Generalized Scattering Matrix Method for Electrostatic Force Microscopy

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Abstract

Understanding the electric field distribution in nanostructured surfaces is a key issue in nanoscience and technology. By applying a voltage between a force microscope tip and a sample, *Electrostatic Force Microscopy* (EFM) has been used to analyze different properties of surfaces at the nanoscale[1,2]. EFM has also been used to study liquid surfaces[3] or to induce the capillary condensation of water bridges between tip and sample[4]. The accurate modelling of electrostatic fields and potentials is of considerable interest not only in EFM but also in electron field emission and field desorption, or in the self-consistent calculation of the electronic image-potential states[5].

Unfortunately, the solution of the Laplace/Poisson equation is analytical only for a few symmetric geometries. Furthermore, even using numerical methods, any geometric element that breaks the symmetry increases the computation time significantly. To overcome this problem, planar or very simple metallic surfaces[6], as well as different approximations to the electric field[7,8] have been proposed before. For flat surfaces, several techniques have been developed to quantitatively predict magnitudes such us the tip radius and shape[9] or to analyze the cantilever influence or the presence of water on the surface[10]. However, some of the most interesting effects at the nanoscale are related to surface defects such as steps on metallic surfaces (for example, the Smoluchowski effect or the condensation of water[11]).

In this poster, we present a method based on the Scattering Matrix (SM) formalism to calculate the exact electric field for non-symmetric three-dimensional systems composed by punctual charges and dielectric samples (see Fig. 1). The main advantage of the method is that the punctual charges located outside the sample only modify the value of the input coefficients (I_1 and R_3 in Fig. 1) and can be changed without calculating the whole system (i.e. SM) again. Although we will focus on the Laplace/Poisson equation, the SM formalism is obtained from a general approach developed for the Sturm-Liouville equation.

To demonstrate the efficiency of the SM method, we calculate the electrostatic potential and capacitance of an EFM non-symmetric system composed by a metallic tip scanning over a nanowire placed on a dielectric surface. We analyze the capacitance as a function of the nanowire dielectric constant. Our results suggest that capacitance measurements could be used to determine the dielectric constant of nanowires. As another interesting application of the SM method, of interest in the study of surface image states and tunnelling currents, we calculate the classical image potential of an electron over a metallic (perfect conducting) stepped surface.

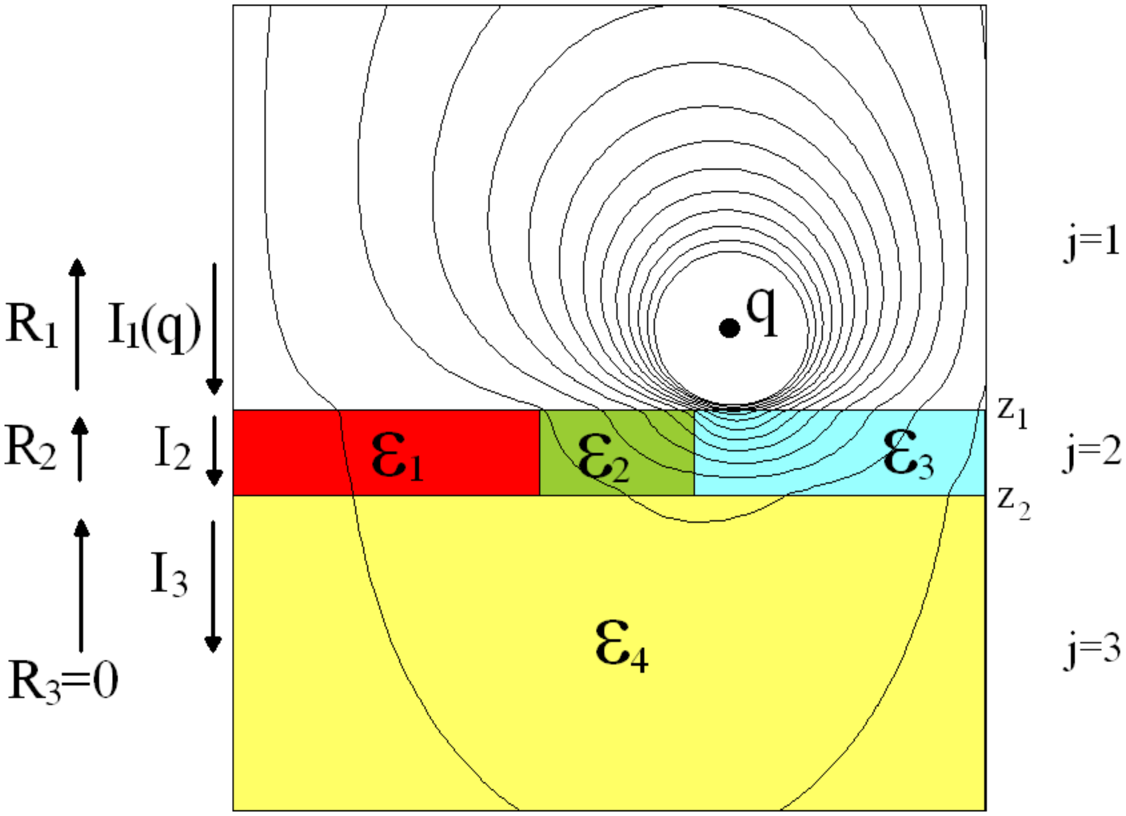

FIG. 1. Electrostatic potential distribution calculated by the Scattering Matrix (SM) method. The system is composed by a punctual charge over a dielectric sample (ε_1=20, ε_2=10, ε_3=5, ε_4=40). The distribution of coefficients for the SM is shown on the left of the image. For this specific geometry, I_1 is given by the punctual charge and R_3 is 0 since there is not any source in region 3.

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