Uniqueness of the complex diffraction amplitude in x-ray Bragg diffraction

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The concept of the complex diffraction amplitude for x-ray Bragg diffraction is discussed in terms of a unique product of its zeros. This formalism allows the inverse scattering problem in x-ray Bragg diffraction to be solved unambiguously. The phase-retrieval technique, via a logarithmic dispersion relation, has associated with it the problem of localization of zeros of the complex diffraction amplitude. The mathematical approach predicts an infinite number of zeros of the complex diffraction amplitude. However, a physical (discrete) representation of the inversion technique limits the number of zeros that should be considered and allows one to obtain a unique solution for the structure-factor profile. Practical examples of the analytical continuation of the complex diffraction amplitude are presented. Distinctions between the artificial, mathematical, and the true, physical, features of the analytical continuation are elucidated. [S0163-1829(98)07017-9]

I. INTRODUCTION

X-ray Bragg diffraction is a powerful diagnostic tool for the nondestructive analysis of crystalline materials. The widely used method of least-squares fitting of a calculated reflectivity to the experimental diffraction profile relies on an *a priori* model of crystal-lattice deformation; see, e.g., Refs. 1 and 2. The method works well for a relatively large class of crystalline structures and allows one to obtain information about the crystal-lattice strain profiles. However, there is no evidence that the solution obtained through least-squares fitting is unique, since it is an intensity that is fitted, while the phase information (representing half of the information) is not taken into account. Since the crystal structure factor is a *complex* function, the analysis of the intensity profile alone, which is a *real* function, is not able to give a physically sound result for a structure factor. Regardless of the relationship between the crystal structure factor and the complex diffraction amplitude profiles, the modulus and phase of the complex diffraction amplitude should be considered in the crystal structure-factor calculation. For instance, Bragg diffraction and specular reflection formalisms have quite different mathematical representation for correspondence between the structure factor and the complex diffraction amplitude.

A method for the solution of the inverse problem based on the calculation of the reflectivity phase profile via a logarithmic dispersion relation[3–5] has been suggested for x-ray Bragg diffraction.[6] Phase-retrieval techniques based on the use of a logarithmic dispersion relation are complicated by the problem of the localization of zeros of the complex diffraction amplitude.[3–6] A self-consistent method for a model-independent determination of the crystal-lattice strains in a single crystal based on this theoretical approach[6] was recently developed experimentally.[7–10] The technique uses a logarithmic dispersion relation to retrieve the phase of the x-ray wave diffracted by a single crystal under Bragg condition. The method has been applied successfully to determine the structure of one- and two-dimensional lattice-strain distributions in silicon crystals that have been implanted with high-energy ions[7–8] and in SiGe/Si superlattices.[9,10] The problem of localization of zeros of the reflection amplitude was not solved in Refs. 7–10, and therefore the technique did not give a unique solution. Often there were two resulting strain profiles that were very similar but not identical.[8,9] A new approach to the unambiguous solution of the inversion problem has been developed recently.[11,12] It was suggested that one must distinguish between the physical and mathematical zeros of the complex diffraction amplitude using experimental data collected for two radiation energies. Only the true zeros should be used in the complete phase-profile calculation.[11,12] Complications in the formalism arising from the nonuniform attenuation in the damaged layer have been addressed in Ref. 12.

The present paper aims to represent the concept of the complex diffraction amplitude in x-ray Bragg diffraction as a unique product of its zeros. We show how physically reasonable assumptions about the complex diffraction amplitude allow us to formulate the inversion procedure[3–6] in terms of a discrete (physical) representation. This discrete formalism, which corresponds directly to an experiment, allows one to obtain a unique solution for the structure-factor profile, which is consistent with the experimental observations. As a practical example, the formalism is applied to x-ray Bragg diffraction data collected at two different radiation energies.

II. AMBIGUITY IN PHASE RETRIEVAL VIA A LOGARITHMIC DISPERSION RELATION

The possibility of retrieving phase from the radiation scattered by an object (in the case of a one-dimensional modulation of the structure-factor distribution) relies on the assumption that the complex diffraction amplitude $R(Q)$ and its logarithm $\ln\{R(Q)\}$ are analytic functions.[3–6] It is important to note that the primary meaning of analyticity is that *physically* this expresses the belief that it is possible to obtain the ''lost'' phase of the scattered intensity. In other words, the modulus and phase of the complex diffraction amplitude *are not independent*. This assumption works directly within the framework of the kinematical theory of x-ray scattering. The problem of the applicability of this phase-retrieval technique to be used for x-ray-diffraction data

exhibiting dynamical features has been addressed elsewhere.[13]

Mathematically, analyticity of the complex diffraction amplitude means that the Cauchy-Riemann equations are satisfied (see, e.g., Ref. 14):

$$\frac{\partial u}{\partial q_r}=\frac{\partial \nu}{\partial q_i}, \quad \frac{\partial u}{\partial q_i}=-\frac{\partial \nu}{\partial q_r}, \tag{1}$$

where $R(Q)=u(q_r,q_i)+i\nu(q_r,q_i)$ and q_r,q_i are the real and imaginary parts of the complex scattering vector $Q=q_r+iq_i$. It is then possible to retrieve the phase $\varphi(Q)$ of the experimentally observed x-ray-diffraction intensity $I(Q)=|R(Q)|^2$ via a logarithmic dispersion relation (i.e., a logarithmic Hilbert transform):[3–6]

$$\varphi(Q)=-\frac{1}{\pi}\,\mathrm{P}\int_{-\infty}^{\infty}\frac{\ln|R(Q')|}{Q'-Q}\,dQ'+2\sum_m \arg(Q-Q^m)$$

$$=\varphi^{\min}(Q)+\sum_m \varphi^m(Q), \tag{2}$$

where Q^m $(m=0,1,2,\ldots,M-1)$ are the zeros of $|R(Q)|$ in the upper half of the complex plane (uhp), that is, $\mathrm{Im}(Q^m)>0$, and P is the Cauchy principal value of the integral. The first term in Eq. (2) can be evaluated simply using a relationship between the Hilbert and Fourier transforms (see, e.g., Ref. 15). The second term presents the major difficulty for the one-dimensional inverse problem based on the phase retrieval via the logarithmic dispersion relation. It is impossible to *a priori* say whether any zero occurs in the diffraction-amplitude profile. We show below that it is not feasible to perform an adequate experiment to determine the occurrence of zeros directly from the intensity measurements. This second term in Eq. (2), which involves the problem of location of the zeros, is the main source of the ambiguity in the one-dimensional inversion formalism.[3–6]

The zeroes Q^m of *unknown* number M are the true, physical, zeros of the complex diffraction amplitude that might occur due to interference suppression of the scattered x-ray wave under certain circumstances. In an experiment, the complex scattering vector Q should be represented as $Q=q+i\mu$, where q is the scattering vector length and μ is the linear attenuation coefficient. Here the q and μ variables are defined to be dimensionless, corresponding to the number of Darwin half-widths for the reflection **h**, so that $\mathrm{Re}(Q)=\Delta\theta\sin 2\theta/|\chi_h|$ and $\mathrm{Im}(Q)=\chi_{oi}/|\chi_h|$, where $\Delta\theta$ is the angular deviation from the exact Bragg position θ and χ_{oi} and $|\chi_h|$ are the imaginary part and the modulus of the corresponding Fourier coefficients of the dielectric susceptibility of the crystal, respectively. Expressions for the real and imaginary parts of the complex scattering vector are written for a symmetric Bragg reflection and can be easily extended to the asymmetric case. Hence, a complex zero Q^m can have real, $\mathrm{Re}(Q)=q^m$, and imaginary, $\mathrm{Im}(Q)=\mu^m$, parts which correspond to some *a priori* uncertain point in the complex plane. To observe a zero in the diffraction amplitude profile we have to perform an enormous number of scans along the scattering vector q for a large set of radiation energies, i.e., different μ. This is the only procedure for determining the true zero locations experimentally. In such an experiment we can cover a reasonably large range of the scattering angles that is along the q coordinate and of the radiation energies that is along the μ coordinate. Such a mesh scan is not feasible since it would take an inordinately long experimental time. However, the fundamental problem is that this set of mesh points is always *finite*. The general mathematical formalism implies that the number of zeros is infinite.[3–6] Thus, we cannot determine all the true zeros experimentally and the second term in Eq. (2) cannot be calculated unambiguously. A formal *continuous* consideration of the problem does not suggest a way to obtain a unique solution to the inversion problem. To resolve this problem we have to consider the complex diffraction amplitude as a unique product of its zeros in its physical, *discrete representation*.

III. DISCRETE REPRESENTATION OF THE COMPLEX DIFFRACTION AMPLITUDE

Analyticity of the complex diffraction amplitude is a physical property. However, as we saw above it has benefited us in a mathematical expression that can be used to retrieve a so-called minimal-phase profile, namely, the first term in Eq. (2), from the experimentally measured intensity distribution. The same analytical nature of the complex diffraction amplitude allows us to represent it as a complex polynomial function of a complex variable (see, e.g., Ref. 14).

In an experiment we collect a certain number K of data points for a reflectivity profile. Then, the complex diffraction amplitude $R(Q)$ can be represented as a complex polynomial function of the degree K:

$$R(Q)=\prod_{k=0}^{K-1}(Q-Q^k), \tag{3}$$

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^m in Eq. (3). In addition, we now have only limited number of zeros to consider. The number of zeros cannot exceed the number of experimentally measured points K.

Thus, to obtain the complex diffraction amplitude profile in the polynomial form (3), first, we collect an experimental intensity profile $I(Q)$ for a range of the scattering vector, q at a particular radiation energy, i.e., fixed μ. Second, we calculate a minimal-phase profile $\varphi^{\min}(Q)$ according to

$$\varphi^{\min}(Q)=-\frac{1}{\pi}\,\mathrm{P}\int_{-\infty}^{\infty}\frac{\ln\sqrt{I(Q')}}{Q'-Q}\,dQ'. \tag{4}$$

Third, we combine a minimal-phase diffraction amplitude profile, $R^{\min}(Q)=\sqrt{I(Q)}\,\exp[i\varphi^{\min}(Q)]$. This profile is a ''slice'' of the complex diffraction amplitude $R(Q)$ along the real axis q of the complex plane at a fixed position on the imaginary axis μ. Finally, we perform an *analytical continuation* of the complex diffraction amplitude in the whole complex plane. This procedure is a representation of the minimal-phase diffraction-amplitude profile $R^{\min}(q)$ in the complex polynomial form (3). Mathematically, we have to interpolate the profile $R^{\min}(q)$ with a complex polynomial

function and calculate the roots of this polynomial. This procedure can be done using standard interpolation routines; see, e.g., Ref. 16.

Once we have collected an experimental Bragg diffraction profile $I(Q)$ as a function of scattering vector length q, we have the data represented in a definite range, $\Delta q^{-\max} \leqslant q \leqslant \Delta q^{+\max}$, of wave numbers. It should be noted that the values $\Delta q^{-\max}$ and $\Delta q^{+\max}$ do not necessarily have to be equal. The influence of asymmetry in the values $\Delta q^{-\max}$ and $\Delta q^{+\max}$ was addressed in Ref. 17. Due to restrictions imposed by the sampling theorem[18,19] we cannot resolve any feature in the resulting structure-factor profile with a spatial resolution ΔT greater than $\Delta T=(\Delta q^{-\max}+\Delta q^{+\max})^{-1}$. Hence, the maximum total thickness T of the analyzed layer that can be considered is $T=\Delta TK/2$. The number 2 appears because real space is divided into two equal halves—vacuum and matter. Thus, we have to divide the layer of thickness T, in which we would want to determine the structure-factor profile, into *not more* than $K/2$ sublayers. We have to consider that the structure factor in every individual sublayer, $\psi_k=|\psi_k|e^{i\phi_k}$, is uniform within the thickness ΔT. It is impossible to resolve a feature within such a sublayer.

We cannot evaluate zeros outside the range $\Delta q^{-\max} \leqslant q \leqslant \Delta q^{+\max}$ simply because we do not have the experimental data outside this range. This fact strictly limits the spatial resolution ΔT that can be achieved in an experiment. However, *all* zeros of the complex diffraction amplitude that should be considered are within the range $\Delta q^{-\max} < \mathrm{Re}(Q^m) < \Delta q^{+\max}$, and the maximum number of these zeros, $N=K/2$, is limited by the number of data points. Hence, for experimental data we always have a *finite* number of zeros that needs to be considered in evaluating the structure-factor profile. It should be noted, however, that the magnitude of the imaginary part $\mathrm{Im}(Q^m)$, corresponding to the zeros, is an unrestricted quantity.

Following this procedure we determine all the zeros of the complex diffraction amplitude that should be taken into account to calculate the *complete* phase profile (2). However, all the roots of the polynomial interpolation of the minimal-phase diffraction amplitude profile $R^{\min}(Q)$ are in the lower half of the complex plane (lhp).[6] This half plane corresponds to a negative imaginary part of the complex scattering vector, hence negative attenuation. Therefore, these zeros are not physically meaningful. The calculated roots (zeros) of the complex polynomial interpolation (3) are always located in the lhp and represent mathematical zeros of the diffraction amplitude profile. We refer to them as the virtual zeros of the complex diffraction amplitude.

The complete phase profile (2) requires that only physical zeros be included in the second term $\Sigma_m \varphi^m(Q)$ that may occur in the complex diffraction amplitude profile due to the interference suppression of the scattered wave. These zeros can only occur in the uhp where attenuation is positive. With the use of the logarithmic dispersion relation (4) and analytical continuation (3), the zeros of the complex reflection amplitude may be calculated. However, so far they are mathematical zeros of the polynomial interpolation of the minimal-phase diffraction amplitude profile $R^{\min}(Q)$ located in the lhp. If one or more true zeros occur in the uhp, they should have imaginary parts that are the complex conjugates of the mathematical (virtual) zeros in the lhp. This is the critical point of the formalism. Due to its analytical properties the complex diffraction amplitude is uniquely determined by its zeros from the analytical continuation into the whole complex plane (3). Some of these zeros are the physical zeros that occur in the uhp that is where the attenuation is positive. The rest of the calculated zeros obtained from the complex interpolation are in the lhp. These latter zeros appear only because of the formal use of the polynomial representation of the complex diffraction amplitude. We do not have to include all zeros in the complete phase profile (2). However, we do not know which zeros in the uhp are the true ones and which are simply formed by the mirror reflection (''flipping'') of the virtual zeros.

Unfortunately, the 2^N solutions for the complex diffraction amplitude $R^m(Q)$ obtained via ''flipping'' of the complex polynomial roots from the lhp into the uhp according to

$$R^m(Q)=R^{\min}(Q)\prod_l^M \frac{Q-\tilde{Q}^l}{Q-Q^l} \tag{5}$$

have the same modulus on the real axis $q=\mathrm{Re}(\tilde{Q}^l)=\mathrm{Re}(Q^l)$. Here a tilde denotes complex conjugation. The problem is that $|(Q-\tilde{Q}^l)/(Q-Q^l)|\equiv 1$, but $\arg\{(Q-\tilde{Q}^l)/(Q-Q^l)\} \neq \mathrm{const}$. Therefore, $|R^m(Q)|\equiv|R^{\min}(Q)|$ and, thus, experimental intensity profiles cannot be distinguished. However, $\arg\{R^m(Q)\}\neq\arg\{R^{\min}(Q)\}$ and, thus, the resulting structure factor should be different. Thus, we obtain the same intensity profile for both the $R^m(Q)$ and $R^{\min}(Q)$ diffraction amplitudes. The index l stands for any combination of M zeros selected from the total number of N. For instance, l can be 3, 5, and 22, hence $M=3$, while N can be any value from 3 to a very large yet finite number. Therefore, according to Eq. (5) we obtain 2^N complex diffraction amplitudes that have the same modulus and, thus, the same intensity profile. For the common case of $N=100$ the number of possible complex diffraction amplitude profiles is more than 10^{30}. Generating and analyzing one solution per second we would spend about 3×10^{22} years to obtain a result using this inversion procedure. The fact that we can obtain an enormous number of identical diffraction intensity profiles, which can be calculated for the same number of crystal structure-factor distributions, shows explicitly the hopelessness of the least-squares-fitting methodology.

Sequential trial of all possible generated solutions obtained via the phase-retrieval formalism does not seem to be feasible either. The problem is that the complex interpolation (3), namely, analytical continuation of the complex diffraction amplitude in the whole complex plane, automatically gives us only negative imaginary parts for the polynomial roots. There is no mathematical criterion for determining whether a particular zero is a virtual or true zero. Thus, we have to determine which zeros are the true by other means.

It was suggested in Refs. 11 and 12 to perform a series of experiments with the same sample for at least two radiation energies in order to determine the true zeros of the complex diffraction amplitude. Here we would like to substantiate the physical meaning of this procedure and, most importantly, to clarify what is true and artefact in the analytical continuation of the complex diffraction amplitude performed at two radiation energies.

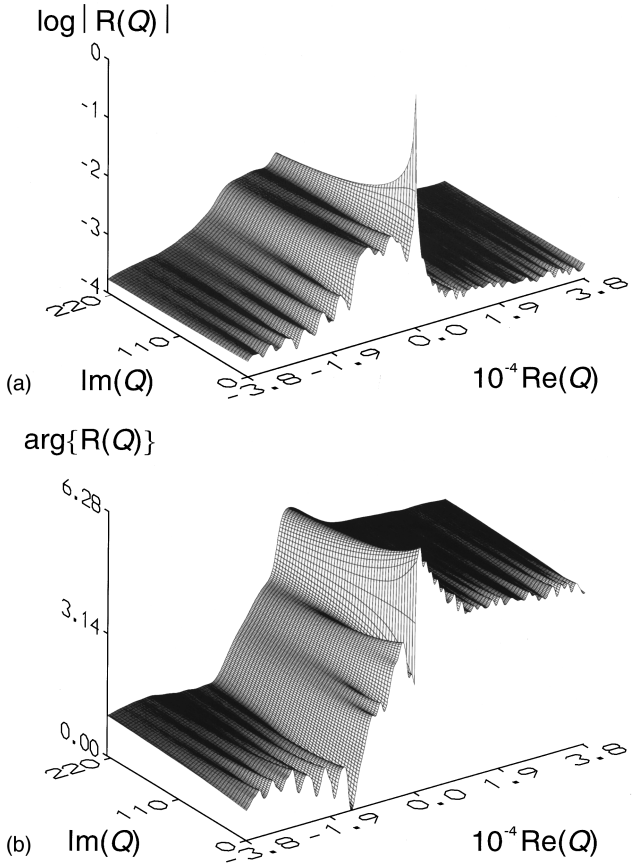

FIG. 1. Analytical continuation of the complex diffraction amplitude evaluated using a logarithmic dispersion relation: (a) is the modulus (on a logarithmic scale) and (b) is the phase of the analytically continued Bragg diffracted profile collected from the $Si_{1-x}Ge_x/Si$ sample for 1.54-Å radiation (Ref. 12). Interpolation has been implemented by a complex polynomial function of degree $N=55$.

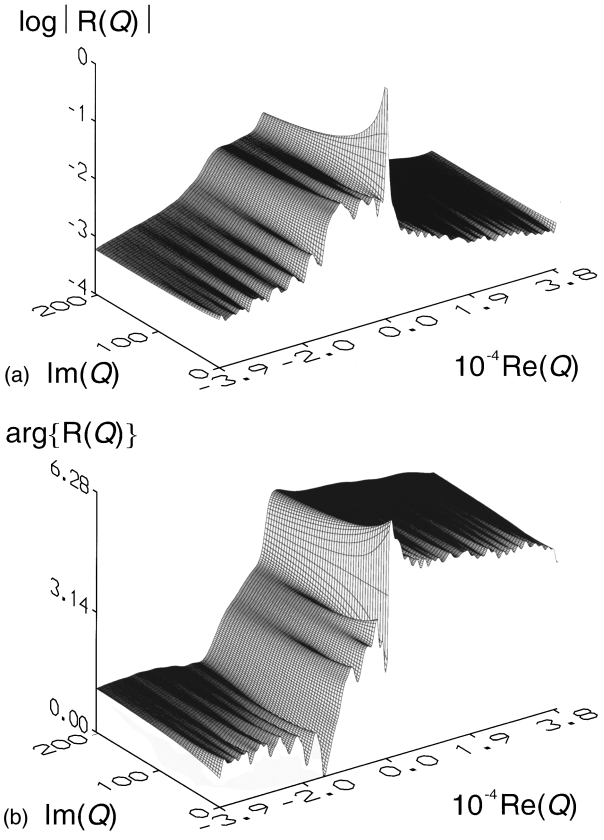

FIG. 2. Analytical continuation of the complex diffraction amplitude evaluated using a logarithmic dispersion relation: (a) is the modulus (on a logarithmic scale) and (b) is the phase of the analytically continued Bragg diffracted profile collected from the $Si_{1-x}Ge_x/Si$ sample for 0.71-Å radiation (Ref. 12). Interpolation has been implemented by a complex polynomial function of degree $N=55$.

IV. ANALYTICAL CONTINUATION OF THE COMPLEX DIFFRACTION AMPLITUDE FOR TWO RADIATION ENERGIES

Figures 1 and 2 represent the analytical continuation in the uhp of the complex diffraction amplitude calculated for the ''high-low'' SiGe/Si sample in the vicinity of the Si(400) reflection for 1.54- and 0.71-Å radiation, respectively.[12] The experimental intensity profiles have been collected at 512 equally stepped points each along the real axis within $q=\mathrm{Re}(Q)\cong\pm 3800$. These experimental parameters correspond to the depth resolution obtained for a structure-factor profile of $\Delta T=15$ Å, which is a record for a nondestructive diagnostic technique.[12] Since the lhp corresponds to a negative absorption coefficient, which does not make physical sense, we present the modulus [Figs. 1 and 2(a)] and phase [Figs. 1 and 2(b)] of the calculated complex diffraction amplitude profiles only in the uhp. Both modulus and phase distributions are plotted on a rectangular grid with 512×50 equal steps along the real and imaginary axes, respectively. Analytical continuation of the diffraction amplitude, shown in Figs. 1 and 2, are calculated for a polynomial function of degree $N=55$.

There is a minimum number of sublayers and, thus, polynomial roots, that needs to be considered. This number can be determined from the ''tail'' of the Fourier transform of the normalized experimental intensity.[9,17] However, improved confidence in the resulting crystal structure-factor profile is obtained by analyzing a slightly larger number of sublayers that is equal to the number of polynomial roots evaluated from the analytical continuation of the complex diffraction amplitude. A larger number of roots, consequently a large number of points in the crystal depth, allows one to explicitly observe a fragment in the resulting crystal structure-factor profile that corresponds to the perfect structure in the substrate. The minimum number of layers that can be analyzed was found to be about 40.[12] The degree of the polynomial function that was used to interpolate the complex diffraction amplitude was selected to be $N=55$.

Having two radiation energies and, thus, two different attenuation coefficients μ_1 and μ_2 we can measure two sets of experimental intensity profiles within the same (or very close) range of wave numbers:[11,12]

$$I_j(Q_j)=|R_j(Q_j)|^2=|R_j(q+i\mu_j)|^2. \tag{6}$$

The phase of $R_j(Q_j)$, where $j=1$ or 2, can be determined via a logarithmic-dispersion relation (2) that in this case has the following form:

$$\varphi_j(Q_j) = -\frac{1}{\pi} \mathrm{P} \int_{-\infty}^{\infty} \frac{\ln|R_j(Q_j')|}{Q_j' - Q_j} dQ_j' + 2\sum_m \arg(Q_j - Q_j^m)$$

$$= \varphi_j^{\min} + \sum_m \varphi_j^m . \quad (7)$$

In practice it is preferable to use the normalized experimental intensity $\hat{R}(Q) = -iQR(Q)$ (Refs. 6 and 9) instead of the directly measured $R(Q) = \sqrt{I(Q)}$ for the evaluation of the integral. The modulus of the Fourier transform of the normalized intensity is zero below a depth corresponding to the thickness of the damaged layer. This useful substitution of the experimentally measured intensity obviously guarantees the convergence of the integral in Eqs. (2), (4), and (7).[9] In addition, it is impossible in practice to measure the experimental intensity profile from minus to plus infinity, as is required for the formal limits of the integral. In practice, however, an evaluation of the integral taken over a range wider than $\Delta q^{-\max} \cong \Delta q^{+\max} \cong 100$ gives an adequate result. This problem has been addressed elsewhere.[17]

The most important question now is what is true and what is artefact in the analytical continuation presented in Figs. 1 and 2? Since we stated that the analytical continuation (3) defines the complex diffraction amplitude uniquely, the modulus and phase should have been identical in the plots 1 and 2. They are similar in major features indeed, but not identical.

To make explicit the last point of the concept of the unique representation of the complex diffraction amplitude via its zeros, we should remember that we do not know and, most importantly, we can never know, all the true zeros of the complex diffraction amplitude. Analytical continuations (Figs. 1 and 2) were calculated using only one true ''slice'' of the modulus of the diffraction amplitude, that is, the experimental data profile for each two-dimensional plot. Therefore, most of the zeros occurring in the calculated analytical continuations (Figs. 1 and 2) are virtual, mathematical, zeros. They do not correspond to the true two-dimensional profile of the complex diffraction amplitude and they are different for each calculation. If, however, there are true zeros in the calculated analytical continuations (Figs. 1 and 2), then the latter might have similar general shapes, which is the case. Thus, the only correct information about the complex diffraction amplitude for these particular calculated analytical continuations (Figs. 1 and 2) is the measured experimental intensity and the physical zeros of the complex diffraction amplitude. They represent a small fraction (or even zero fraction) of the total number of virtual zeros calculated from the polynomial interpolation (3). The general shape of the profiles (Figs. 1 and 2) is, strictly speaking, incorrect. To determine the correct general shape of the complex diffraction amplitude we must know all the physical zeros, which are fundamentally unobtainable.

However, to solve the inverse problem, that is, to determine the crystal structure factor, it is sufficient to localize only those true zeros which occur within the measured range of the $\Delta q^{-\max} < \mathrm{Re}(Q^m) < \Delta q^{+\max}$. Thus, the problem now is to distinguish between the true and virtual zeros in the analytical continuations (Figs. 1 and 2). To resolve this issue we make another physical assumption, namely, the presence and location of the true zeros due to interference suppression of the scattered wave within the analyzed layer is intrinsic to a particular discrete representation of the structure-factor profile $\psi = \Sigma_{k=0}^{N} |\psi_k| e^{i\phi_k}$. This assumption allows us to determine the true zero locations in the analytical continuation of the complex diffraction amplitude (Figs. 1 and 2). Since the true zeros are intrinsic to the structure-factor profile and their locations do not depend on a mathematical/numerical implementation of the technique, analytical continuation of two complex diffraction amplitudes, obtained using two different radiation energies, should produce the *same* locations for the true zeros.

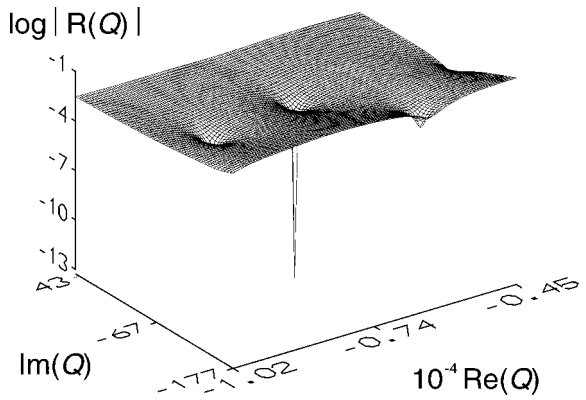

FIG. 3. Modulus (on a logarithmic scale) of the analytical continuation of the complex diffraction amplitude obtained from the experimentally measured Bragg diffracted profile from the $Si_{1-x}Ge_x$/Si sample for 1.54-Å radiation (Ref. 12) in the vicinity of zero No. 21.

Figures 3 and 4 show enlargements of the modulus of the analytical continuations (Figs. 1 and 2) in the lhp—the only place where the zeros can be calculated. This represents the narrow area around zero No. 21, which was found to be one of the true zeros and was included in the complete phase profile (7).[12] Zero No. 21 is in the center of each plot in Figs. 3 and 4. To improve the visibility of the plots in order to allow direct observation of the zeros, calculations were performed on a rectangular grid with 300×150 steps along the real and imaginary axes, respectively. There are other zeros that can be seen in the calculated profiles (Figs. 3 and 4).

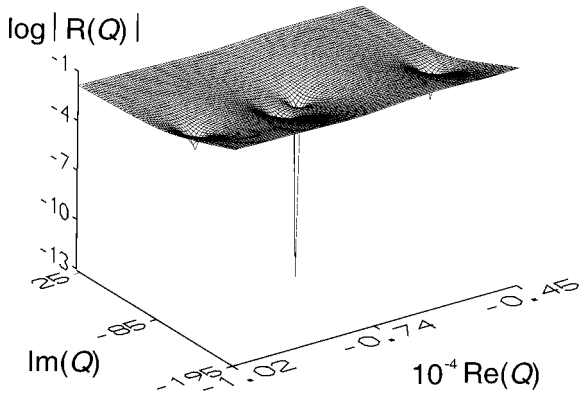

FIG. 4. Modulus (on a logarithmic scale) of the analytical continuation of the complex diffraction amplitude obtained from the experimentally measured Bragg diffracted profile from the $Si_{1-x}Ge_x$/Si sample for 0.71-Å radiation (Ref. 12) in the vicinity of zero No. 21.

However, even the greatly improved spatial resolution used for the calculation (Figs. 3 and 4) is not sufficient to resolve the locations of other zeros. The radiation energy must be selected with very high precision in order to observe a zero of the complex diffraction amplitude in an experiment. Yet, this is the only procedure for determining the true zero locations experimentally.

However, we can see from Figs. 3 and 4 that all other zeros, except for the central one, have quite different locations in the complex plane. This means that they are virtual (mathematical) zeros which should not be ''flipped'' in the uhp. The central zero, No. 21, in the calculation performed for the polynomial interpolation of degree $N55$, seems to be the true (physical) zero. Indeed, this zero was included, together with a few other true zeros, in the complete phase profile (7).[12] The crystal structure factor calculated for that complex diffraction amplitude gave remarkable agreement with the *a priori* knowledge of the sample under analysis and with results obtained by other means.[12]

Ideally, every zero calculated from Eq. (3) should be checked experimentally to determine whether it is located in the uhp. If the experiment, using the required radiation energy, shows a zero in the experimental intensity profile, this zero is the true one. If the experiment does not show the presence of a zero, this zero is not physical, but appears only because of the analytical properties of the complex diffraction amplitude and its analytical continuation (3). The position of such a zero in the analytical continuation depends on the numerical procedure used to approximate the solution. However, such a comprehensive experimental procedure does not seem to be feasible.

The problem of the zeros occurring in the experimental intensity is also intrinsic to other inversion methods, e.g., using the transport of intensity equation.[20,21] Imaging techniques usually deal with two-dimensional intensity distributions. It was shown in Ref. 22 that in the presence of zeros the phase-reconstruction problem cannot be solved uniquely. It seems that for some cases involving imaging based on inversion methods the suggested multi-energy formalism can be useful.

V. CONCLUSION

The complex diffraction amplitude in Bragg diffraction is represented as a unique product of its zeros. The analytical property of the complex diffraction amplitude allows the phase to be retrieved via a logarithmic dispersion relation. However, this creates a large number of virtual zeros that are difficult to distinguish from the true zeros. To determine the locations of the true zeros of the complex diffraction amplitude it is necessary to consider the analytical continuation of the diffraction amplitude in the whole complex plane. Since an experimental intensity profile always has a discrete representation, a comprehensive examination of the limited number of complex zeros allows one to determine the locations of the true zeros unambiguously. The inverse problem can then be solved uniquely, which allows the direct model-independent characterization of modern sophisticated semiconductor devices with a remarkable spatial resolution of about 10–15 Å.

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