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An Efficient Spectral-Element Spectral-Integral Method for Modeling Doubly Periodic Objects Embedded in Stratified Media

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Scattering analysis of doubly periodic structures with background layered media is required in applications including frequency selective surfaces (FSSs), metasurfaces (MSs) and extreme ultraviolet lithography (EUV). For a finite periodic structure, as the number of periods increases, the solution approaches that of an infinite periodic structure, except for the unit cells near edges.

Rigorous numerical methods, including FDTD, FEM, MOM and rigorous coupled wave analysis (RCWA), have been applied to solve the scattering problem of an infinite periodic structure. Each of them has certain disadvantages. A method that is highly efficient and accurate for the above type of problems is desired. First, this method should be able to model complex scatterers with arbitrary shapes and material distributions. Second, it should avoid the discretization of background layered media, because there can be nearly a hundred layers in a real EUV mask simulation. Moreover, it should maintain a low computational complexity, since one unit cell in MS and EUV sometimes can be tens or hundreds of wavelengths large.

The hybrid finite-element boundary-integral (FEBI) [1, 2] method with a periodic layered medium Green's function (PLMGF) satisfies most of the above requirements. However, its computation cost grows fast as the unit cell extends in the periodic directions, because a direct solver is utilized to solve a FEBI system where the dense BI matrices are assembled into the FEM system.

We present a method that dramatically reduces the computational complexity of FEBI for doubly periodic structures. In the proposed method, the domain decomposition method is applied to the FE-BI interface to facilitate nonconformal meshes and a two-fold iterative solver. In the iterative solver, the FE submatrix and BI submatrix are solved separately. Furthermore, a Calderon multiplicative preconditioner (CMP) and fast-Fourier transform (FFT) algorithm effectively reduces the computational complexity of BI subsystem to roughly linear. The overall complexity of SESI reduced by roughly one order compared to the basic FEBI and becomes comparable to solving a sparse FEM system that only contains the complex scatterer without background stratified layers.

A numerical example verifies the low complexity of SESI. More examples on EUV and MSs are provided to validate the accuracy of SESI with a commercial solver.

1. T. F. Eibert, J. L. Volakis, D. R. Wilton, D. R. Jackson, "Hybrid FE/BI modeling of 3-D doubly periodic structures utilizing triangular prismatic elements and an MPIE formulation accelerated by the Ewald transformation," *IEEE Transactions on Antennas and Propagation*, **47**, 5, 1999, pp. 843-850, doi: 10.1109/8.774139.

2. J. Niu, Y. Ren, and Q. H. Liu, "Spectral Element Boundary Integral Method with Periodic Layered Medium Dyadic Green's Function for Multiscale Nano-optical Scattering Analysis," *Optics express*, **25**, 20, 2017, pp. 24199-24214, doi: 10.1364/OE.25.024199.