Reply to "Comment on 'Three-dimensional imaging of a phase object from a single sample orientation using an optical laser' "

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In a technical comment to our paper [Phys. Rev. B **84**, 224104 (2011)], Wei and Liu criticized our work without providing theoretical, numerical, or experimental evidence. Furthermore, we believe they misinterpreted our matrix rank analysis of ankylography and their statements about our experiment are inaccurate. Below is our detailed point-by-point response to their criticisms.

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Wei and Liu commented on the section of "Matrix Rank Analysis of Ankylography" in Ref. 1, saying "The sum of the presented equations amount to reformulating the equation of far-field diffraction

$$F(k_x,k_y,k_z) = \int \rho(x,y,z)e^{-2\pi i(k_x x+k_y y+k_z z)}dx\,dy\,dz \qquad (1)$$

into a matrix equation $BX = A$ or $B'X' = A$"[2] This statement is incorrect. Equation (1) represents the three-dimensional (3D) Fourier transform of an object and the discretization of this equation (i.e., the discrete form of the 3D Fourier transform) is well known. However, our matrix analysis in Ref. 1 is to related a 3D real object, $\rho(x,y,z)$, to the Fourier components, $F(k_x,k_y,k_z)$, oversampled on a spherical shell with one voxel thick. In our paper,[1] we specifically stated that "*Eq. (1) (in Ref. 1) is not the discrete Fourier transform relation as the reciprocal-space vectors on the spherical shell* (k_x, k_y, k_z) *are not independent, but related via* $(N-1/2)^2 \leqslant k_x^2 + k_y^2 + (k_z+N)^2 < (N+1/2)^2$." In the derivation, we separated the real and imaginary parts of $F(k_x,k_y,k_z)$ as each part corresponds to an independent equation. We then obtained a matrix relation $BX = A$ [i.e., Eq. (2) in Ref. 1], where X is a matrix representing the real object, A is a matrix representing the Fourier components oversampled on a spherical shell, and B is a 2D (but not a square) matrix consisting of the sine and cosine functions. In order to perform a quantitative analysis, we padded X with zeros to obtain $B'X' = A$ where B' is a square matrix, allowing us to calculate the rank of matrix B'. Padding an object with zeros is equivalent to oversampling of its Fourier transform, which has been well established in coherent diffraction imaging (CDI),[3,4] and is also an important requirement in ankylography.[5]

By using $B'X' = A$, we first calculated the rank of B' for a $7 \times 7 \times 7$ voxel object. With the oversampling degree (O_d, defined in Ref. 5) of 1.14 and tolerance of 10^{-3}, we computed the rank of B' to be larger than the total number of unknown variables. We also calculated the rank of B' for a $14 \times 14 \times 14$ voxel object with $O_d = 2.06$. In this case, the rank of B' is larger than the number of unknown variables with tolerance of 10^{-6}, but smaller with tolerance of 10^{-3}. When O_d is increased to be ∼4.0, the rank of B' (with tolerance of 10^{-3}) is larger than the number of unknown variables. The matrix rank analysis suggests that when the object array is larger, the tolerance becomes smaller in order to maintain full rank of the sampling matrix, and the ankylographic reconstruction becomes more challenging without additional constraints and information, which is consistent with the numerical experiment results[5,6] as well as the statement "we also noted that when the array size of the 3D object becomes larger, the ankylographic reconstruction requires additional constraints," that we made in Ref. 5. The matrix rank calculation was computed by using a MATLAB routine, $k = \text{rank}(A, tol)$,[1] where k is the rank, A is a matrix, and tol is tolerance. This routine returns the number of singular values of A that are larger than tol. In matrix rank calculation, tolerance defines a level such that the number of singular values greater than this level is the rank of input matrix. This definition is well known (see, e.g., Refs. 7 and 8) and can also be found in a MATLAB manual.

Wei and Liu also commented on our experiment, saying "However, the authors seem to have confused a 3D-supported scattering object of actually 2D complexity with a 3D-distributed scattering object of truly 3D complexity. Although the employed phase object is 3D-supported, namely, occupying a 3D volume, its structure is too simple to represent a general 3D distribution of a scattering object, which has 3D complexity and exhibits variations inside the support volume. By contrast, the weak phase object in question remains constant inside its support volume, and belongs to a class of sparse 3D objects with 2D complexity…".[2] This statement is inaccurate. First, in our experiment, a phase object consists of a dense raftlike arrangement of four alphabet letters (*WWWA*) in close proximity; as fabricated, each platelike letter is about 4 μm wide $\times$ 7 μm tall $\times$ 1 μm thick.[1] The sample was supported on a silicon nitride membrane of 100 nm thickness. To increase the depth of the sample along the Z (beam) axis, the silicon nitride membrane was tilted about 45° relative to the incident beam. The projection length of the object in the X, Y, and Z axes is ∼19 μm, ∼23 μm, and ∼23 μm, respectively. Thus the depth of the object is as large as that of the width and length. Second, the phase object in our experiment is *not* constant inside its support volume. In the ankylographic reconstruction, we started with a loose support to determine a tight support. The tight support was then used to reconstruct a 3D structure. In our reconstruction, we did not enforce the density inside the support to be constant. As shown in Fig. 4

in Ref. 1, the variation of the reconstructed 3D structure is clearly visible inside the object.

As described in our report,[9] ankylography, which under certain circumstances recovers 3D structure information from oversampled diffraction intensities on a spherical shell, is an ill-posed problem and inherently not a general method. However, an ill-posed problem does not mean it cannot be practically dealt with. For example, 3D structure may be determined from a 1D atomic pair distribution function[10] or powder diffraction patterns[11] through the use of constraints. Both methods aim to reconstruct a 3D structure from a 1D diffraction intensity distribution (i.e., an ill-posed problem), which is in principle more difficult than ankylography. Furthermore, a recent paper shows that the atomic position of a two-layer graphene structure can be determined at subangstrom resolution along the Z direction from a single view.[12] This work exploited in real space is conceptually related to ankylography implemented in Fourier space as both use the curvature of the Ewald sphere to extract the three-dimensional information.

In conclusion, we believe that Wei and Liu misinterpreted our matrix rank analysis and their statements about our experiment are inaccurate. To facilitate a better understanding of ankylography, we have posted the ankylographic reconstruction codes in MATLAB on a public website[6] and encourage interested readers to download the codes and test the method.

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[6] www.physics.ucla.edu/research/imaging/Ankylography. [Three numerical experiments of ankylographic reconstructions and the MATLAB source codes have been posted on this website: (i) numerical simulation on the ankylographic reconstruction of a 3D "UCLA" pattern with 7 × 7 × 7 voxels; (ii) numerical simulation on the ankylographic reconstruction of a continuous 3D object with 14 × 14 × 14 voxels; and (iii) numerical simulation on the ankylographic reconstruction of a sodium silicate glass structure with 25 × 25 × 25 voxels consisting of 365 atoms.]

[7] http://www.itl.nist.gov/div898/software/dataplot/refman2/ch4/mat_rank.pdf.

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