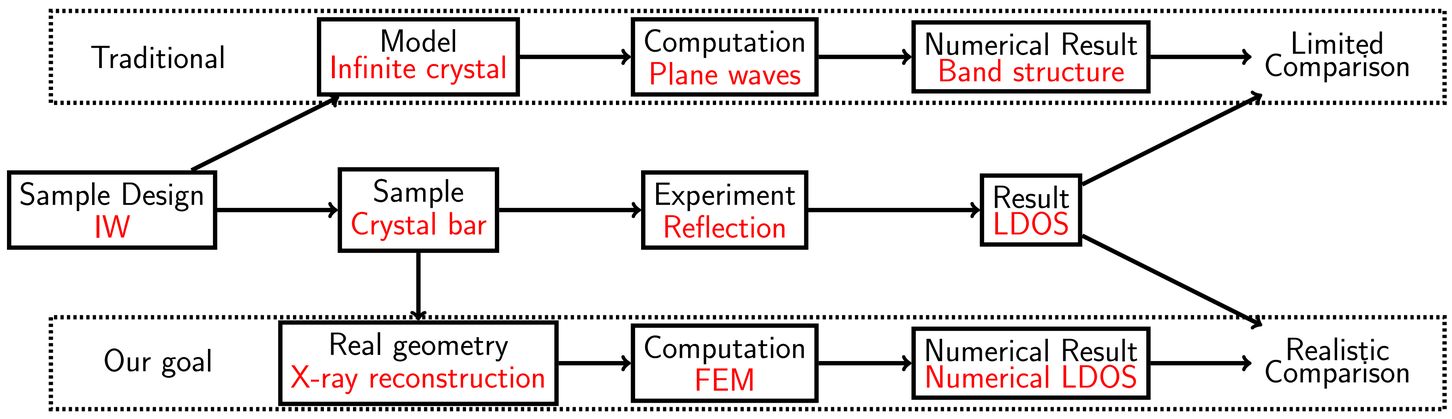
Simulating light propagation in a real photonic crystal: The first attempt

Lars J. Corbijn van Willenswaard[1,2], Jens Wehner[3], Nicolas Renaud[3], Matthias Schlottbom[1], Peter Cloetens[4], Jaap J.W. van der Vegt[1], and Willem L. Vos[2]

[1]Mathematics of Computational Science (MACS), University of Twente, The Netherlands
[2]Complex Photonic Systems (COPS), University of Twente, The Netherlands
[3]Netherlands eScience Centre, The Netherlands
[4]ESRF – The European Synchrotron, France

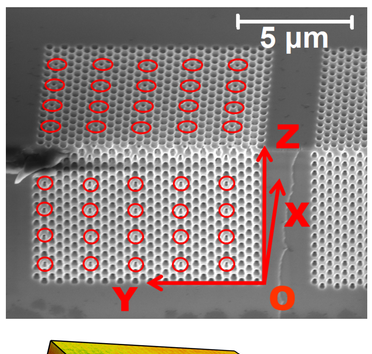
Introduction

- Typical simulations of photonic crystals use the idealized models of a perfect (infinite) crystal.
- Differences between simulation and experiments on real nanostructures are attributed to manufacturing effects and modelling assumptions.
- We aim to perform simulations based on the geometry of a real crystal, allowing for comparison with experiment with as little assumptions as possible.
- Here we discuss how to make the X-ray suitable as input for simulations and show first proof of principle results.

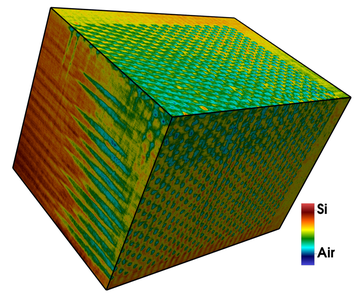


X-ray holotomography dataset

Scanning Electron Microscope (SEM) image of a photonic crystal with an Inverse Woodpile (IW) design consisting of 15^3 unit cells. The red circles highlight pores with intentionally reduced radius.

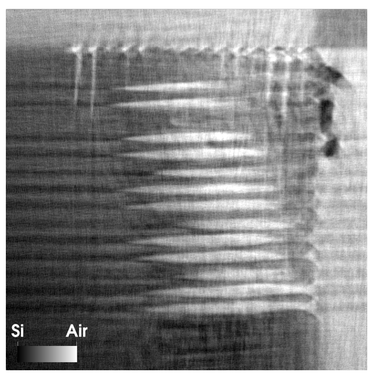


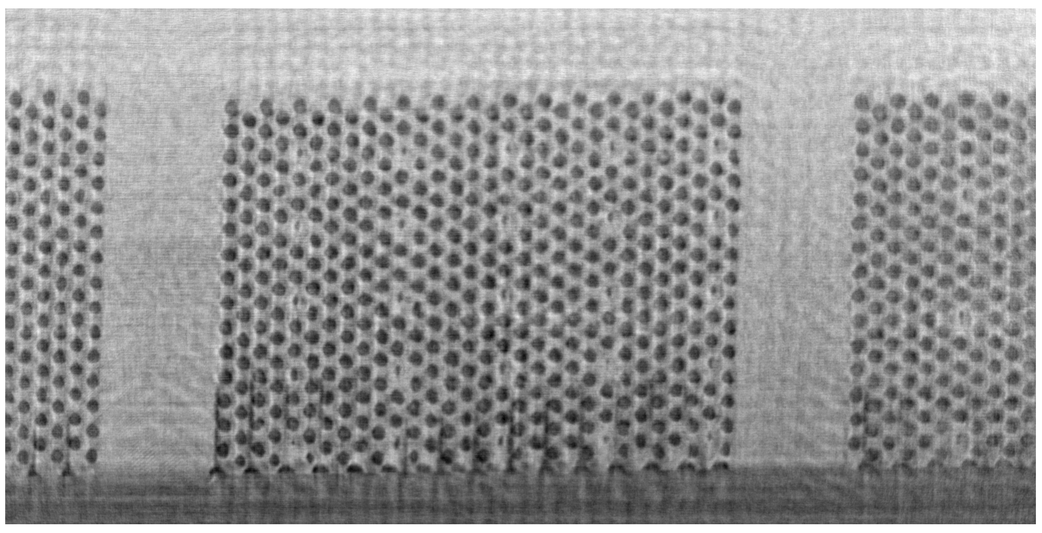
3D reconstruction from X-ray holotomography at the ESRF (ID-16A). Reconstruction is a two step process of phase retrieval followed by filtered back-projection [1]. A subvolume of 1108×800^2 voxels of $(10\,\text{nm})^3$ gives a birds-eye view of a single crystal.



Cross sections in XZ (right) and YZ (below) of the dataset reveal both manufacturing and reconstruction effects.

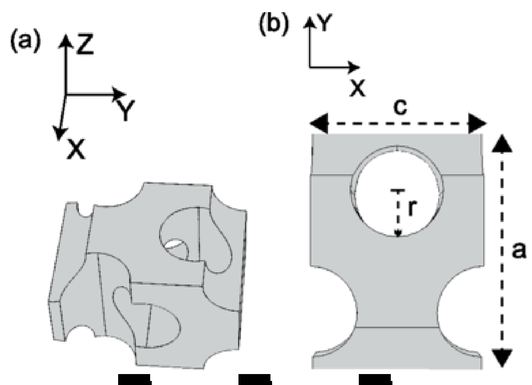
- Pores in the Z direction are much shorter due to manufacturing problems.
- Pores deviate from the perfect cylindrical design.
- Reconstruction artifacts from missing angles and periodicity of the structure [1].



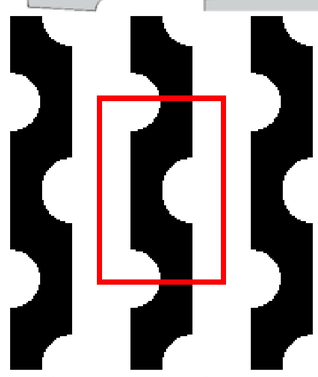


Proof of concept computation

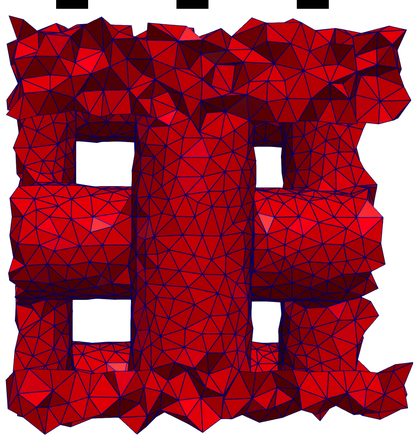
Design of a single unit cell of an Inverse Woodpile crystal [2]. The grey region corresponds to the silicon substrate, in which cylindrical pores are made. Typical values are $a = \sqrt{2}c = 680\,\text{nm}$ and $r = 0.24a \approx 160\,\text{nm}$.



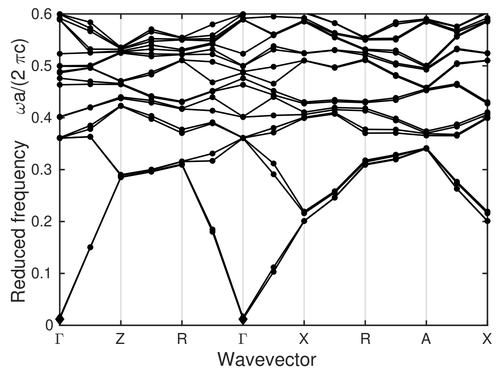
The design is converted into voxels to create a **synthetic** tomography dataset (white = air, black = silicon). The central unit cell is outlined in red. The lattice constants are such that the dataset is perfectly periodic, but does not match the real crystal sizes due to an inadvertent error.



A single unit cell from the synthetic X-ray dataset is selected. This unit cell is meshed using pygalmesh (CGAL [3]) to serve as input for a FEM computation. The tetrahedral mesh for the air fraction of the mesh is shown.



A photonic band structure is computed using our in-house Discontinuous Galerkin FEM (DGFEM) solver [4]. The generalized eigenvalue problems are solved using Krylov-Schur (SLEPc [5]) with shift-and-invert (direct solver MUMPS).



Further challenges (1)

Full crystal is too large for an accurate computation

- Truncate the domain → introduces artificial boundary
- Introduce artificial periodicity → Only possible in two directions
- Use 2D region of the crystal → reduces realism

Further challenges (2)

Only ONE dataset of the crystal:

- How to verify the accuracy of the results?
- How to minimize the effect of reconstruction artifacts?
- What to compute to gain the most knowledge?

references

[1] D.A. Grishina, C. Harteveld,..., P. Cloetens & W.L. Vos, ACS Nano 13 (2019) 13932
[2] K. M. Ho, C. T. Chan, ..., R. Biswas & M. Sigalas, Solid State Commun. 89 (1994) 413
[3] CGAL, Computational Geometry Algorithms Library, https://www.cgal.org
[4] Z. Lu, A. Cesmelioglu & J.J.W. van der Vegt, J. Sci. Comput. 70 (2017) 922
[5] V. Hernandez, J. E. Roman & V. Vidal, ACM Trans. Math. Software 31 (2005) 351