

INVESTIGATIONS OF SOME DIRECT AND INVERSE PROBLEMS IN X-RAY IN-LINE PHASE-CONTRAST IMAGING AND TOMOGRAPHY

by **Jelena Schmalz**

MSc (Mathematics) Moscow State University

A thesis submitted for the degree of Doctor of
Philosophy of the University of New England

October 2013

Abstract

In the present thesis several direct and inverse problems of X-ray in-line phase-contrast imaging and computed tomography are studied.

A general method for finding the fundamental solution of the Helmholtz equation subject to Sommerfeld radiation conditions is developed. Unlike the established techniques, this method provides all solutions to the Helmholtz equation before selecting the one that satisfies the chosen valid boundary conditions.

Sufficient conditions for the validity of Teague's method for solving the Transport of Intensity Equation are derived and an example of a solution, which cannot be obtained using this method, is provided.

Teague's method is also applied to tomography for the reconstruction of the three-dimensional refractive index distribution in a generic sample from in-line X-ray projections. The proposed solution simplifies and stabilises the reconstruction process. A formula is derived for the single-step reconstruction of a newly introduced auxiliary function. This function contains information about both the absorption index and the refractive index decrement. The reconstruction is obtained directly from the intensity measurements, without the intermediate step of phase retrieval for each illumination angle. A precise relationship is established between the newly introduced function and the complex refractive index distribution. The physical meaning of this function is examined for phase objects and for generic objects with slowly varying distributions of absorption index.

Some examples of possible applications of our results are discussed in Conclusions.

I certify that the substance of this thesis has not already been submitted for any degree and is not currently submitted for any other degree or qualification.

I certify that all help received in preparing this thesis and all sources used have been duly acknowledged in this thesis.



Acknowledgements

I am grateful to my supervisors Konstantin Pavlov and Timur Gureyev for their guidance and patience throughout the course of the PhD project.

I wish to thank my collaborators.

Chapter 7 is the result of collaboration with Gerd Schmalz, Timur Gureyev and Konstantin Pavlov.

Chapter 8 is the result of collaboration with Timur Gureyev, David Paganin and Konstantin Pavlov.

Chapter 9 is the result of collaboration with Thomas Baillie, Timur Gureyev and Konstantin Pavlov.

I am grateful to Gerd Schmalz and David Vine for their help with L^AT_EX. Imi Bokor helped me with questions concerning English usage.

This PhD was supported by an Australian Postgraduate Award, which I gratefully acknowledge.

Contents

Contents	1
List of Figures	4
List of Tables	5
1 Introduction	6
1.1 Historical and Theoretical Background of Phase Retrieval . . .	6
1.2 Application of the Propagation-Based Phase-Retrieval Method to X-Ray Computed Tomography	10
1.3 Structure of this Thesis	12
2 Helmholtz Equation	14
2.1 Introduction	14
2.2 Derivation of the Helmholtz Equation	14
2.3 Paraxial Helmholtz Equation in the Presence of Matter	17
3 X-ray Imaging	19
3.1 Introduction	19
3.2 Refractive index	20
3.3 Absorption Cross Section, Attenuation Coefficient, Absorption Index	21
3.4 Scattering, Refractive Index Decrement, Phase Contrast	23
3.5 Summary	24
4 Phase-Retrieval Methods	25
4.1 Introduction	25
4.2 X-Ray Interferometry	25
4.3 Analyser-Based Phase Retrieval	30
4.4 Grating-Based Method	33

4.5	Propagation-Based Phase-Retrieval Methods	35
4.6	Summary	38
5	The Transport of Intensity Equation	39
5.1	Introduction	39
5.2	Derivations of the Transport of Intensity Equation	40
5.3	Methods for Solving the TIE	42
5.4	Summary	43
6	X-ray Computed Tomography	44
6.1	History of the Development of Tomography	44
6.2	Mathematical Basis for Computed Tomography (CT)	45
6.3	Reconstruction of the Absorption Index β	49
6.4	Phase-Contrast X-Ray CT	50
7	Derivation of a Green's Function for the Helmholtz Equation Using Generalised Functions	51
7.1	Introduction	51
7.2	Generalised Functions	52
7.3	General Solution for Green's Functions for the Helmholtz Equation in Fourier Space	54
7.4	Green's Function for the Helmholtz Equation Subject to the Sommerfeld Boundary Conditions	57
7.5	Comparison with the ie-Technique	59
7.6	Summary	60
8	Teague's Method for Phase Retrieval, its Validity Conditions	61
8.1	Introduction	61
8.2	Notation	62
8.3	Teague's Solution of the Transport of Intensity Equation	63
8.4	Helmholtz's Theorem in 2D and the TIE	66
8.5	General Conditions for the Validity of Teague's Assumption . .	70
8.6	Solutions that Cannot Be Obtained Using Teague's Assumption	74
8.7	Summary	78

9 Simplifying the Reconstruction Algorithm for the Refractive Index Decrement	81
9.1 Introduction	81
9.2 Theoretical Background	81
9.3 Definition of an Auxiliary Function $\tilde{\delta}$	87
9.4 Physical Nature of the Auxiliary Function $\tilde{\delta}(\mathbf{x}, \mathbf{y}, \mathbf{z})$	88
9.5 Methods and Results	90
9.6 Summary	95
10 Conclusions	98
10.1 Green's Functions	98
10.2 Teague's Method	99
10.3 Auxiliary Function $\tilde{\delta}$	99
10.4 Future Applications	101
Bibliography	102
Appendix	120
A Definition and Properties of the Fourier Transform	120
B Solutions of the homogeneous Helmholtz equation	121
C Rotational symmetry and the Fourier transform	122
D Rotationally invariant generalised functions on the sphere	123
E Lemmata for Chapter 9	124

List of Figures

1.1	Generic phase-retrieval scenario using radiation or matter wavefields	7
3.1	Object plane illuminated by an X-ray plane wave	20
4.1	Bonse-Hart X-ray interferometer	26
4.2	Peaks in Fourier space, corresponding to summands of Equation (4.8)	28
4.3	(a) Wrapped phase (b) Unwrapped phase	29
4.4	Experimental scheme of analyser-based phase-contrast imaging . .	30
4.5	Rocking curve of the analyser for non-absorbing crystals	31
4.6	X-ray grating interferometer	34
4.7	Propagation-based phase-contrast imaging setup	36
6.1	Tomosynthesis or photographic laminography	45
6.2	Projection $P_\theta(f)$ maps a function $f(x, y, z)$ of the three-dimensional space into the set of its line integrals	46
6.3	The two-dimensional Fourier transforms of the projections $\mathbf{F}_2[P_\theta f](\xi', \eta)$ are defined on the planes which fill the three-dimensional Fourier space	48
8.1	Phase distribution, defined in $\Omega = (-10, 10) \times (-10, 10)(\mu\text{m}^2)$ as in the counter-example	75
8.2	Intensity distribution defined in Ω as in the counter-example . . .	76
8.3	Distribution of the function $-\text{div}(I(x, y)\nabla_\perp \phi(x, y))$ in Ω as in the counter-example	77
8.4	Distribution of the function $\psi(x, y) = \nabla_\perp^{-2} \text{div}(I(x, y)\nabla_\perp \phi(x, y))$ in Ω as in the counter-example	78
8.5	Distribution of the function $\tilde{\phi}(x, y) = \nabla_\perp^{-2} \text{div}(I^{-1}(x, y)\nabla_\perp \psi(x, y))$ in Ω as in the counter-example	79

8.6	Distribution of the error function $\epsilon(x, y) = \phi(x, y) - \tilde{\phi}(x, y)$ in Ω as in the counter-example	80
9.1	Generic layout of the in-line CT experimental setup	82
9.2	Structure of the simulated object	90
9.3	Reconstructed values using $\tilde{\delta}$ for the three objects with constant β	93
9.4	Reconstructed values using $\tilde{\delta}$ for the three objects with constant β and 5% Poisson noise	94
9.5	Auxiliary function $\tilde{\delta}$ and the reconstructed values of δ	95
9.6	Typical projection with an object-to-detector propagation distance of 10 cm	96

List of Tables

9.1	Components of refractive indices of certain real materials at a wavelength of 1 Å	92
9.2	Best-fit parameters used in Figures 9.3 and 9.4	93
9.3	Best-fit parameters used in Figure 9.5	94