

Understanding & Exploiting Diffraction in Optical Radiation Measurements

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COAM

ABSTRACT

Optical diffraction has been used for the first time to measure aperture area. The results are compared to measurements made using several other techniques, including a new radiometric technique developed during the course of this project. Diffraction code based on a Feynman path integral formulation and valid in the Fresnel regime has been written. This is a first step in the anticipated future development of more accurate diffraction code for radiometry.

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1 INTRODUCTION

Optical diffraction is a mature topic in physics. Many theoretical treatments of varying degrees of complexity are well known, ranging from the Huygens wavelet approach to numerical solutions of Maxwell's equations. Nevertheless in several situations of practical importance and/or theoretical interest the full effects of diffraction have either not yet been computed to the accuracies desired or have not been measured. Furthermore while diffraction is often regarded as a complicating factor in optical measurements, the sensitivity of diffraction to apparatus dimensions raises the question of whether diffraction can play a useful and direct role in measurement. The potential exploitation of diffraction for metrology is an unexplored avenue.

One of the most important measurements in radiometry is the measurement of *radiance*. Since an aperture of some sort is necessary for this measurement in order to construct a solid angle, the effects of diffraction must be accurately calculable for the highest accuracy radiance measurements. Even the most sophisticated primary standard radiometer which minimises diffraction effects by creating a pseudo-infinite radiating source requires a diffraction correction. At present diffraction is one of the main uncertainties limiting primary and secondary standard radiometric accuracy.

For the relatively large aperture sizes used in radiometers, classical diffraction theory is adequate in principle even though work is required to achieve lower computational uncertainties. On the other hand, for very small apertures approaching sizes of a few wavelengths the assumptions of most diffraction theories break down. In particular chromatic and polarisation effects become pronounced and both calculations and experiments with useful accuracy are extremely difficult to achieve. Nevertheless arrays of ultrasmall apertures have been considered for use as spectral filters.

Diffraction by apertures of intermediate size (i.e. of order 100 wavelengths) is theoretically tractable, since small-scale effects are negligible and the far field case, which generally allows significant simplification of the equations, is realisable in the laboratory. In this case the intriguing possibility exists of working "backwards" from diffraction in order to determine the dimensions of the aperture itself. This would be metrologically important as a new kind of dimensional measurement technique based on the use of light.

These considerations have led to a two pronged investigation of unresolved issues in diffraction: to exploit diffraction for measuring aperture size, and to develop more accurate diffraction code for radiometry.

2 APERTURE MEASUREMENT BY DIFFRACTION

2.1 Aperture Measurement by Diffraction: Theory

The aperture measurement technique based on diffraction exploits the well known fact that far from the diffracting aperture, the light field of the diffraction pattern is the fourier transform of the light field in the aperture plane.¹ In principle then, the distant diffraction field, both amplitude and phase, can be measured and transformed by fast fourier transform code to yield the complete two dimensional aperture function. In practice, however, measuring the *phase* of the light field would introduce great complexity into the experimental apparatus. It is doubtful that sufficient measurement accuracy

could be attained.

To solve this problem, we have adopted a technique developed for high resolution astronomical imaging called *phase retrieval*. In this technique only the modulus (squared) of the diffraction pattern is measured. An iterative fourier transform process yields a reconstruction of the phase of the field, which in turn enables the reconstruction of the diffracting aperture.

The fourier transform phase retrieval (FTPR) method has been described in the literature.² A flowchart outlining the method is shown in Figure 1. The far-field diffraction pattern is measured and the modulus is straightforwardly obtained. A mock phase for the diffracted field is multiplied by the actual modulus and the product (DF1) is fourier transformed. Certain constraints can be applied to the resultant expression, such as boundary conditions for the field based on a rough knowledge of the aperture size. The constrained field then represents a first-round approximation of the field in the aperture plane (AF1). AF1 is then fourier transformed and the resultant modulus is replaced by the true modulus to yield a new approximation of the diffracted field (DF2). This cycle is iterated until convergence is achieved, at which point $AF(j) = AF(j+1)$. In practice convergence is normally achieved in a reasonable time on desktop computer. On a 266 MHz Pentium II machine, 100 iterations takes 18 seconds for a 128x128 diffraction pattern, 400 seconds for a 512x512 pattern, and 27000 seconds for a 1024x1024 pattern. Convergence was not achieved in some cases when the diffraction data was noticeably distorted either by drift in the baseline or by a “washing out” of the pattern when insufficient time was allowed for each measurement.

The FTPR software was developed into an executable named PHASERET with an easy to use front-end which reads data from a standard spreadsheet format. It will run on any standard issue NPL PC.

2.2 Aperture Measurement by Diffraction: Experiment

Several factors affecting the FTPR calculation were tested by numerical simulation experiments:

- The number of diffraction zones measured, e.g. the number of rings in the diffraction pattern of a disk. When only 3 zones were put into the calculation, an error of 2% resulted. This error dropped to 0.2% for 8 zones and 0.1% for 16 zones. Typically 10-12 zones of diffraction were measured in the actual optical experiments.
- The number of data points per zone. The calculation was less sensitive to this factor. In actual diffraction measurements an average of 10 measurements per zone were typically acquired. Numerical results indicated the resultant uncertainty to be ca. 0.05%.
- Small random or cyclical fluctuations in the laser power. Mock data was generated by computing diffraction patterns from analytical expressions with fluctuations of up to 2% imposed. The effect on the FTPR calculation was trivial, typically 0.05%.
- Baseline subtraction. The FTPR code automatically finds the baseline, so baseline drift can lead to unpredictable errors or, as stated above, non-convergence.

The apparatus constructed to measure diffraction is shown schematically in Figure 2. A 30mW helium neon laser ($\lambda=632.8$ nm) was spatially filtered and intensity stabilised to better than 0.2% over 12 hours. The polarisation incident on the aperture was either vertical or horizontal, depending on the orientations of the half waveplate and polarisers. The beam exiting the spatial filter was 4-6 mm in $1/e^2$ diameter and collimated, so the central portion of the field incident on an aperture of

order 100 μm was essentially uniform. The distance from the aperture to the measurement plane was measured by a calibrated inside micrometer. The detector unit was mounted on a 2-D translation stage with incremental encoders and maximum translation of 100 mm per axis. The stated accuracy of each stage (3 μm) was confirmed prior to use via a calibrated micrometer. The detector was a Hamamatsu model 1337 photodiode. A box with matt black interior enclosed the light-sensitive parts of the apparatus.

In order to determine aperture size by FTPR, it is important to ensure that the measured diffraction pattern is indeed a far-field pattern. An intuitive approach to identifying the far-field regime can be gleaned from Figure 3. Rays A and B emanate from the one edge of the aperture, while ray C emanates from the other. In an observation plane a distance L from the aperture, rays B and C interfere to contribute to the point in the diffraction pattern which is in the angular direction Θ with respect to the aperture normal. In the far-field ($L \rightarrow \infty$) rays A and C interfere to contribute to the analogous point in the diffraction pattern. Therefore, the far-field is effectively reached when A and B become equal to within a small fraction of a wavelength. For an aperture of dimension 100 μm and a wavelength 633 nm, the far-field is on the order of 0.5 meter from the aperture. This was confirmed by numerically generating diffraction patterns of disk and square apertures and comparing these via least-squares fitting to patterns generated by analytical expressions for far-field diffraction by these shapes.

A diffraction pattern of a few square inches typically took 6-12 hours to measure. Data was almost always acquired overnight in order to minimise thermal drift due to the intermittent presence of people, opening and closing the lab door, etc. Thermal stability was also found to be better with the room air conditioner switched off, since this unit's proportional control leads to pronounced temperature oscillations of ± 1 degree. (Although the laser stability was typically better than $\pm 0.1\%$, the laser power as measured through a small aperture mounted directly in front of the detector was typically no better than $\pm 0.5\%$ over several hours. This is believed to be due to fluctuations in local areas of the laser cross section originating in the crystal within the laser stabiliser module. The local environment within this crystal is temperature dependent.)

2.2 Aperture Measurement by Diffraction: Uncertainty Contributions

The following ($k=2$) uncertainty contributions to the aperture size measurement were determined for the experimental conditions outlined above. Types A & B uncertainties are to be added in quadrature.

Type B

• # zones measured:	0.15%
• # points per zone:	0.05%
• measurement of aperture-to-detector distance:	0.1%
• laser power fluctuation:	0.05%
• translation stage positioning uncertainty:	0.05%

Type A

(aperture dependent)

3 APERTURE MEASUREMENT BY MICROSCOPY

Measurements made by the FTPR method have been compared to those made by three types of microscopy: electron microscopy (EM), normal optical microscopy (OM), and calibrated image analysis (CIA). These microscopy measurements were done by the length metrology section at NPL. Additional OM measurements were done by us in order to test for long term degradation of the apertures.

In both EM and OM the aperture is mounted on a translatable platform. The position of the platform is measured to a small fraction of an optical wavelength by a laser interferometer. The aperture is viewed through a high power lens system and the length of line segments connecting two points on the aperture edge are measured. Thus these techniques are in essence “sampling” techniques in that a complete 2-D image can be built up only by measuring many 1-D sections. The ultimate accuracy of an aperture area measurement is limited by (1) the number of samples acquired and (2) the accuracy of each 1-D measurement. The severity of the first limitation depends on how much the aperture shape deviates from an ideal one. The second limitation is a result of fundamental wave physics. Since both EM and OM rely on imaging the aperture edge, the accuracy of each 1-D measurement is limited by the ultimate resolution of this image. For the case of OM this resolution is on the order of an optical wavelength (0.5 μm) whereas for EM it is on the order of the deBroglie wavelength of an energetic electron (5 nm).

In CIA a CCD chip is mounted in the focal plane of a lens system and the complete system (lens + CCD) is calibrated by viewing a 2-D object of known size. The calibrated system is then used to view the test aperture. The main limitation with CIA is, as in OM, the finite resolution in principle of the aperture image.

4 APERTURE MEASUREMENT BY INTEGRATED IRRADIANCE METHOD

4.1 Integrated Irradiance Method: Theory

As a further test of the accuracy of the FTPR method, a new radiometric aperture measurement technique was developed. This *Integrated Irradiance Method* (IIM) compares the measurement of the power in a laser beam with the power of the same beam incident on the aperture in question measured at an array of points. The two powers will be equal if the correct aperture size has been assumed. This simple method yields uncertainties better than 1% for the area of small (150 μm) apertures and should also be adaptable with lower uncertainty to larger apertures.

The method can be explained in one-dimension with the aid of Figure 4. The curve at the top of the figure represents the cross sectional irradiance $I(y)$ of a laser beam propagating parallel to the z-axis and incident on an aperture array parallel to the y-axis. The aperture array has a grid spacing of $c \equiv a + b$ and each aperture is a wide. The average irradiance of the beam across the i -th aperture is represented by the height of the i -th grey pillar and equals:

$$\frac{1}{a} \int_{y_i - \frac{a}{2}}^{y_i + \frac{a}{2}} I(y) dy \equiv A_i \quad (1)$$

where y_i is the midpoint of the i -th aperture.

The total power incident on the i -th aperture is simply the area of the i -th pillar:

$$aA_i \equiv P_{ai} \quad (2)$$

The irradiance between grey pillars, i.e. where the beam is incident on opaque sections of the aperture array, is not measured. However if the beam cross section is smooth between adjacent apertures, then the irradiance between any two apertures can be assumed to be the average of the irradiance on these two apertures. In other words, the average irradiance at the i -th opaque section of the array (B_i) is the average of the height of the i -th and the $(i+1)$ -th grey pillars,

$$\frac{A_i + A_{i+1}}{2} \equiv B_i \quad (3)$$

and the power incident on the i -th opaque section of the array is:

$$bB_i \equiv P_{bi} \quad (4)$$

In the figure B_i is represented by the height of the i -th white pillar.

Combining (2) and (4), the total power in the beam is then:

$$\sum_i (aA_i + bB_i) \equiv P_{tot} \quad (5)$$

This expression is essentially equivalent to the “rectangular rule” in elementary calculus for calculating the area under a curve. As a and b approach zero, the expression becomes more exact.

By substitution and rearrangement, equation (5) leads to the following expression for the aperture size:

$$a = \frac{\frac{c}{2} \sum_i (P_{ai} + P_{a(i+1)})}{P_{tot} - \frac{1}{2} \sum_i (P_{ai} - P_{a(i+1)})} \quad (6)$$

Therefore a can be straightforwardly calculated if the following quantities are measured:

- the grid spacing c
- the power transmitted through each aperture in the array P_i
- the total power in the beam P_{tot}

The three quantities listed above are generally easier to measure than a small aperture size. The total power in a laser beam can be measured by a single uniform photodiode. Similarly the laser power transmitted through a small aperture can also be accurately measured with a photodiode. Lastly, the aperture array can be simulated by moving a single aperture to all positions on the grid by means of a precision translation stage. The grid spacing c is then set by the user and read from the stage's encoder.

The generalisation to 2-D is straightforward (Refer to Figure 5). Here a square aperture of area a^2 oriented with sides parallel to the x - and y -axes has been assumed. (This assumption is made purely to simplify the equations. In fact the method can be shown to work equally well with

apertures of other shapes.) In the equations below, i is the row index of the array and j is the column index.

The irradiance and power at aperture position (i,j) are related as

$$a^2 A_{ij} = P_{ij} \quad (7)$$

and the irradiance and power at the adjacent opaque position are related as

$$abB_{ij} = P_{bij} \quad (8)$$

where

$$\frac{A_{ij} + A_{i(j+1)}}{2} \equiv B_{ij} \quad (9)$$

The power in row i is:

$$a \cdot \sum_j (aA_{ij} + bB_{ij}) \equiv P_{rowi} \quad (10)$$

The power in the opaque region between rows i and $(i+1)$ is:

$$\frac{b}{a} \cdot \frac{P_{rowi} + P_{row(i+1)}}{2} \equiv P_{browi}$$

The total integrated power is then:

$$\sum_i (P_{rowi} + P_{browi}) = P_{tot} \quad (11)$$

After substitution and rearrangement, equations (7)-(11) yield the following expression:

$$\begin{aligned} P_{tot} = & \frac{1}{a^2} \left\{ \frac{c^2}{4} \sum_i \sum_j \left(P_{ij} + P_{i(j+1)} + P_{(i+1)j} + P_{(i+1)(j+1)} \right) \right\} + \\ & \frac{1}{a} \left\{ \frac{c}{2} \sum_i \sum_j \left(P_{ij} + P_{i(j+1)} - P_{(i+1)j} - P_{(i+1)(j+1)} \right) \right\} + \\ & \left\{ \frac{1}{4} \sum_i \sum_j \left(P_{ij} - P_{i(j+1)} - P_{(i+1)j} + P_{(i+1)(j+1)} \right) \right\} \end{aligned} \quad (12)$$

(Note that for $a=c$, equation (12) reduces to $P_{tot} = \sum_i \sum_j P_{ij}$ as expected.)

Equation (12) is a quadratic equation in $\frac{1}{a}$, so just as in the 1-D case the aperture area can be directly calculated in terms of:

- the grid spacing c
- the power transmitted through each aperture in the array P_{ij}
- the total power in the beam P_{tot}

The final result of IIM is the aperture area, which for any aperture shape is a^2 .

4.2 Integrated Irradiance Method: Experiment

The diffraction measurement apparatus was used for all IIM measurements. The only modification was that the test aperture was mounted directly onto the translation stage a few centimeters in front

of the detector. The total laser beam power measurement was made using the same detector with the aperture removed. (The beam diameter was small enough so that at least 99.95% of its energy landed on the detector.) Special care was taken to minimise multiple reflections between the detector and the aperture mounting assembly, as these would lead to an anomalously large calculated aperture area.

Several numerical tests were done to test the sensitivity of IIM to experimental conditions.

- Since the laser beam is diffracted by the test aperture, the silicon detector sees a spread of angles of incidence. Calculations showed that the resultant error was less than 0.01%.
- Mock data, generated assuming a gaussian laser profile and a perfectly spaced grid, was fed into the IIM calculation. Surprisingly the beam need cover as few as 9 grid points to achieve better than 0.1% accuracy in the aperture size determination.
- Since the translations stages have finite positioning uncertainty, mock data was generated assuming some fluctuation in the grid spacing. Fluctuations on the order of the translation stage specification lead to errors of less than 0.03% when the grid spacing was less than twice the aperture size. Fluctuations twice as large led to errors of less than 0.05%. Increasing the grid spacing to several times the aperture size led to marginally increased errors.
- Calculations were also made assuming rectangular and circular aperture shapes with equivalent accuracy to the square aperture case.

5 APERTURE MEASUREMENT SUMMARY

Complete sets of aperture measurements by all of the techniques discussed above were acquired for a 150 μm square aperture and a 40 μm disk aperture. The results are shown in Figures 6 & 7.

These comparisons provide an important link in the traceability chain for the new technique. The results for apertures of dimension 150 μm diameter showed excellent agreement (i.e. agreement well within error bars) between all the measurements, with uncertainties at the 1% level for all techniques.

The major source of uncertainty in the optical microscopy techniques is the fundamental imaging resolution limit for a given wavelength, whereas for FTPR it is Type A uncertainty due to non-diffractive scattering by imperfections in the aperture. In principle electron microscopy is capable of orders of magnitude lower uncertainty. However, since this technique measures the distance from one edge to another, small imperfections in the aperture rim cannot be accurately mapped unless typically hundreds or thousands of individual measurements are made. When only a small number of measurements are made, which even then can take a day, the uncertainty is dominated by the size of the imperfections, which are typically of order 1% for this size aperture.

The FTPR results for a 40 μm aperture agreed with the microscopy results only to within a few percent. In this size regime the aperture thickness is comparable to the cross sectional size. Thus significant non-diffractive scattering occurs which distorts the diffraction measurement and the resulting fourier transform.

The IIM for the 150 μm square aperture were in excellent agreement with the results of the other measurement methods. The dominant uncertainty was due to the apparently random spread in the calculated aperture size after many trials. This is believed to be due to scattering from imperfections

in the aperture edge and land. Imperfections in the laser side of the aperture can scatter additional light into the aperture. On the other hand, imperfections on the detector side can scatter transmitted light such that it misses the detector.

The IIM results for a nominally 50 μm diameter disk aperture were in much poorer agreement with the microscopy results. This is not surprising given the much higher thickness-to-diameter ratio of this smaller aperture and the large edge imperfections resulting from its production by laser drilling.

A chart summarising key aspects of the various measurement techniques is shown in Figure 8.

6 FRESNEL DIFFRACTION CODE

Another strand of the diffraction project was to begin development of diffraction code. There were two motivations for this:

- Comparing measured and calculated diffraction patterns is one means by which aperture size can be determined.
- High accuracy diffraction code is required for the calculation of diffractive loss in radiometric apparatus.

After some initial work on the first of the above aims, it was decided to be unworkable. A huge number of calculated patterns would need to be generated quickly, and image comparison software would need to be developed.

The second of the aims remains a high priority and new code developed in this project is a good starting point. The new code is computationally efficient and can calculate Fresnel (and of course Fraunhofer) diffraction from any two dimensional object illuminated by a point source. A laser source can be simulated by moving the point source far from the diffracting object. This code was based upon the work of Dauger.³ Its novelty is the use of a Feynman Path integral formulation. The code was tested by computing diffraction patterns in cases where the result is known analytically, namely the far field cases for disks and rectangles.

This aspect of the project will continue as a CASE student project at Imperial College. In the preliminary phase of the studentship, diffraction code developed at NIST will be investigated.⁴

7 ULTRASMALL APERTURES

Diffraction theories come at various levels of sophistication. Generally the Kirchhoff model, which assumes an infinitely thin, perfectly opaque diffraction screen and a sharply delineated aperture edge, is capable of high enough accuracy for radiometric calculations. The next level up treats the diffraction screen as an infinitely thin, perfectly conducting plane. Then the diffraction problem is treated by solving Maxwells equations.^{1,5} However for apertures on the order of a wavelength in size, neither theory is sufficient to account for the effects of finite thickness, which is typically greater than the size parallel to the diffraction plane. Measurements by Butler of the transmittance of optical

radiation through a 10 μ m aperture shows rough agreement with the Maxwell theory and confirms the disparity between the physical size of the aperture and the effective size measured by spectral transmittance.⁶ A further anomaly of the optical properties of ultrasmall apertures was reported in measurements of the spectral transmittance of aperture arrays.⁷ Peak transmittances greater than the ratio of total aperture area to total beam cross sectional area were reported and attributed to surface plasmons. Measurements made at NPL on arrays of ultrasmall holes manufactured for ESA showed no evidence of anomalous transmittance peaks. At all wavelengths transmittance was lower than the ratio of total aperture area to total beam cross sectional area.

8 CONCLUSIONS

The Strategic Research project on diffraction has demonstrated that optical diffraction can be exploited to measure medium size apertures ($\geq 100\ \mu\text{m}$) with uncertainties comparable to those of microscopy methods. This new technique is of interest for several reasons.

- It measures area rather than distance, and so is inherently suited to 2-D measurements.
- It is fundamentally optical, providing the best evidence we know of to date of the agreement between physical and optical area for apertures of this size.
- The apparatus is relatively inexpensive to build and to maintain. Measurement costs are comparable to those of microscopy methods.
- Diffraction patterns can provide a diagnostic tool, in some cases via simple visual inspection, of the deviation of nominally round or square apertures from ideality.
- In the future high resolution pixel-by-pixel calibrated detector arrays may make diffraction measurements extremely rapid and accurate, making the FTPR method more attractive as a measurement tool.

The Integrated Irradiance Method is an unanticipated spin-off of this SR project. While FTPR is limited by reasons of practicality to aperture sizes on the order of 100 μ m, IIM can also be applied to larger apertures, perhaps even as large as several millimeters. Further development is necessary to determine the upper bound on aperture size and the ultimate uncertainty achievable. The lower bound on aperture size measurable by IIM is not limited by fundamental physics, as are FTPR and optical microscopy. However, the increased thickness-to-size ratio and edge defects of very small apertures does increase uncertainties of measurements obtained by IIM.

The diffraction calculation code developed in this project has provided a springboard for a CASE student project devoted to diffraction in radiometry.

9 FIGURES

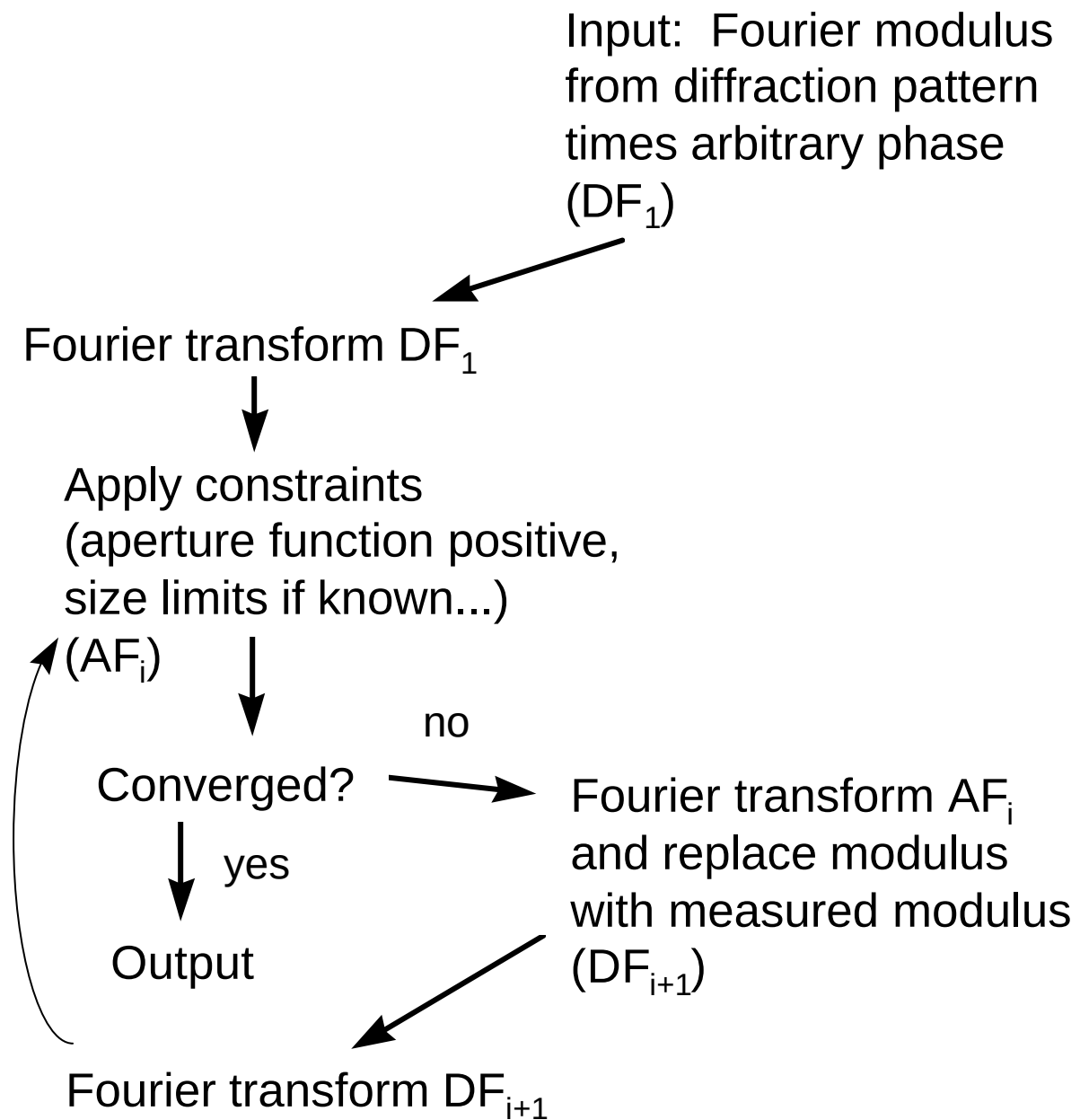
FIGURE 1: FOURIER TRANSFORM PHASE RETRIEVAL FLOWCHART

FIGURE 2: DIFFRACTION MEASUREMENT APPARATUS SCHEMATIC

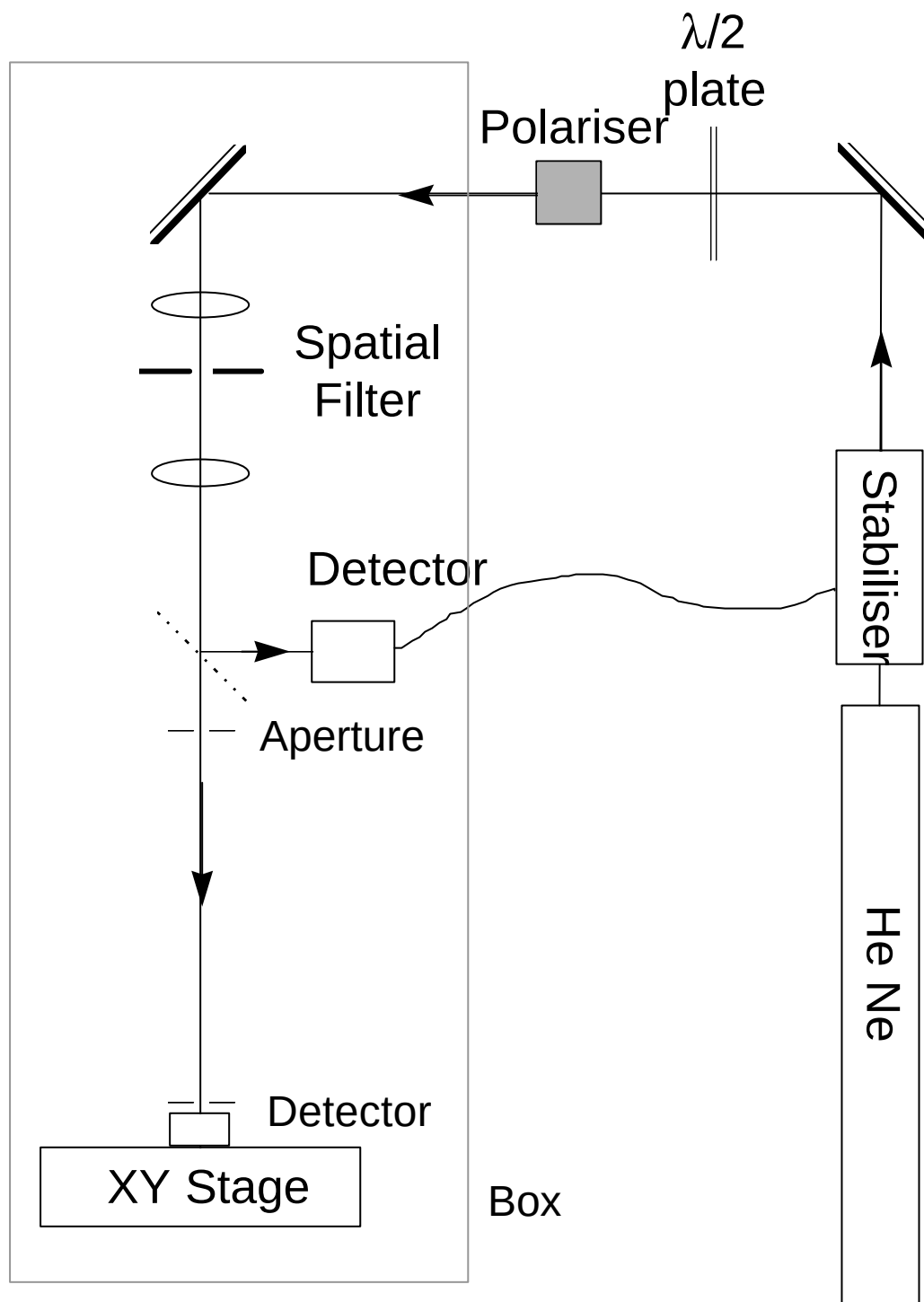


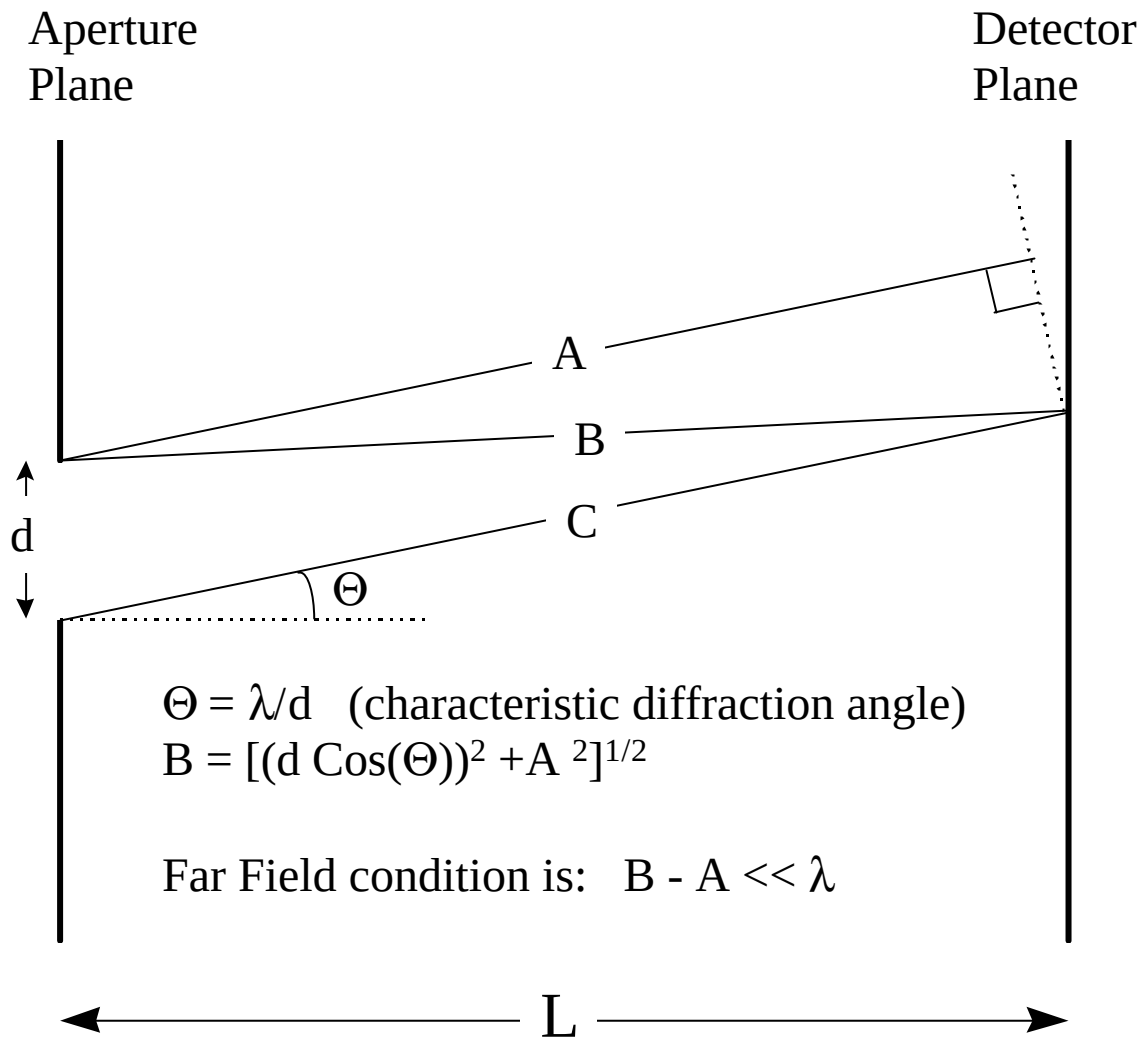
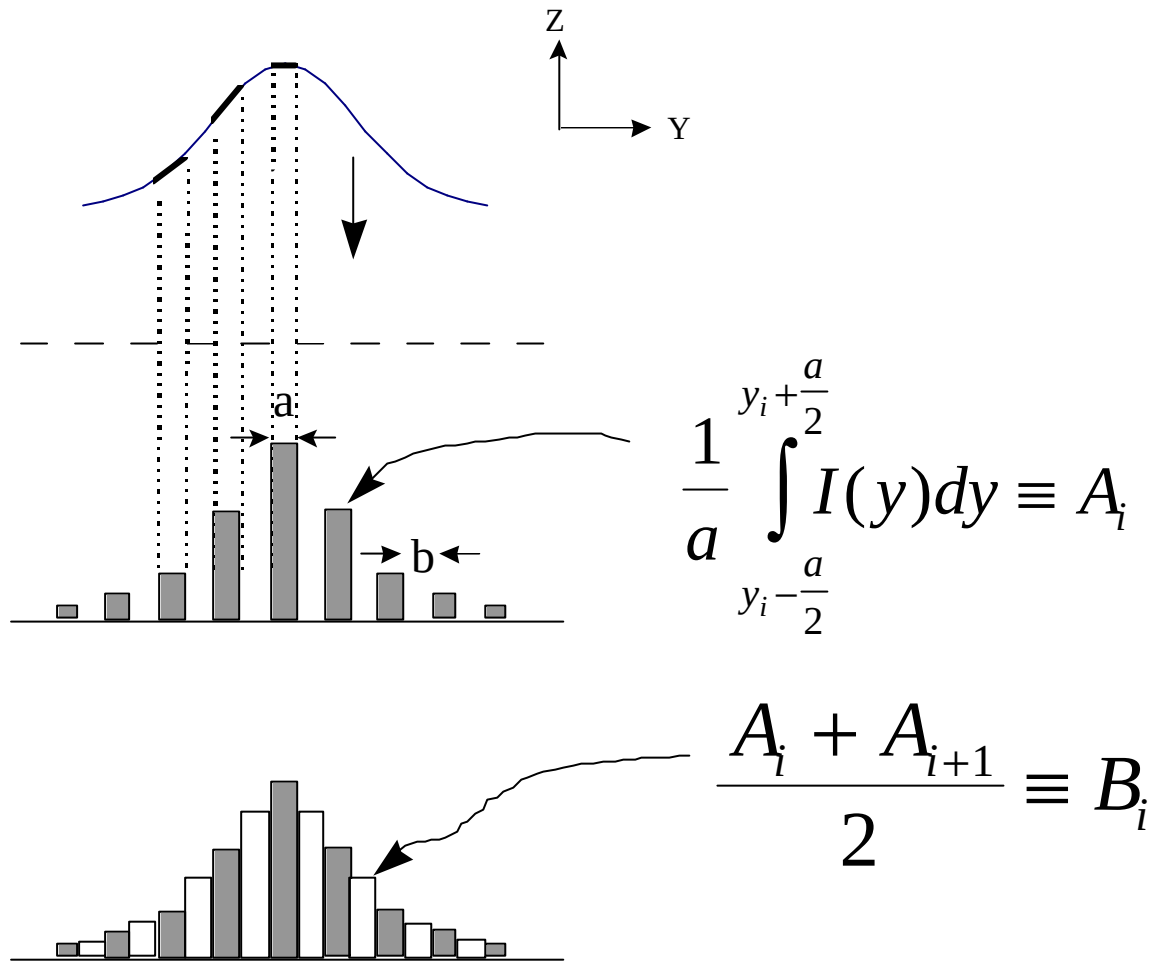
FIGURE 3: FAR FIELD REGIME SCHEMATIC

FIGURE 4: INTEGRATED IRRADIANCE METHOD IN ONE DIMENSION

$$TotalPower = \sum_i (aA_i + bB_i)$$

FIGURE 5: INTEGRATED IRRADIANCE METHOD IN TWO DIMENSIONS

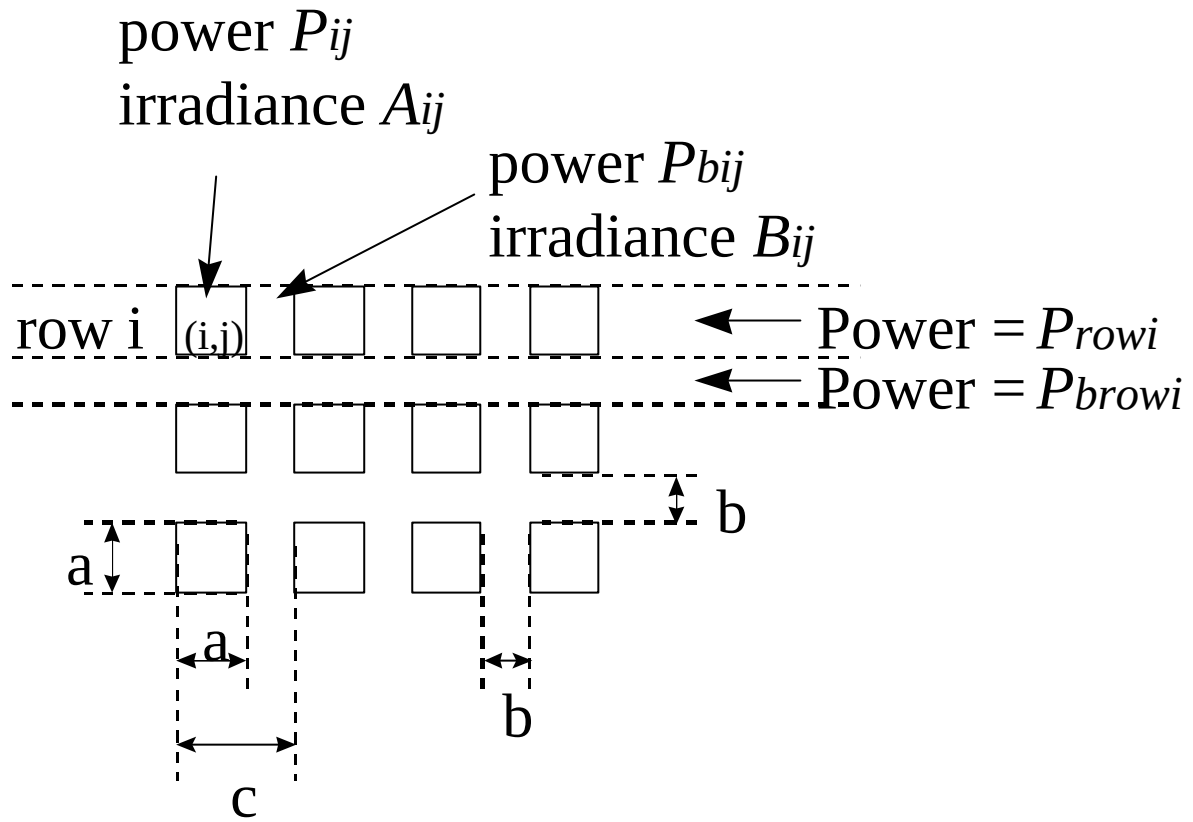


FIGURE 6: 150 μm SQUARE APERTURE MEASUREMENT RESULTS

nominally 150 μm square (copper, ca. 15 μm thick)	# measurements	Average width or Sqrt(Area) in μm	Uncertainty (k=2)
Electron Microscopy	6	144.60	0.7% per width
Optical Microscopy	8	145.6	1% per width
Calibrated Image Analysis	1	144.79	0.7%
Diffraction: FT Phase Retrieval	10	144.66	0.7%
Integrated Irradiance	3	144.63	0.2%

FIGURE 7: 40 μm DISK APERTURE MEASUREMENT RESULTS

nominally 40 μm dia disk (stainless steel, 13 μm thick)	# measurements	Average diameter in μm	Uncertainty (k=2)
Electron Microscopy	3	41.40	1.2%
Optical Microscopy	240	40.5	1%
Calibrated Image Analysis	----	----	----
Diffraction: FT Phase Retrieval	12	38.9	2.4%
Integrated Irradiance	11	40.5	1.5%

FIGURE 8: 40 μm DISK APERTURE MEASUREMENT RESULTS

	Dimensionality	Size Range	Accuracy	Measurement Person-Time
Electron Microscopy	1-D	> 100 nm	10 nm	1 day for 1 % of 100 μm
Optical Microscopy	1-D	10 μm - few mm's	1 μm 1% of 100 μm	1 day
Calibrated Image Analysis	2-D	10 μm - few mm's	1 μm 1% of 100 μm	1/2 day
Diffraction FT Phase Retrieval	2-D	50 μm - 400 μm	0.7 % of 150 μm	1 day
Integrated Irradiance	2-D	50 μm - few mm's	0.2 % of 150 μm 0.05% target	1/2 day

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