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Simulating physics of tomographically reconstructed photonic crystals

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

1. Complex Photonic Systems (COPS), MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

2. Mathematics of Computational Science (MACS), MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

3. Netherlands eScience Center, Science park 140, 1098 XG Amsterdam, The Netherlands

4. ESRF–The European Synchrotron, CS50220, 38043 Grenoble, France

Computational methods have proven to be essential in the design of three-dimensional (3D) photonic crystals [1]. They have allowed the prediction of the properties of the photonic crystal design without expensive manufacturing steps. Additionally, computations are used to interpret experimental results from real crystals. Interestingly, the fabrication of photonic crystals is necessarily never perfect as structural differences from the design are inevitable [2,3]. This structural mismatch between design and realization means that experimental results (transmission, reflection) are not faithfully interpreted, as the physical model (plane-wave expansion) does not have the true structural realization as input.

Here we propose a procedure to overcome this mismatch by using a reconstruction of the structure of a real photonic crystal. As starting point we use the reconstructed electron density of an 3D inverse woodpile crystal Fig. 1a that was obtained by X-ray holotomography [2]. Several preprocessing steps are taken to remove artifacts from the reconstruction. A small part of the reconstructed crystal is chosen as input for computations, as the whole crystal volume is so large that computations exceed memory and CPU needs. For the computation we want sufficient accuracy to study the fabrication effects , hence discretiztion effects should be smaller than real structural details. Therefore, we use a Discontinuous Galerkin Finite Element Method [1,4], as such a method can accurately handle the sharp and detailed boundary between air and silicon. We show first results based on synthetic perfect structures, see Fig. 1b since this allows comparison with previous work [4,5].

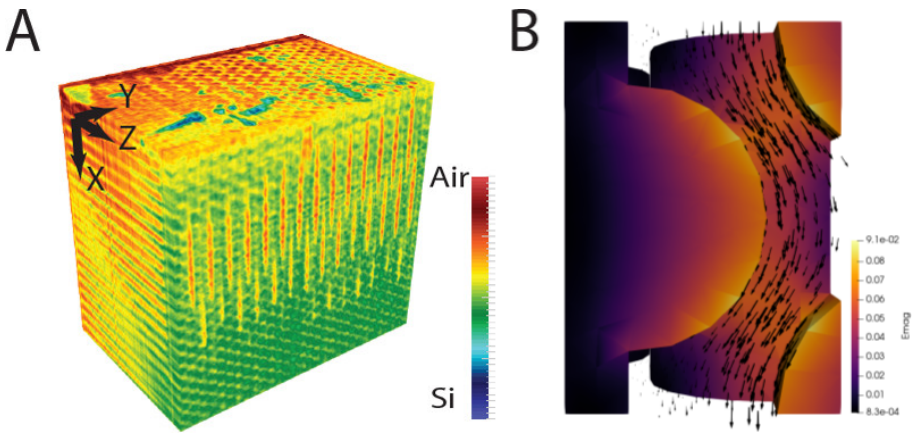

Fig. 1 a) Reconstruction of the electron density of a Si inverse woodpile photonic crystal obtained using X-ray holotomography [2]. b) Electric field from the lowest Bloch mode inside an inverse woodpile, computed using DivDGMax. The magnitude of the normalized electric field inside the pores is shown in color, and arrows in the Si region show the real part of the electric field.

To validate our novel approach, we analyze assumptions (numerical, physical) that are inevitable in each step and that affect the computational result. We will discuss the choices, and how they impact the goal of making computations that are as close as possible to experimental reality.

References

[1] K. Busch, M. König, J.Niegemann, "Discontinuous Galerkin Methods in nanophotonics," Laser Photonics Rev. **5**, 773 (2011)

[2] D.A. Grishina, C.A.M. Harteveld, A. Pacureanu, D. Devashish, A. Lagendijk, P. Cloetens and W. L. Vos, "X-ray Imaging of Functional Three-Dimensional Nanostructures on Massive Substrates," ACS Nano **13**, 13932 (2019)

[3] W. Bogaerts, R. Baets, P. Dumon, V. Wiaux, S. Beckx, D. Taillaert, B. Luyssaert, J. Van Campenhout, P. Bienstman and D. Van Thourhout, "Nanophotonic waveguides in silicon-on-insulator fabricated with CMOS technology," J. Lightwave Tech **23** 401 (2005)

[4] Z. Lu, A. Cesmelioglu, J.J.W. van der Vegt, and Y. Xu, "Discontinuous Galerkin approximations for computing electromagnetic Bloch modes in photonic crystals," J. Sci. Comput. **70**, 922 (2017)

[5] D. Devashish, S. B. Hasan, J. J. W. van der Vegt, and W. L. Vos, "Reflectivity calculated for a three-dimensional silicon photonic band gap crystal with finite support," Phys. Rev. B **95**, 155141 (2017)