

## Reply to ‘‘Comment on ‘Uniqueness of the complex diffraction amplitude in x-ray Bragg diffraction’ ’’

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In their Comment Li *et al.* have tried to propose an alternative procedure to solve the phase problem. This Reply addresses the issues raised by Li *et al.* [S0163-1829(99)06621-7]

In their Comment, Li *et al.* attempt to argue that the x-ray phase-retrieval formalism discussed in Ref. 1 is ‘‘questionable.’’ We will show below that their examples are completely irrelevant to the formalism.<sup>1</sup>

The formalism discussed in Ref. 1 is based on the theorem that all causal functions are analytical.<sup>2</sup> The complex diffraction amplitude (CDA) is a causal function. ‘‘Mathematically, analyticity of the complex diffraction amplitude means that the Cauchy-Riemann equations are satisfied:

$$\frac{\partial u}{\partial q_r} = \frac{\partial v}{\partial q_i}, \quad \frac{\partial u}{\partial q_i} = -\frac{\partial v}{\partial q_r}, \quad (1)$$

where  $R(Q) = u(q_r, q_i) + iv(q_r, q_i)$  and  $q_r, q_i$  are the real and imaginary parts of the complex scattering vector  $Q = q_r + iq_i$ .<sup>1</sup> If these conditions are satisfied, the real and imaginary parts of such a function are uniquely linked via a Hilbert transform (see Ref. 3):

$$\begin{aligned} \text{Re}\{R(Q)\} &= -\frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\text{Im}\{R(Q')\}}{Q' - Q} dQ' \quad \text{and} \\ \text{Im}\{R(Q)\} &= \frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\text{Re}\{R(Q')\}}{Q' - Q} dQ'. \end{aligned} \quad (2)$$

If the logarithm of such a complex function is also an analytic function, then the phase is linked to the modulus via a logarithmic Hilbert transform:<sup>4</sup>

$$\begin{aligned} \varphi(Q) &= -\frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\ln|R(Q')|}{Q' - Q} dQ' + 2 \sum_m \arg(Q - Q^m) \\ &= \varphi^{\min}(Q) + \sum_m \varphi^m(Q), \end{aligned} \quad (3)$$

where  $Q^m$  ( $m=0,1,2, \dots, M-1$ ) are the zeros of  $|R(Q)|$  in the upper half of the complex plane (u.h.p.), that is  $\text{Im}(Q^m) > 0$ , and P is the Cauchy principle value of the integral. However, it must be reiterated that Eq. (3) can only be applied to analytical functions, that is the conditions (2) must be valid. Bochner and Martin<sup>5</sup> use another criterion for analyticity—a complex polynomial series. ‘‘Then, the complex diffraction amplitude,  $R(Q)$ , can be represented as a complex polynomial function of the degree  $K$ :

$$R(Q) = \prod_{k=0}^{K-1} (Q - Q^k), \quad (4)$$

where  $k$  denotes the indices. The major advantage of this representation is that due to its analyticity the complex diffraction amplitude is now *uniquely* defined by its zeros,  $Q^k \dots$ ’’<sup>1</sup> Li *et al.* claim that polynomials of power 512 are employed in their calculations. In fact, we see only 20 ‘‘zeros’’ in Figs. 2 and 3. However, if Li *et al.* ‘‘employed’’ a polynomial of power 512, the *Fundamental Theorem of Algebra* [Carl F. Gauss, circa 1811] would imply that there must be 512 zeros in the polynomial, not 20 as in their Figs. 2 and 3. In addition, Li *et al.* claim that their zeros have been ‘‘flipped’’ in Fig. 3 of the Comment. However, imaginary parts of the ‘‘rest zeros’’ and ‘‘flipped’’ ones have the same negative sign. ‘‘Flipping’’ a zero means that imaginary part must change its sign.<sup>4,1,8</sup>

Integral

$$R(q) = \int_0^d \frac{\partial u}{\partial z} e^{2\pi i H u(z)} e^{-2\pi \mu_i z} e^{2\pi q z} dz \quad (5)$$

[see Eq. (3) in the Comment of Li *et al.*] is not a Fourier transform because its lower and upper limits are finite. We reproduced the calculations of Li *et al.* in Figs. 1–3. It is clear from Figs. 2 and 3 that this function (5) is not analytic, because the conditions (2), above, are not valid. Since the examples discussed by Li *et al.* are not analytical functions, further speculations by Li *et al.* in their Comment on an al-

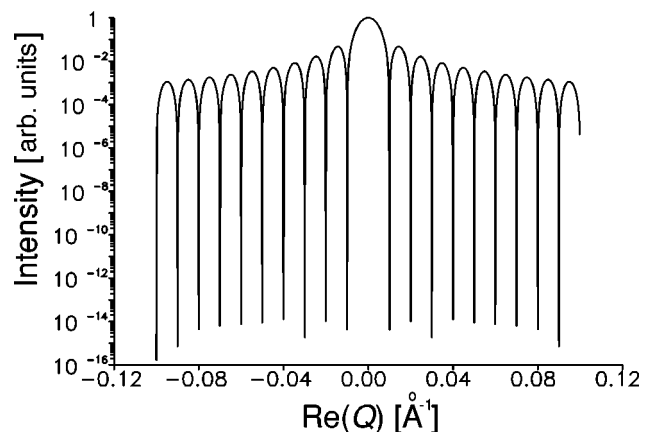


FIG. 1. Calculated ‘‘intensity’’ for the parameters used by Li *et al.* in their Comment.

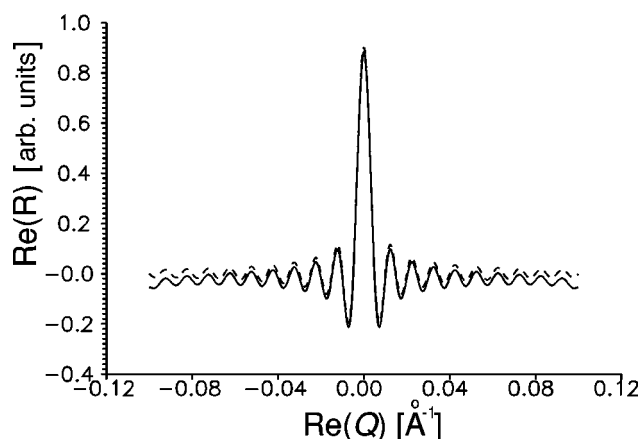


FIG. 2. Real part of the calculated “amplitude” for the parameters used by Li *et al.* in their Comment. The dashed line represents the calculated real part and the solid line represents a Hilbert transform of the imaginary part according to conditions (2).

ternative procedure to solve the phase problem are completely irrelevant to the entire formalism discussed in Ref. 1.

The regularization procedure suggested in Ref. 6 and cited by Li *et al.* is not discussed in Ref. 1. Since the phase retrieval via a logarithmic Hilbert transform<sup>1-4</sup> is not applicable to nonanalytic functions such as presented in the Li *et al.* Comment, we cannot comment on their resulting lattice mismatch profile.

Li *et al.* correctly mention in their Comment that experimental noise, etc., may affect the resulting structure profile, and this was also stated in Ref. 7. The major problem with the two radiation energies approach<sup>1,7,8</sup> is that “the difference in the radiation energies used for the diffraction data

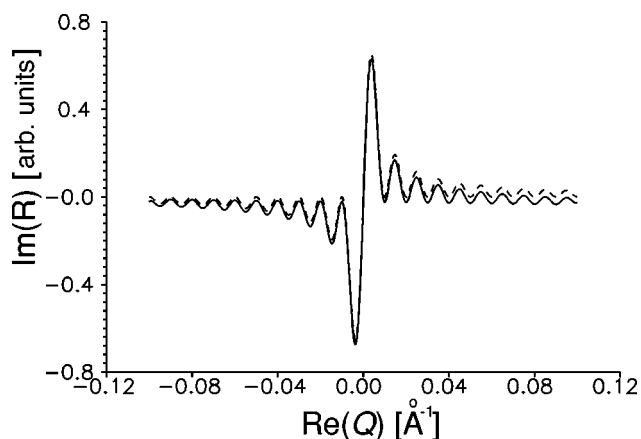


FIG. 3. Imaginary part of the calculated “amplitude” for the parameters used by Li *et al.* in their Comment. The dashed line represents the calculated imaginary part and the solid line represents a Hilbert transform of the real part according to conditions (2).

... causes not only a difference in the linear attenuation coefficients to be sufficient for the numerical data analysis, but also introduces a considerable difference in all the parasitic scattering phenomena such as thermal diffuse scattering, inelastic scattering, surface and interface roughness scattering, etc. All these parasitic effects blur the location of the true zeros of the CDA so that the phase-retrieval analysis technique is sensitive to the experimental setup.”<sup>9</sup> In order to keep the contribution from the parasitic phenomena the same, and yet have a large enough difference in the absorption values, we collect the Bragg diffraction data near an absorption edge of the material.<sup>9</sup>

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