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Computing Gabor coefficients for a scattering problem: super exponential converging accuracy and a more localized representation

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Optical scatterometry is a non-destructive inspection technique to evaluate possible production deformations for integrated circuits. A key component of optical scatterometry is a Maxwell solver to obtain accurate information regarding the electromagnetic scattering from the structures of interest. This Maxwell solver also needs to be capable to quickly adapt the geometrical details of these structures to take various possible deformities into consideration for the fast computation of electromagnetic scattering. A fitting Maxwell solver [1] takes the form of a spatial-spectral domain integral equation such that its computational domain is comparable to the volume of the scattering objects of interest, e.g. parts of an integrated circuit. The spatial-spectral representation in terms of Gabor frames allows to analytically and efficiently incorporate the response of a planarly layered background medium, since the setting of optical scatterometry for integrated circuits is characterized by such a background description. The Gabor frames as in [1] make it possible to describe the electromagnetic fields and scattering objects as weighted sums of shifted and modulated Gaussian window functions, where the so-called Gabor coefficients are the weighting coefficients. We want to make more efficient use of the Gabor frames, which requires the computation of Gabor coefficients, such that the Maxwell solver [1] becomes faster and more suitable for optical scatterometry applications.

Computing Gabor coefficients is one of the computationally dominant parts within this Maxwell solver [1], since each coefficients requires the evaluation of an integral. Especially, the Gabor coefficients for the scattering objects with discontinuous boundaries are tedious to compute due to their discontinuous behavior. A clear example can be found in [2]: the Gabor-frame representation of 144 scattering objects required a computation time of 146 seconds from the total 181 seconds of the whole preprocessing phase of the Maxwell solver, which is used to also compute the Green's function, incident field and more. This timing is achieved by using the spectral transformation method [2], where the Gabor coefficients of a scattering object are computed in the spectral domain instead of the spatial domain. The spectral transformation method displayed an absolute error that decayed as $O(exp(-\tau/h))$ instead of the original $O(h)$ with respect to an analytical reference, where $\tau \in \mathbb{R}$ represents the decay parameter of the so-called dual window function within a Gabor frame and h is used as the stepsize within the repeated trapezoidal rule in the spectral domain.

To achieve a further reduction in computation time, we extend the work of [2]. We propose to interchange the two relevant window functions within the Gabor frame, i.e. the Gaussian window function and the dual window function. We perform this interchange of window functions, since the decay of the window function within the Gabor coefficient integral dictates the decay of the absolute error within the repeated trapezoidal rule, owing to the use of the spectral transformation method. The decay of a Gaussian window function is superior to that of the dual window [2]. Consequently, we achieve super exponential convergence regarding the Gabor coefficients, which reduces the computational burden while maintaining accurate results. A numerical benchmark is used to show the performance in terms of computation time and accuracy of the original implementation, as in [2], versus the representation with interchanged window functions. Additionally, we look into the impact of interchanging the window functions within the Gabor for a 2-dimensional (2D) transverse electric (TE) scattering problem[1,pp.95-116]. We perform a benchmark in form of solving a 2D TE scattering problem given the original implementation and interchanged implementation to show that the interchanged implementation leads to a more localized solution owing to the Gabor coefficient integrals decaying super exponentially.

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[2] S. Eijsvogel, L. Sun, F. Sepehripour, R.J. Dilz, and M.C. van Beurden "Describing discontinuous finite 3D scattering objects in Gabor coefficients: fast and accurate methods", JOSA A, 39, 1, 2022, 86-97.