The diffraction of light is an important phenomenon with wide physical and engineering applications and diffraction gratings are optical components with a periodic structure which are used to diffract light into several beams propagating in various directions. Direct methods like AFM or SEM proved to be insufficient to study the shape of planar diffraction gratings and therefore they must be supplemented with results obtained from optical spectroscopy. Computer simulations are the integral part of this method. This Thesis is focused on two particular simulation methods—the RCWA and the C-Method. It gives a rich theoretical introduction, discusses the weaknesses of these methods and also describes improvements of the RCWA using the Airy-like series and proper Fourier factorization. Both methods are implemented, tested on simple examples and afterwards the convergence for particular cases is investigated. The C-Method and the modified RCWA algorithm exhibit excellent convergence. At the end, the numeric results are compared with experiments, giving a very good agreement in the ellipsometric parameters.