Forward Diffraction Modelling:

Analysis and Application to
Grating Reconstruction

The semiconductor industry uses lithography machines for manufacturing complex integrated circuits (also called ICs) onto wafers. Because an IC is built up layer by layer it is very important to align the wafer each time it enters the machine. Today, gratings are used for this alignment step. Gratings are tiny periodic structures printed on a wafer and are even smaller than ICs. These gratings are illuminated with a laser and by measuring the scattered field one can get information on the position of a wafer. In a similar way gratings can also be used for various other lithographic metrology tasks such as overlay metrology and CD metrology which give additional information on the production process. All in all it becomes increasingly more important to develop and use a rigorous mathematical model that solves optical diffraction problems for periodic gratings.

In this thesis we model the optical diffraction problem (both planar diffraction as well as conical diffraction are considered) starting from Maxwell's equations. A reduced model is derived by simplifying both the grating and the incident electromagnetic field. The former is approximated with an infinitely periodic layered structure where the materials are linearly reacting and isotropic. The latter is approximated with a time-harmonic incident plane wave. The reduced model is discretised using two different mode-expansion methods, Bloch and RCWA (Rigorous Coupled-Wave Analysis), that expand the electromagnetic fields in each layer in terms of the (approximate) eigenfunctions. After truncation a transmission problem is derived by matching the fields at the layer interfaces. Having solved the linear system of this transmission problem the scattered field can be computed.

This thesis examines and extends both mode-expansions methods. Although Bloch in principle is a more accurate discretisation using the exact eigenfunctions, it is much harder to generalise this method to arbitrary gratings. Therefore we will use this method mainly as a reference for simple geometries. On the other hand RCWA based on Fourier theory only approximates the exact eigenfunctions but is much more flexible. We investigate and present numerical results of two RCWA extension that have the potential of improving its convergence and get better approximations. ASR (Adaptive Spatial Resolution) transforms the Maxwell equations by introducing a stretching parameter. The stretching increases the resolution around a material interface which results in a faster converging Fourier series. FD (Finite Differences) removes the Fourier discretisation completely and replaces this with a finite difference approximation in the periodic direction only. This allows one to capture the material interface even better. On the basis of Fourier theory and numerical tests we also derive some convergence criteria for the truncation parameters. Since both the original as well as the modified formulations still result in a similar transmission problem, special care is taken in the solution process of the linear system. We mathematically prove that the linear system can be stably condensed, thereby optimising the speed of the algorithm, with a decoupling algorithm. Next we show that the resulting algorithm is actually the same as the enhanced transmittance matrix approach and thereby confirming the stability of the original RCWA formulation.

Finally we apply the forward diffraction model to a new sensor concept of grating reconstruction. Here one tries to reconstruct the shape of a grating by measuring the reflected field only as a function of angle of incidence, wavelength and polarisation.