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Fast Numerical Shape Reconstruction of Highly Conductive Submicron Particles on Substrates

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Abstract— Optical characterisation of nano- and submicron structures often requires rapid numerical solution of inverse scattering problems. This is the case, e.g., in the production and quality control of functional nanomaterials. A commonly used approach in inverse scattering is the Kirsch-Kress Method (KKM). Here, the scattered near field is reconstructed from the given measurement data using a forward scattering model based on layer potentials, whereafter the position and shape of the scatterer are estimated by minimising a boundary condition error within a class of admissible boundaries.

In KKM, the radiation integrals representing the reconstructed scattered near field are used in the objective functional for the boundary-error minimisation, and they are therefore repeatedly evaluated during the inversion. Thus, the efficiency of the computation of these integrals greatly influences the overall efficiency of the inversion method. This is especially important in the shape estimation of structures *on substrates*, since the scattered near field in this case is given by radiation integrals that involve half-space Green's functions. Such Green's functions are namely given by Sommerfeld-type integrals, and are therefore computationally expensive.

We here present an efficient Kirsch-Kress type numerical method for shape reconstruction of highly conductive penetrable nano- and submicron particles on substrates. To speed up the inversion, the method eliminates or simplifies numerical integration wherever possible. First, to avoid integration of surface current densities, the forward model is based on the so-called Method of Auxiliary Sources (MAS). Here, the surface current densities in the radiation integrals are approximated by spatially impulsive sources: line currents in the 2D case and Hertzian dipoles in the 3D case. Next, matching of the sources with the measured scattered far field is done at discrete testing points, and finally, the relevant half-space Green's functions are approximated using Fresnel reflection and complex image theory. The particles to be reconstructed are either approximated as perfectly electrically conducting (PEC), or an appropriate Surface Impedance Boundary Condition (SIBC) is used.

We apply the inversion method to actual angular-resolved bistatic scatterometric data provided by the Danish Fundamental Metrology. Here, cross-sections of three platinum (Pt) submicron wires on silicon (Si) substrate are estimated based on the scattered far-field intensity measured in a narrow angular range. The samples are illuminated by a 325 nm HeCd laser. In addition, we present an analysis of the accuracy and efficiency of the inversion for families of circular PEC and silver (Ag) submicron wires on Si substrate, using numerically simulated measurement data. An example of shape estimation of a 3D Ag submicron particle on an Si substrate is also shown. Finally, we discuss the suitability of different approximations of the half-space Green's function in the forward model.