Numerical Modeling of Electrostatic Force Microscopes

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Abstract

In this paper a two dimensional simulation model of an electrostatic force microscope (EFM) is presented. An approach to couple several numerical methods is proposed for its calculation.

Introduction

Due to the rapid miniaturization of integrated devices into the mesoscopic regime and the increasing interest in very small structures, high resolution measurement instruments have become very important within the last years. An example is the atomic force microscope (AFM). Its ability to scan surfaces with nearly atomic resolution and it's versatility make it one of the most important measurement devices in nanotechnics. If the sample under investigation holds a charge distribution and the distance between the AFM tip and the sample is kept large, other interaction forces can be neglected due to the much larger influence of the electrostatic force. In this case the AFM is called electrostatic force microscope (EFM) [8]. Several approaches to calculate the electric field in order to model this interaction have been made, such as in [7] the author carries out a multipole expansion by using the program MMP. In this paper a two-dimensional model for an EFM is presented and several numerical methods are applied to calculate the electrostatic field.

2D Model of the EFM

In order to develop a simulation model for the EFM (Fig. 1) it is evident to understand its components and their interaction. During the scanning process the tip at the end of the cantilever is run over the sample. The forces acting on the cantilever and the tip are determined by the electrostatic field. The electrostatic fields and forces will be referred to as the electrostatic part of the model in the following. The other part of the model will be called the mechanical part. It is used to calculate the mechanical behavior. The approach to calculate the electrostatic part and the mechanical part separately requires a coupling between both parts (Fig.2). For this purpose the electrostatic forces that are calculated by

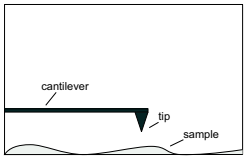

Figure 1: Two Dimensional EFM Model

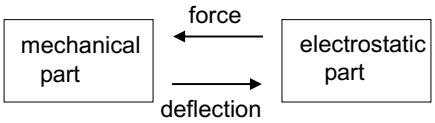

Figure 2: Mechanical and Electrostatic Part

the electrostatic part are passed to the mechanical part during a simulation. Using these forces as input the mechanical part is able to calculate the deflection of the cantilever and pass it to the electrostatic part. Taking into account this updated position of the cantilever the electrostatic field has to be calculated again. To find a convenient numerical simulation approach we will take a closer look at the electrostatic part and point out the difficulties that may occur in the model. In an uncharged region the electrostatic potential φ can be obtained by solving Laplace's equation

$$\Delta\varphi = 0. \tag{1}$$

In the sample charge distributions and possible nonlinearities of the dielectric properties may have to be taken into account. Therefore a versatile numerical method as the finite element method (FEM) has to be applied in region 2 (Fig. 3). For modeling the high values of the electric field near the tip (region 1) more accurately at low computational cost the method of fundamental solutions (MFS) or alternately the charge simulation method (CSM) will be used while the long distance interaction (region 3) can conveniently be treated using the boundary element method (BEM). During the calculation of the electrostatic potential the numerical methods mentioned above have to be coupled to each other. The FEM for-

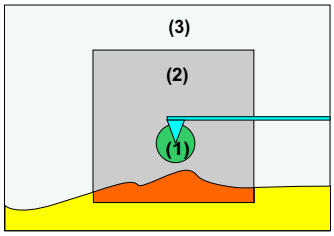

Figure 3: Simulation Regions

mulation of Eq. 1 in region 2 leads to

$$\sum_j K_{ij}\varphi_j + \sum_n K_{in}\varphi_n = 0\,. \tag{2}$$

Here φ_j are the values of the electric potential to be calculated and φ_n are the potential values on the nodes with Dirichlet boundary condition. The stiffness matrix $\mathbf{K}$ is defined by

$$K_{ik} = \int_\Omega \left[\frac{\partial\psi_i}{\partial x}\left(\varepsilon\sum_{k=1}^{n}\frac{\partial\psi_k}{\partial x}\right) + \frac{\partial\psi_i}{\partial y}\left(\varepsilon\sum_{k=1}^{n}\frac{\partial\psi_k}{\partial y}\right)\right] d\Omega\,, \tag{3}$$

where n is the number of nodes and ψ are the FEM shape functions [3].
The use of FEM in region 1 would require a very fine mesh to take into account the high field values near the tip. In order to keep computational cost low two alternative numerical methods are applied in region 1 and coupled to the FEM. One of these methods is the CSM which is based on the fact that boundary conditions can be approximated by placing virtual charges outside the calculation domain [10]. This leads to

$$\varphi(\mathbf{r}) = \frac{1}{2\pi\varepsilon_0}\sum_j q_j \ln\frac{\|\mathbf{r}-\mathbf{r_j}\|}{r_0}\,, \tag{4}$$

where the values of the virtual charges q_j can be obtained by using the boundary conditions while their positions $\mathbf{r}_j$ are fixed. r_0 is the radius with zero potential. The result of a CSM calculation of the electrostatic potential near the cantilever is shown in Fig. 4.

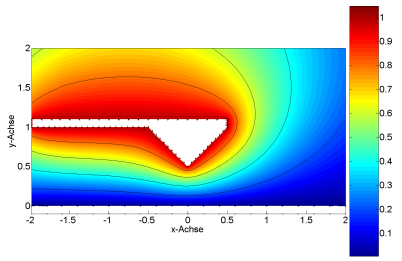

Figure 4: Electrostatic Potential by CSM

Coupling between FEM and CSM is achieved by

$$\varphi_i = \frac{1}{\varepsilon}\sum_l q_l\, G(||\mathbf{r}_i - \mathbf{r}_l||) - \sum_k \varphi_k \oint_s \left[G(ik)\,\nabla\,\psi(\mathbf{r}_k) - \psi(\mathbf{r}_k)\,\nabla\,G(ik)\right]\,\mathbf{n}\,ds\,. \tag{5}$$

Here $ik = G\|\mathbf{r_i} - \mathbf{r_k}\|$, φ_i are the boundary conditions, φ_k are the coupling nodes, G is the associated Green function and $\mathbf{n}$ is the normal vector on the coupling surface s [6].

The other approach investigated here to deal with the high field values near the tip is the MFS. In polar coordinates the electrostatic potential at any point (ρ, ϕ) in region 1 can be approximated by

$$\varphi(\rho,\phi) = \varphi_0 + \sum_{m=1}^{m_{max}} a_m \rho^{\frac{m\pi}{\beta}} \sin(\frac{m\pi\phi}{\beta}). \tag{6}$$

Here m_{max} is the number of ansatz functions and β is the angle outside the tip [6]. The coefficients a_m can be found by using the boundary conditions. To couple the MFS to the FEM Eq. 6 is applied to the coupling points and used in Eq. 2 [9]. This leads to

$$\sum_j K_{ij}\varphi_j + \sum_l K_{il}\left(\varphi_0 + \sum_{m=1}^{m_{max}} a_m \rho_j^{\frac{m\pi}{\beta}} \sin(\frac{m\pi\phi_j}{\beta})\right) = \sum_n K_{in}\varphi_n\,, \tag{7}$$

where l are the coupling nodes and n are the nodes with Dirichlet boundary condition. The sum j includes the nodes that are neither coupling nodes nor nodes with Dirichlet boundary conditions. Fig. 5 shows the electrostatic potential near the tip calculated by the coupled FEM / MFS. For the use of FEM in region 2 the whole domain has to be meshed

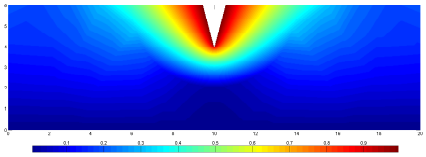

Figure 5: Electrostatic potential simulated by coupled FEM / MFS

and calculated. Therefore, to save computational cost, it is convenient to keep the FEM simulation domain small and apply the BEM in region 3. For the calculation both methods have to be coupled. The BEM formulation of the setup can be written as

$$\sum_{i=1}^{M}\sum_{j=1}^{N} H^{ij}\varphi^j = \sum_{i=1}^{M}\sum_{j=1}^{N} G^{ij}q^j \tag{8}$$

$$H^{ij} = -\frac{1}{2\pi}\frac{(\underline{x}_j - \underline{\xi}_i)\cdot\underline{n}}{|\underline{x}_j - \underline{\xi}_i|^2}\frac{l_e}{2} \tag{9}$$

$$G^{ij} = -\frac{1}{2\pi}\ln|\underline{x}_j - \underline{\xi}_i|\frac{l_e}{2}\,. \tag{10}$$

Here N and M are the total number of elements and nodes, respectively, φ is the potential, q is the potential derivative, l_e is the length of the element, i and j are node indices. Since the 2D simulation by BEM requires 1D discretization, the discretization only on the boundary is necessary. BEM provides improved accuracy in the calculation of electric field and exterior problems. Now let us define φ_B^I , φ^B and q_B^I , q^B as the interface and the non-interface

potential and the flux of the BEM region respectively, φ_F^I and φ^F as the interface and the non-interface potential of the FEM region and q_F^I as the interface flux of the FEM region. The necessary coupling condition for potential is $\varphi_B^I = \varphi_F^I = \varphi^I$ and for flux is q_B^I = - q_F^I = q^I. Applying these coupling conditions and the converting matrix $\mathbf{M}$ the resulting coupling equation for the whole system is

$$\begin{bmatrix} \mathbf{[H]}^{II} & \mathbf{[H]}^{IB} & -\mathbf{[G]}^{II} & -\mathbf{[G]}^{IB} & 0 \\ \mathbf{[H]}^{BI} & \mathbf{[H]}^{BB} & -\mathbf{[G]}^{BI} & -\mathbf{[G]}^{BB} & 0 \\ \mathbf{[K]}^{II} & 0 & \mathbf{M} & 0 & \mathbf{[K]}^{IF} \\ \mathbf{[K]}^{FI} & 0 & 0 & 0 & \mathbf{[K]}^{FF} \end{bmatrix} \begin{Bmatrix} \{\varphi\}^I \\ \{\varphi\}^B \\ \{q\}^I \\ \{q\}^B \\ \{\varphi\}^F \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix}, \quad (11)$$

where I indicates the coupling nodes, F and B indicate the nodes which are in the FEM and BEM region respectively [1] [2]. Now implying all boundary conditions the unknown potential and the flux can be determined from this equation. By using the BEM boundary potential and flux the internal potential at any point in the BEM region can be determined from

$$\varphi^i = \sum_{j=1}^{N} G^{ij} q^j - \sum_{j=1}^{N} \hat{H}^{ij} \varphi^j \,. \quad (12)$$

The result of the coupled FEM-BEM simulation is shown in Fig. 6.

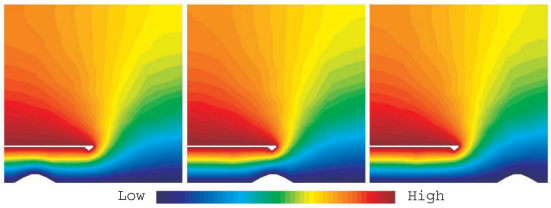

Figure 6: Electrostatic potential simulated by coupled FEM-BEM

Since the scanning process of an EFM is dynamic, the FEM mesh in region 2 has to be changed during the calculation which is achieved by using the arbitrary Lagrangian Eulerian (ALE) method [5] and modeling the mesh as a massless elastic. The resulting vector Laplace equation for the mesh deformation is solved by FEM [3]. In Fig. 7 the deformation of the mesh can be observed.

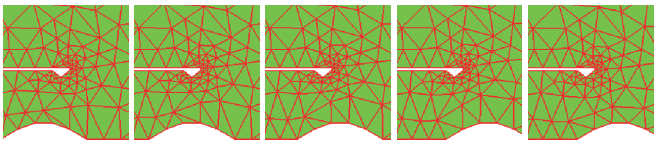

Figure 7: ALE

Conclusion

In this paper a concept of physical and numerical electrostatic modeling of a 2D EFM is presented. The simulation domain is divided in three parts in each of which a different numerical method is applied in order to combine the advantages of each method. Some typical simulation results obtained by a coupled FEM-MFS and FEM-BEM are presented.

Acknowledgements

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References

[1] *Brebbia, C.A., Dominguez, J.*: Boundary Elements An Introductory Course. McGraw-Hill Book Company (1989)

[2] *Beer, G., Watson, J.O.*: Introduction to Finite and Boundary Element Methods for Engineers. Wiley (1992)

[3] *Reddy, J.N.*: Finite Element Method. McGraw-Hill International Editions, Singapore (1993)

[4] *Gaul, L., Kögl, M., Wagner, M.*: Boundary Element Methods for Engineers and Scientists. Springer Verlag (2003)

[5] *Belytschko, T., Kam Liu, W., Moran, B.*: Nonlinear Finite Elements for Continua and

[6] *Jackson, J.D.*: Classical Electrodynamics. Wiley (1975)

[7] *Jacobs, H.O.*: Leuchtmann P., Homan O.J., Stemmer A.: Resolution and contrast in Kelvin probe force microscopy. Journal of Applied Physics Vol. 84, num. 3 (1998)

[8] *Morita, S.*: Wiesendanger, R., Meyer, E.: Noncontract Atomic Force Microscopy. Springer (2002)

[9] *Zi-Cai, Li*: Numerical Methods for Elliptic Problems with Singularities. World Scientific (1990)

[10] *Zhou, P.* : Numerical Analysis of Electromagnetic Fields. Springer Verlag (1993)