COMMENTS

Comments are short papers which criticize or correct papers of other authors previously published in **Physical Review B.** *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Comment on ''Uniqueness of the complex diffraction amplitude in x-ray Bragg diffraction''

Ming Li,* W. Faschinger, and G. Landwehr
Physikalisches Institut der Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Z. H. Mai
Institute of Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100080, People's Republic of China
(Received 3 August 1998)

Nikulin in his recent paper [Phys. Rev. B **57**, 11 178 (1998)] reviewed their attempts to solve the phase problem in x-ray Bragg diffraction. Through three numerical examples, we show that the phase-retrieval procedure proposed in that paper may lead to contradictory results. [S0163-1829(99)06521-2]

The phase problem in light scattering has attracted much attention in the last few decades.[1–4] Phase-retrieval techniques based on the use of a logarithmic dispersion relation have been suggested long before.[1–4] These methods are complicated by the problem of localization of zeros of the complex scattering amplitude.[2,4] In a recent paper[5] Nikulin reviewed their attempts[6–9] to solve the phase problem in x-ray Bragg diffraction. A procedure was proposed to retrieve the complex diffraction amplitude by analyzing x-ray diffraction intensity profiles collected for two different radiation wavelengths. Polynomials were employed to fit the *minimal-phase diffraction amplitudes* in order to produce the zeros. These zeros were categorized into physical (*true*) and mathematical (*virtual*) ones. The true zeros in Ref. 5 meant those which should be flipped into the upper half-plane. The rule for distinguishing the true zeros from the virtual ones was the following: if the zeros produced by the two polynomials used to fit the two minimal-phase amplitudes are *at the same location*, they are true; but if they *have quite different locations in the complex plane*, they are virtual.[5] However, the assumption suggested and used by the author of Ref. 5 is questionable. We shall give three numerical examples to show this point in the present comment.

We consider first a mathematical model, namely, a very simple function,

$$\rho(z)=\begin{cases}\exp(2\pi\xi z), & \text{if } z\in(0,d),\\ 0, & \text{otherwise,}\end{cases} \tag{1}$$

the Fourier transform of which has the form,

$$R(q)=\frac{\exp(2\pi\xi d)\exp(2\pi i q d)-1}{2\pi(iq+\xi)}. \tag{2}$$

If $R(q)$ in Eq. (2) is analytically continued from real axis to the entire complex plane, it has zeros in the upper half-plane. In a scattering experiment, the phases at the sampling points are lost and only the modulus $|R|$ is measurable. Suppose that we utilize two radiation energies to perform the scattering experiments, each of which corresponds to an absorption coefficient μ_i, $i=1,2$. We follow Ref. 5 to retrieve the phases from the data given by $|R_i|$, $i=1,2$, at 1024 sampling points. The logarithmic dispersion relation results in two *minimal-phase diffraction amplitudes* $R_i^{\min}$, $i=1,2$. Two polynomials of power 500 are then employed to fit the two amplitudes, respectively. Figure 1 indicates that the polynomials can reproduce the minimal-phase amplitudes very accurately. Figure 2 shows the modulus of the analytical continuation near some zeros, which correspond to the absorption coefficient μ_1. The inset in Fig. 2 is a map of the zeros in the sampling range which are produced by the two polynomials; the rest of the zeros lie outside of the sampling range. One can see that the zero pairs which have equal real values have almost the same imaginary value. Therefore, these zeros are *true* ones according to Ref. 5 and should be flipped into the upper half-plane. This is correct according to Eq. (2).

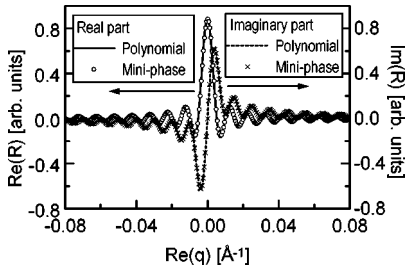

FIG. 1. Interpolation of the minimal-phase amplitude (symbols) with a polynomial (lines). The parameters for the profile in Eq. (1) are $d=100$ Å and $\xi=6\times10^{-5}$ Å^{-1}. The corresponding absorption coefficient is $\mu_1=1\times10^{-5}$ Å^{-1}.

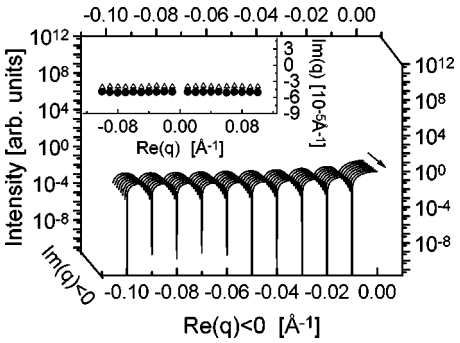

FIG. 2. Modulus of the analytical continuation of the minimal-phase amplitude showing a part of the zeros in the lower half-plane. The structural parameters are the same as in Fig. 1. Inset: Map of a part of the zeros. Circles represent $\mu_1=1\times10^{-5}$ Å^{-1} and triangles represent $\mu_2=2\times10^{-5}$ Å^{-1}.

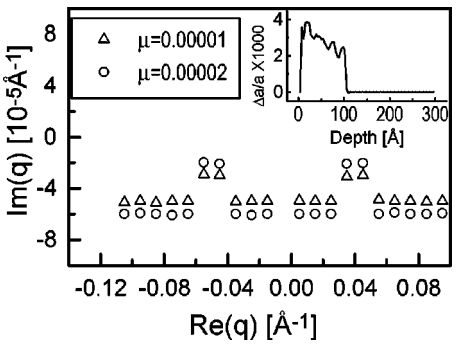

FIG. 3. Map of zeros for the structure in the inset. Inset: a complicated strain profile showing significant strain fluctuations within the layer. Its corresponding diffraction amplitude has four zeros in the upper half-plane with $\mathrm{Im}(Q_j)=4\times10^{-5}$ Å^{-1}. The rest of the zeros are in the lower half-plane. The layer is 100 Å thick with a mean lattice mismatch $\Delta a/a=2.6\times10^{-3}$.

Now we consider the x-ray reflection amplitude of a thin epitaxial layer on a thick substrate. In Refs. 5–7 normalized intensities were used instead of the directly measured intensities. It can be easily shown that the normalized diffraction amplitude for our structure is just the following Fourier transform:[10]

$$\mathcal{R}(q)=\int_0^d \frac{\partial u}{\partial z}e^{2\pi iHu(z)}e^{-2\pi\mu_i z}e^{2\pi iqz}dz, \tag{3}$$

where H is the reciprocal lattice vector, $u(z)$ is the atomic plane displacement field, μ_i is the linear absorption coefficient, d is the thickness of the layer, and $\partial u/\partial z=\Delta a/a$ represents the lattice mismatch which is nonzero within the layer only. The same process as above produces two sets of zeros in the lower half-plane. If we let $d=100$ Å, $\mu_1=4\times10^{-5}$ Å^{-1}, and $\mu_2=5\times10^{-5}$ Å^{-1}, the map of zeros is the same as the inset in Fig. 2 except for a shift by $-H(\Delta a/a)$ along the real axis. *Are these zeros true*? In order to be consistent with the first example, they should be *true*. But it is easy to prove that $\mathcal{R}(q)$ in Eq. (3) has no zeros in the upper half-plane. If one flips all the zeros into the upper half plane, one gets a physically meaningless result that the absorption coefficient is negative.

Therefore, we have shown that the rule for selecting the true zeros used in Ref. 5 is quite questionable. It leads to contradictory results for the two examples above. Actually, it is not necessary to divide the zeros of the polynomials into true ones and virtual ones. Each zero is equally significant and should be independent of the numerical implement. The effect of the absorption is just to shift the zeros along the imaginary axis. If two corresponding zeros produced by two polynomials have quite different locations, higher power polynomials should be used to make the fitting more accurate. The author of Ref. 5 used polynomials of power as low as 55 to fit the somehow more complicated curves. We have used a polynomial of power 250 to fit the dots (the minimal-phase amplitude) in Fig. 1. The resulting locations of the zeros are quite different from those produced by the polynomial of power 500. The zeros shown in the inset of Fig. 2 deviate a little bit from the theoretically expected positions. The deviation becomes smaller when we fit the dots in Fig. 1 by a polynomial of power 1000 or higher. These results indicate that the artifact in calculations modifies the position of the zeros. In principle, Eq. (2), which is an entire function,[3] has an infinite number of zeros; and the number of zeros which can be taken into account is equal to the number of sampling points according to the Sec. III of Ref. 5. However, the author of Ref. 5 interpolated a polynomial of power 512 with a polynomial of power 55. This is quite similar to fitting the points on a parabola by a straight line. Another source which influences the position of the zeros is noise. The quite different positions for the corresponding ''virtual'' zero pairs in Refs. 5–8 may result from both the noise and the low power polynomials used.

If the positions of the zeros are not correctly calculated, no correct scattering profile can be obtained. Surprisingly, it seems that the procedure had been successfully utilized to retrieve the diffraction amplitudes in Refs. 6–8, which were cited to support the mathematics in Ref. 5. However, the success was achieved with the aid of a *trick*, namely, a regularization procedure.[6,8] If one reads Ref. 8 carefully, one would find that the regularization procedure is not independent of the *a priori* knowledge about the sample, which makes the statement of being model-independent meaningless. We give an example to elucidate it. Shown in the inset of Fig. 3 is a strain profile $\Delta a/a$ as a function of depth,[11] which fluctuates significantly. The curve is similar to that in Fig. 3 of Ref. 8. But the fluctuations were suppressed by the regularization procedure in Ref. 8. The complex diffraction amplitude corresponding to the strain profile in the inset has four zeros in the upper half-plane, which is the reason for the fluctuations.[12] The regularization procedure is effectively equivalent to flipping the four zeros into the lower half-plane for our example. If one flips these zeros into the lower half-plane, one obtains a smooth strain profile. But without any *a priori* information, who can make sure that there are no fluctuations in the layer?

We have calculated the absolute diffraction amplitude $|\mathcal{R}|$ by using Eq. (3) with the integrand being replaced by the profile in the inset of Fig. 3. The same procedure as above results in two sets of zeros which correspond to two different wavelengths, respectively. The map of zeros is shown in Fig. 3. One can see that there are four specific zeros in Fig. 3, corresponding to those which should be flipped into the upper half-plane. The different behavior of the four specific

zeros suggests that there is an alternative way to decide which zeros should be flipped into the upper half-plane. The effect of the absorption is to move the zeros by $-\mu_i$ along the imaginary axis. Therefore, if a zero lies in the upper half-plane, its actual position is nearer to the real axis if the diffraction was measured by using a wavelength with larger absorption; and vice versa. Therefore, if two zeros have the same real value, and one of them which corresponds to a larger absorption coefficient is nearer to the real axis than the other which corresponds to a smaller absorption coefficient, this pair of zeros locate in the upper half-plane; and vice versa.

In summary, the phase-retrieval procedure in Ref. 5 is questionable and the regularization procedure used to support the mathematics of Ref. 5 is problematic. An alternative rule can be adopted to determine which zeros should be flipped into the upper half-plane. Of course, the difference in absorption coefficient between the two radiation energies practically used should be large enough to ensure that the shift along the imaginary axis can be resolved by the numerical implement.

One of the authors (M.L.) extends his gratitude to the Volkswagen Foundation for financial support.

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*Permanent address: Institute of Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100080, P. R. China.

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[10] The unnormalized amplitude is given by $R(q)=-1/[2\pi i(q-\mu)]-\mathcal{R}(q)H/(q-\mu)$.

[11] We flip four zeros of the polynomial which corresponds to the profile of Eq. (3) to obtain a new diffraction amplitude. The inverse Fourier transform produces the strain profile in the inset of Fig. 3. The distance of the zeros to the real axis is 4×10^{-5} Å^{-1}.

[12] Mathematical details for the fluctuations can be found in Ref. 3.