly varying function of x. The visibility of $I(x)$ is given by

$$V(x) = \frac{I_{\max} - I_{\min}}{I_{\max} + I_{\min}} = \frac{|\gamma(x)|}{A/2}, \quad (5)$$

where $I_{\max}$ and $I_{\min}$ are the maximum and the minimum of $I(x)$ within $x \pm 1/2k_0$, respectively.

As discussed before, $\varphi(x)$ cannot be determined, because the measuring system does not have an accuracy of $1/k_0$. The first term in the cosine of (2) is out of control. Thus the available information is $|\gamma(x)|$. When the missing phase, $\varphi(x)$, is recovered, the original spectrum could be reconstructed by Fourier transform, $s(\Delta k) = \mathcal{F}\{|\gamma(x)| \exp[i\varphi(x)]\}$.

2.2. Iterative method

In the numerical iterative method (Fienup, 1978), Fourier transform and inverse Fourier transform are performed iteratively under suitable constraints to make the phase converge. Each iteration consists of four steps:

(i) Calculate the nth spectrum using $s_n(\Delta k) = \mathcal{F}[\gamma_{n-1}(x)]$.

(ii) Apply the spectrum space constraint: the spectrum is non-negative inside the bandwidth and zero outside the bandwidth.

(iii) Calculate the nth interferogram by $\gamma_n(x) = \mathcal{F}^{-1}[s_n(\Delta k)]$.

(iv) Apply the interferogram space constraint: replace $|\gamma_n(x)|$ with the measured $|\gamma(x)|$, leaving the calculated phase, $\varphi_n(x)$, *i.e.* $\gamma_n(x) = |\gamma(x)| \exp[i\varphi_n(x)]$.

Usually the iteration starts from a guessed initial spectrum, $s_1(\Delta k)$, which is made from a series of random numbers.

There is another constraint that $s_n(\Delta k)$ must be real, which requires

$$\gamma_n(-x) = \gamma_n(-x)^*. \quad (6)$$

When the interferogram of the sample is discussed, the spectrum space constraint of step (ii) becomes tighter such that $s_n(\Delta k) < s_I(\Delta k)$, where $s_I(\Delta k)$ is the white-beam background spectrum of the interferometer, *i.e.* the spectrum of back reflection of the mirror crystal.

The iterative method is powerful and insensitive to noise; however, it has a problem of uniqueness. The solution in the one-dimensional phase problem is known to be multiple (Fienup, 1978).

2.3. Logarithmic Hilbert transform method

Another method for phase recovery is an analytic method. Consider the logarithm of the interferogram,

$$\ln \gamma(x) = \ln |\gamma(x)| + i\varphi(x). \quad (7)$$

The imaginary part is expressed by the real part using the logarithmic Hilbert transform as

$$\varphi(x) = \frac{2x}{\pi} P \int_0^{\infty} \frac{\ln |\gamma(\xi)|}{\xi^2 - x^2}\, \mathrm{d}\xi + \sum_j \arg\left(\frac{x - z_j}{x - z_j^*}\right) - 2\pi\kappa_0 x, \quad (8)$$

where P denotes the Cauchy principal value at $\xi = x$, z_j is the location of the jth zero of $\gamma(z)$ in the complex upper half plane, and κ_0 is a non-negative constant (Wolf, 1962). The shift of the spectrum by the additional term, κ_0, is not important in the present problem and can be neglected. If the location of the zeros or absence of zeros was known in the complex upper half plane, the spectrum could be calculated using the phase determined by (8). Bates (1969) presented a procedure to recover the possible distributions of zeros. However, to date, there is no method of determining the location of zeros from knowledge of $|\gamma(x)|$.

One optimistic fact is that the effect of zeros far from the measured region, $-x_m \le x \le x_m$ on the real axis, is small and might be negligible. So the number of zeros may be limited or, in some cases, there is no zero which affects the spectrum. When the theoretical spectrum is known, information on the zeros is available. For example, the interferogram of blackbody radiation is known to have no zeros in the complex upper half plane (Kano & Wolf, 1962).

In the present case, we calculated $|\gamma(z)|$ numerically in the complex plane from the theoretical spectrum of the Si 14 6 0 back reflection and the Fabry-Perot interferometer investigated below. We found no zero in the region of interest for both cases. Therefore the logarithmic Hilbert transform method would be reliable for the present cases.

3. Simple spectrum

For the first example we discuss the white-beam background spectrum of our Michelson interferometer without sample (Fig. 1*a*). In this case the spectrum is merely the reflectivity spectrum of the Si 14 6 0 back reflection used as the mirror. Fig. 2 shows the normalized intensity correlation measured at the RIKEN synchrotron radiation physics beamline (BL19LXU) of SPring-8 (Yabashi, Mochizuki *et al.*, 2001). The normalized intensity correlation, C, relates to the modulus of the interferogram, *via* $|\gamma(x)| \propto [2(C-1)]^{1/2}$ (Tamasaku *et al.*, 2003). The path difference was scanned from $x = 0$ to $x_m = 1.575$ mm in 0.025 mm steps (64 points). The wavenumber (energy) resolution was $1/2x_m = 317\ \mathrm{m}^{-1}$ (394 μeV).

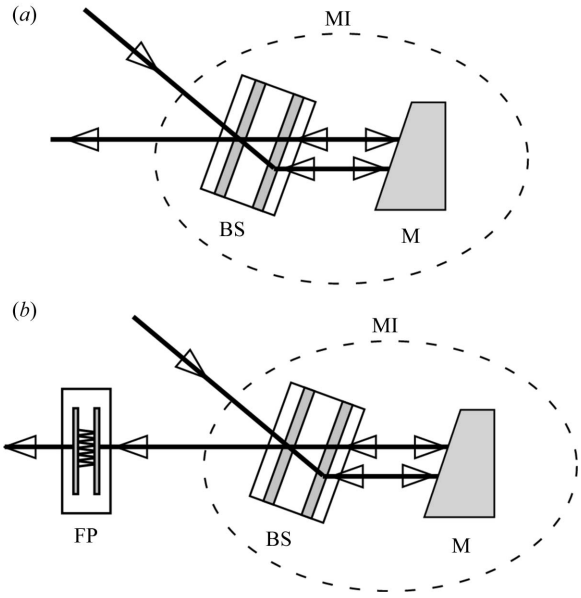

Figure 1
Schematic view of (*a*) the experimental set-up for the simple spectrum measurement, and (*b*) the set-up used to calculate the complicated spectrum. MI: Michelson interferometer; M: mirror; BS: beam splitter; FP: Fabry-Perot interferometer.

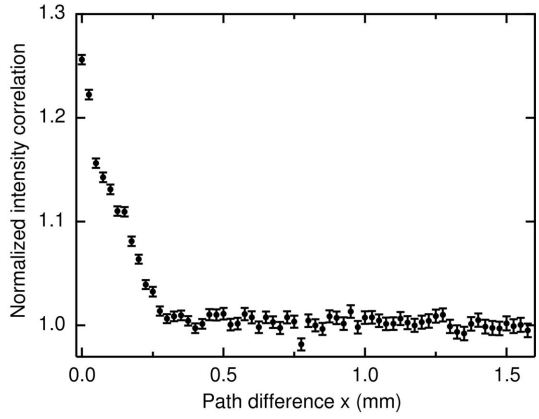

Figure 2
Measured normalized intensity correlation of the Si 14 6 0 back reflection. Vertical bars indicate the statistical error.

From the measured $|\gamma(x)|$, the autocorrelation function of the spectrum was calculated by $\mathcal{F}[|\gamma(x)|^2]$. The width of the spectrum was estimated as the half width at the half-maximum of the autocorrelation function, which was $\Delta k_0 = 2500\ \mathrm{m}^{-1}$. The width was in good agreement with the theoretical width, $2521\ \mathrm{m}^{-1}$.

3.1. Iterative method

We used Δk_0 for the Δk-space constraint, *i.e.*

$$s(k) = 0 \quad \text{if} \quad |\Delta k| > \Delta k_0. \tag{9}$$

Fig. 3(*a*) shows the typical reconstructed spectrum after 100 iterations. The reconstructed spectrum was in good agreement with the theoretically calculated spectrum of the Si 14 6 0 back reflection, though there were many fine structures and negative parts on the tail of the spectrum.

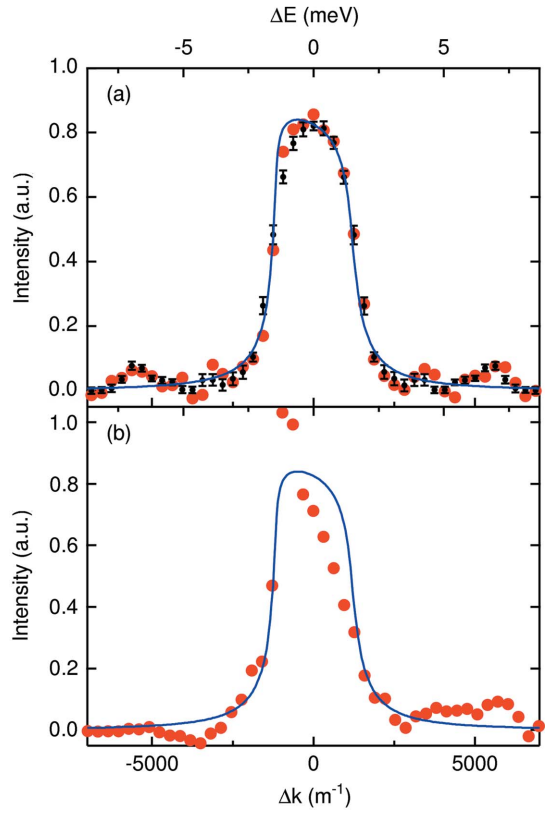

Figure 3
(*a*) Reconstructed spectrum using the iterative method (circles), the averaged spectrum of 500 independent reconstructions with the standard deviation (circles with vertical bars) and the theoretical spectrum of the Si 14 6 0 back reflection (solid line). (*b*) Reconstructed spectrum using the logarithmic Hilbert transform method (circles) and the theoretical spectrum of the Si 14 6 0 back reflection (solid line).

We found that the reconstruction depended slightly on the initial spectrum, $s_1(\Delta k)$. The ambiguity of the reconstruction was evaluated by the standard deviation of 500 independent reconstructions which was plotted with respect to the averaged spectrum (Fig. 3*a*). The dependence of the initial spectrum on the reconstructed spectrum was considered to be reasonably small and may be acceptable. It should be noted that the averaged spectrum cannot be the solution of the phase problem because, in general, $|\mathcal{F}^{-1}\{[s_a(\Delta k) + s_b(\Delta k)]/2\}| \neq |\gamma(x)|$ for $s_a(\Delta k) \neq s_b(\Delta k)$ where $|\mathcal{F}^{-1}[s_a(\Delta k)]| = |\mathcal{F}^{-1}[s_b(\Delta k)]| = |\gamma(x)|$. The averaging was just used to estimate the ambiguity of the reconstruction.

3.2. Logarithmic Hilbert transform method

The integral (8) needs values of $|\gamma(x)|$ up to $x = +\infty$, which requires extrapolation. We used constant extrapolation, *i.e.* $|\gamma(x)| = |\gamma(x_\mathrm{m})|$ for $x > x_\mathrm{m}$. In fact this extrapolation does not include any contribution, because the first term of the right-hand side of (8) can be rewritten as

$$\frac{2x}{\pi} P \int_0^\infty \frac{\ln|\gamma(\xi)|}{\xi^2 - x^2}\,\mathrm{d}\xi = \frac{1}{\pi}\int_0^\infty \mathrm{d}\xi \frac{\mathrm{d}^2 \ln|\gamma(\xi)|}{\mathrm{d}\xi^2}\Big[(\xi - x) \times \ln|\xi - x| - (\xi + x)\ln(\xi + x)\Big]. \tag{10}$$

The right-hand side of (10) may be convenient for numerical calculations because it does not have any singularity like the left-hand side.

The missing phase was recovered by neglecting the last two terms of (8), because the absence of zeros near the region of interest is expected from the numerical analysis discussed above. The measured normalized intensity correlation, C, was less than unity at 14 data points (Fig. 2), which were physically meaningless. These data points were replaced by a small value (C = 1.005), corresponding to the noise level of the measurement.

Fig. 3(b) shows the reconstructed spectrum. The width and the single asymmetric peak structure of the spectrum were reconstructed properly. The overall reconstruction was poorer than the iterative method because the numerical calculation was considered to be sensitive to the signal-to-noise ratio.

The logarithmic Hilbert transform method had no ambiguity in principle, and had the advantage of uniqueness compared with the iterative method. However, the extrapolation needed for the actual experiment may cause a small ambiguity. We had to try several different extrapolations since we could not know the behavior of $|\gamma(x)|$ outside the measured region. Fortunately we found that the effect of extrapolation was small, because $|\gamma(x)|$ was measured up to sufficiently large x.

4. Complicated spectrum

For the complicated spectrum, we used a calculated spectrum from a Fabry-Perot interferometer (Shvyd'ko, 2004) with a blade thickness of 0.2 mm, a gap of 0.5 mm and the Si 14 6 0 back reflection. The spectrum was calculated as $R_M T_{FP}$, where R_M is the reflectivity spectrum of the mirror (Si 14 6 0 back reflection) and T_{FP} is the transmissivity spectrum of the Fabry-Perot interferometer (see Fig. 1b). The calculated modulus of the interferogram is shown in Fig. 4. The maximum pathlength was set to x_m = 6.08 mm, corresponding to that of the present Michelson interferometer. The wavenumber (energy) resolution was $1/2x_m$ = 82 m^{-1} (102 μeV). The number of points was set to 256.

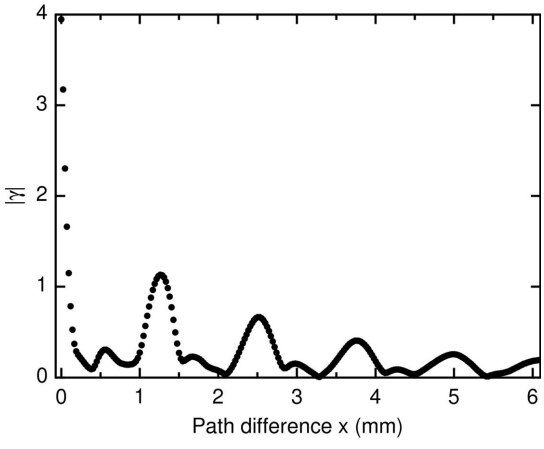

Figure 4
Calculated modulus of the interferogram, $|\gamma(x)|$, for the complicated spectrum, $R_M T_{FP}$.

Some information on the spectrum was deduced from $|\gamma(x)|$. First, the spectrum should have several peaks. From the fact that the peaks of $|\gamma(x)|$ were separated by Δx = 1.26 mm, the separation of the peaks of the spectrum was deduced to be $1/\Delta x$ = 804 m^{-1} (Fig. 5). The spectral width of each peak relates to decay of the envelope of $|\gamma(x)|$, and may be estimated.

4.1. Iterative method

The white-beam background spectrum of the interferometer (the spectrum of the 14 6 0 back reflection) was used for the Δk-space constraint instead of the width of the autocorrelation of the spectrum, resulting in better convergence.

Fig. 5(a) shows a typical reconstruction after 20000 iterations. Most features of the spectrum, the width and the number of the peaks, and the height of the peaks, were reconstructed well. However, it was difficult to determine which of the three peaks around the origin was highest.

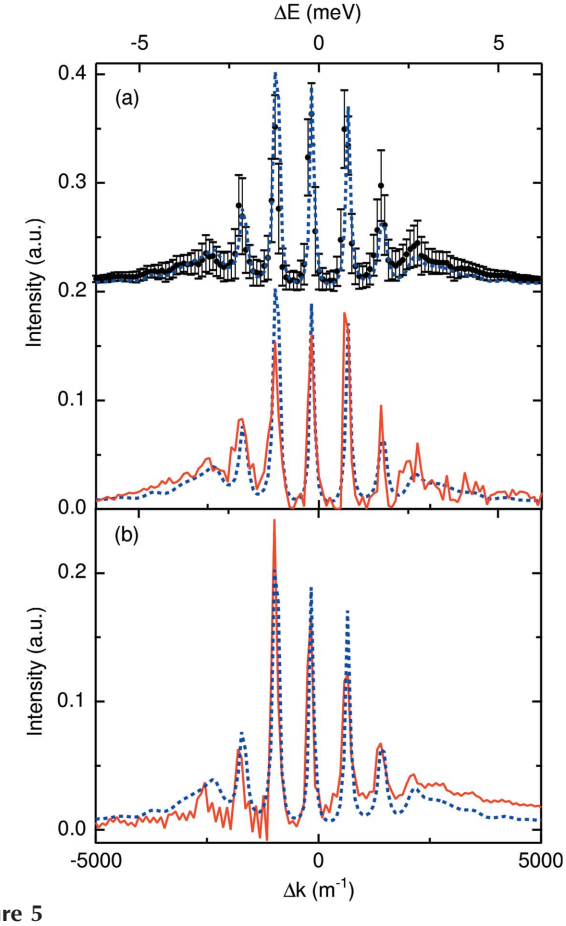

Figure 5
(a) Reconstructed spectrum using the iterative method (solid line) and the original spectrum (dotted line), $R_M T_{FP}$. The averaged spectrum of 500 independent reconstructions with the standard deviation (circles with vertical bars) is shifted by 0.2 for clarity. (b) Reconstructed spectrum using the logarithmic Hilbert transform method (solid line) and the original spectrum (dotted line), $R_M T_{FP}$.

The ambiguity of the reconstruction was evaluated in the same manner for the simple spectrum. For complicated spectra, such as the spectrum of the Fabry-Perot interferometer, the ambiguity of the origin was serious because the sharp structure of the spectrum was smeared out after averaging. To avoid such ambiguity, we aligned each reconstructed spectrum with respect to a reference spectrum, which was chosen arbitrarily from the reconstructed spectra. Each alignment was carried out by calculating a cross-correlation function between the reference and each reconstructed spectrum. Using this procedure the standard deviation of 500 independent reconstructions was estimated (Fig. 5*a*). The error bars were reasonably small, except for the main peaks around the origin.

4.2. Logarithmic Hilbert transform method

The reconstruction by the logarithmic Hilbert transform method was satisfactory (Fig. 5*b*). The reconstructed spectrum showed the same number of peaks, and the correct asymmetry owing to dynamical absorption. We tried several polynomials for the extrapolation, $|\gamma(x)| \propto x^{-m}$ $(m \geq 0)$; however, we observed negligible difference in the reconstructed spectra.

5. Discussion

Both the iterative and the logarithmic Hilbert transform methods showed satisfying reconstruction for two kinds of spectra. When $|\gamma(x)|$ is measured with sufficient signal-to-noise ratio, the logarithmic Hilbert transform method was more determinate than the iterative method as seen in the calculated spectrum of the Fabry-Perot interferometer. On the other hand, the iterative method was useful for noisy data. However, we consider that the use of the two completely independent methods is necessary for reliability of reconstruction. This is because the origin of the ambiguity of the iterative method is completely different from that of the logarithmic Hilbert transform methods. Agreement of the two independent methods enhances the reliability of the reconstruction. A combination of the two methods may be useful, especially for asymmetric spectra. The reconstructed spectrum by the logarithmic Hilbert transform method can be used for the spectrum space constraint of the iterative method.

The problem of the logarithmic Hilbert transform method is the fact that the absence of zeros of $|\gamma(z)|$ on the complex upper half plane is not guaranteed in general. Bates' procedure (Bates, 1969) is helpful for searching the possible locations of zeros. However, it seems straightforward to understand the physical meaning of zeros of $|\gamma(z)|$ in the complex upper half for application of the logarithmic Hilbert transform to the present problem. Although the nature of zeros is still not understood well, it has been believed to have a physical significance (Wolf, 1962). Investigation of spectra of the diffractive process should provide complementary information to that of the optical spectra for a full understanding of the zeros of $|\gamma(z)|$.

We consider that the maximum entropy method (MEM) may be a potential supplementary technique. The technique cannot be applied to the phase problem; however, it is useful to refine the reconstructed spectrum by the iterative method. We applied MEM to the interferogram $\{|\gamma(x)| \exp[i\varphi(x)]\}$ of the Si 14 6 0 back reflection reconstructed by the iterative method. Most fine structure arising from the noise of the measurement became smoother, and the negative parts of the spectrum were removed. This is because MEM reproduces the spectrum with the simplest structure from the given interferogram, and treats non-negative values. Other possibilities of MEM are the super-resolution (Kawata *et al.*, 1983) and the phase refinement (Ikeda *et al.*, 1998).

A quite different approach to the present problem may be converting the problem to a two-dimensional phase problem, which may be solved using the iterative method. Such an approach was successful for measurements of ultrashort laser pulses (Trebino *et al.*, 1997).

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