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Abstract

Purpose – The purpose of this paper is to present a hybrid numerical simulation approach for the calculation of potential and electric field distribution considering charge and dielectric constant.

Design/methodology/approach – Each numerical method has its own advantages and disadvantages. The idea is to overcome the disadvantages of the corresponding numerical method by coupling with other numerical methods. An augmented finite element method (FEM), linear FEM and boundary element method are used with an efficient coupling.

Findings – The simulation model of microstructured devices is not so simple. During the simulation various types of problems will occur. It is found that by using several numerical methods these problems can be overcome and the calculation can be performed efficiently.

Research limitations/implications – The present approach can be applied in 2D cases. But, in 3D cases the calculation of augmented FEM in a spherical coordinate becomes quite elaborate.

Practical implications – The proposed hybrid numerical simulation approach can be applied for the simulation of the electrostatic force microscope (EFM) which is a very high-resolution measuring tool in nanotechnology. This approach can be applied also to other micro-electro-mechanical systems.

Originality/value – Since the scanning process of the EFM is dynamic, it requires the updating of the FEM mesh in each calculation time step. In the present paper, the mesh updating is achieved by an arbitrary Lagrangian-Eulerian (ALE) method. The proposed numerical approach can be applied for the simulation of the EFM including this remeshing algorithm ALE.

Keywords Finite element analysis, Numerical analysis, Simulation, Nanotechnology, Electrostatics, Measuring instruments

Paper type Research paper

Introduction

A rapid advancement in nanotechnology has been observed over the last few years. This progress has also been influenced by the development of new high-resolution measurement instruments. Since, the present trend is the rapid miniaturization of integrated devices into the mesoscopic regime, these instruments become very important.

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An interesting example of such high-resolution measuring instrument is the atomic force microscope (AFM). Based on the design of the scanning tunneling microscopes, the first AFM was developed in 1986 by G. Binning and his coworkers in collaboration between IBM and Stanford university. After then AFM rapidly developed into a powerful and invaluable surface analysis technique in micro- and nanoscales and even in atomic and molecular scales. As a result a new era of topological imaging, as well as for measuring force-separation interactions between a probe and substrate began. Its ability to scan surfaces with nearly atomic resolution and its versatility makes 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 then all other interaction forces except the electrostatic force can be neglected. This special working mode of AFM is known as electrostatic force microscope (EFM) which can be used for scanning electric field. Since the coupled electrical and mechanical behaviors have to be taken into account, the numerical modeling of the EFM is divided into an electrical and mechanical part. The interaction between them can conveniently be realized by using a staggered simulation approach. In this paper, a numerical model of the EFM is presented considering charge distribution inside the measuring sample and different dielectric constant inside the simulation region. In the present model a more detailed description is given on the electrical part, i.e. the cantilever is kept fixed.

Basic working principle of EFM

The working modes of EFM are mainly classified into three groups. These are contact mode, non-contact mode and tapping mode. Atomic defects such as atomic vacancies can not be observed in the contact mode AFM (Morita, 2002; Pethica and Oliver, 1987). In the present work, the non-contact mode of EFM is considered. For EFM the interaction force is the electrostatic force between the biased atomically sharp tip and the sample. In addition, the van der Waals force is always present between the tip and the sample. The van der Waals force and the electrostatic force have two different dominant regions. The van der Waals force is proportional to $1/r^6$ and the electrostatic force is proportional to $1/r^2$ where r is the distance between the tip and the sample. Thus, when the tip is closed to the sample the van der Waals force is dominant and when the tip is moved away from the sample the electrostatic force is dominant. So for contact mode van der Waals force is dominant where as for non-contact mode electrostatic force is dominant. The scanning of the EFM is usually done in two ways. Firstly the topology of the sample is performed by tapping scanning mode which is known as "intermittent-contact" mode. In this case the van der Waals force is dominant. Secondly using this topological information a constant tip sample distance is maintained while scanning where the electrostatic force is dominant which is known as "lift-scanning" (Yan and Bernstein, 2006). In this case it is assumed that the influence of all short range forces can be neglected and only the electrostatic force plays the vital role for imaging. To detect the electrostatic force a voltage is applied between the cantilever tip and the sample. The cantilever oscillates near its resonance frequency which changes in response to any additional force gradient. Changes in any cantilever resonant frequency can be detected using phase detection, frequency modulation, amplitude modulation, etc. (Bhushan, 2004). A diode laser is focused on the back of the cantilever and the reflected light is collected by a position sensitive photo detector. These usually consist

of two closely spaced photodiodes. Due to any angular displacement of the cantilever, one photodiode will receive more or less light than the other photodiode which results in different output voltage. This output voltage will be used to plot the potential, electric field distribution, etc. on the measuring sample.

Numerical model

For modelling and simulation of EFM multi-physics aspects must be taken into consideration. From the numerical point of view additional problems arise since we are frequently confronted with multi-scale problems. Therefore, the application of advanced numerical methods is necessary. For developing a numerical model of the EFM different effects have to be considered. For example, long distance interaction, charge distribution and non-linearity of the material properties, singularity, etc. In order to take into consideration these effects the simulation region is divided into three regions as shown in Figure 1.

As high values of the electric field occurs at the peak of the tip, a special numerical method is needed to calculate this electric field more effectively. For this reason an augmented finite element method (FEM) method will be applied to region 1. Since charge distribution and nonlinearities of the dielectric properties may need to be considered, a versatile numerical method such as FEM should be applied to region 2. As boundary element method (BEM) works well when the boundary is infinite or semi-infinite, the large distance interaction between the tip and the cantilever can be conveniently treated using BEM in the region 3. Later all these three numerical methods will be coupled with each other.

In this paper, a coupled simulation will be presented considering charge distribution and dielectric constant (permittivity) of the measuring object. If the simulation model of Figure 1 is applied to a model which includes a silicon made measuring object and contains locally charged domains then the corresponding schematic diagram results in Figure 2.

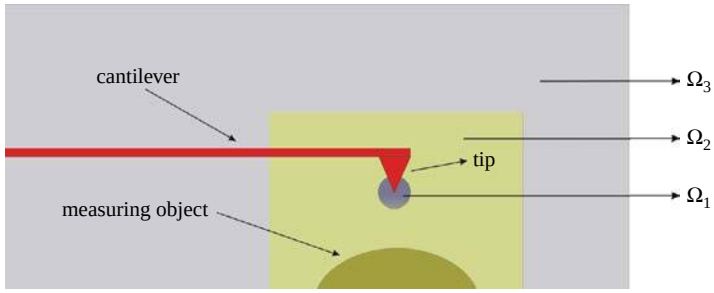

Figure 1.
2D model of EFM

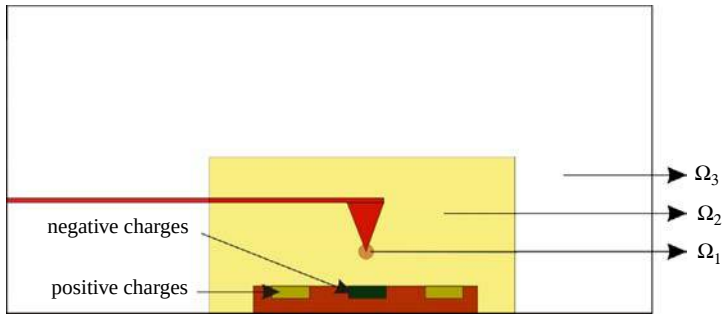

Figure 2.
Schematic diagram

Here, the positive charges exist inside the left and right side whereas the negative charges exist in the middle of the measuring object. This model is same as like the *p*-type and *n*-type materials where there exists excess of positive and negative charges, respectively. In the case of measuring such object, the applied voltage and the distance between the tip and the sample are such that there occurs no corona effect.

Numerical formulation

The energy related functional in the electrostatic calculation domain Ω can be written as (Greiff *et al.*, 2006):

$$W = \int_{\Omega} (\nabla u)^2 \mathrm{d}\Omega - \oint_{\Gamma} u \frac{\partial u}{\partial n} \mathrm{d}\Gamma \quad \text{for} \quad u \in H_D^1(\Omega) : \left\{ u \in H^1 \middle| u_{|\Gamma_D} = u_0 \right\} \tag{1}$$

where $u(a_1, a_2, \ldots, a_m, x, y)$ is an approximation of the potential u (x, y). In the present case the boundary integral of equation (1) is zero. It is well known that the solution of:

$$\frac{\partial W}{\partial a_i} = 2 \int_{\Omega} \nabla u \frac{\partial \nabla u}{\partial a_i} \mathrm{d}\Omega = 0 \tag{2}$$

yields an approximative solution for the Laplace equation in region Ω. The approximation solution in the circular region Ω_1 of radius R can be described by:

$$u(\rho, \phi) = \sum_{i=1}^{m} c_i \left(\frac{\rho}{R} \right)^{i\pi/\beta} \sin\left(\frac{i\pi\phi}{\beta} \right), \quad (\rho, \phi) \in \Omega_1 \tag{3}$$

where β is the outer opening angle of the tip (Strang and Fix, 1973) and ρ is the distance of any point on Ω_1 as shown in Figure 3.

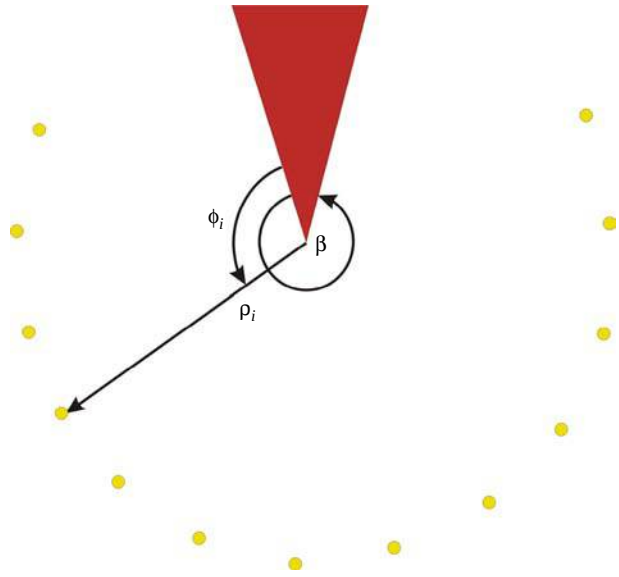

Figure 3.
Representation of augmented FEM near the EFM tip

In the region Ω_2 linear FEM:

$$u(x,y) = \sum_{j=1}^{m} u_j \psi_j(x,y), \quad (x,y) \in \Omega_2 \tag{4}$$

is applied. Since, the approximation of equation (3) will be kept only near the tip and the approximation of equation (4) will be applied to the total region, the global approximation function for both ansatz functions becomes:

$$u(x,y) = \sum_{j=1}^{n} u_j \psi_j(x,y) + A(\rho) \sum_{k=1}^{m} c_k f_k(\rho, \phi) \tag{5}$$

where $A(\rho)$ is applied to reduce the influence of equation (3) away from the tip which is shown in Figure 4 and defined by:

$$A(\rho) \begin{cases} 0 & \rho > R \\ 1 & \rho \leq R/2 \\ \frac{1}{2}\left(1 + \cos\left(\frac{2}{\mathrm{R}}\,\rho - 1\right)\pi\right) & \frac{\mathrm{R}}{2} < \rho < R \end{cases}$$

Now applying equation (5) into equation (2) leads to a set of linear differential equations which can be represented in matrix form as:

$$\begin{pmatrix} \mathbf{M} & B^{\mathrm{T}} \\ B & \mathbf{F} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \tag{6}$$

where $\mathbf{M}$ is the matrix resulting from the augmented FEM and $\mathbf{F}$ is the stiffness matrix expressed by:

$$\mathbf{F}_{ij} = 2 \int_{\Omega_2} \nabla \psi_i \nabla \psi_j \mathrm{d}\Omega. \tag{7}$$

On the FEM-BEM transmission interface (Bala *et al.*, 2007) $\Gamma_T = \Gamma_3 \cap \Gamma_2, u_2 = u_3$ and:

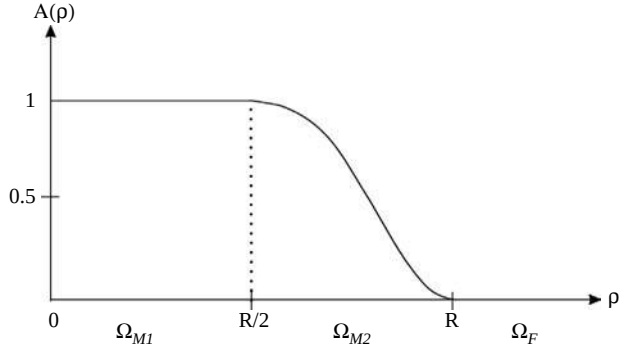

Figure 4.
Cut-off function

$$\frac{\partial u_3}{\partial n} + \frac{\partial u_2}{\partial n} = 0.$$

Using the Gauss theorem on the augmented finite element and finite element domain one obtains (Reddy, 1993):

$$\int_{\Gamma_2} \frac{\partial u_{12}}{\partial n} v \mathrm{d}\Gamma = \int_{\Omega_{12}} \mathrm{div}\ (\nabla u_{12} \cdot v) \mathrm{d}\Omega = \int_{\Omega_{12}} \Delta u_{12} \cdot v \mathrm{d}\Omega + \int_{\Omega_{12}} \nabla u_{12} \cdot \nabla v \mathrm{d}\Omega \tag{8}$$

i.e. for all:

$$v \in H^1_{D,0}(\Omega_{12}) := \{v \in H^1(\Omega_{12}) : v|_{\Gamma_D \cap \Gamma_2} = 0\}$$

$$a(u_{12}, v) := \int_{\Omega_{12}} \nabla u_{12} \cdot \nabla v \mathrm{d}\Omega = \int_{\Omega_{12}} f \cdot v \mathrm{d}\Omega + \int_{\Gamma_2} \frac{\partial u_{12}}{\partial n} v \mathrm{d}\Gamma =: (f, v)_{\Omega_{12}} + \left\langle \frac{\partial u_{12}}{\partial n}, v \right\rangle_{\Gamma_2} \tag{9}$$

where u_{12} includes u_1 and u_2. The representation formula of the Laplace equation for the solution of u_3 inside Ω_3:

$$u_3(x) = \int_{\Gamma_3} \left\{ \frac{\partial}{\partial n(y)} G(x,y) u_3(y) - G(x,y) \frac{\partial u_3}{\partial n(y)} \right\} \mathrm{d}\Gamma, \quad x \in \Omega_3 \tag{10}$$

with the fundamental solution of the Laplacian in 2D is given by:

$$G(x,y) = -\frac{1}{2\pi} \log|x - y|. \tag{11}$$

For the Poisson problem the two well known boundary integral equations are (Reddy, 1993):

$$V \frac{\partial u_3}{\partial n} = (I + K) u_3 - N_0 f \tag{12}$$

$$W u_3 = (I - K') \frac{\partial u_3}{\partial n} - N_1 f \tag{13}$$

where the single layer potential V and the hypersingular operator W are symmetric and the double layer potential K has the dual K' (Stephan, 2004). The integral operators N_0 and N_1 are defined by:

$$N_0 f(x) := \int_{\Omega_3} G(x,y) f(y) \mathrm{d}y \tag{14}$$

$$N_1 f(x) := \frac{\partial}{\partial n_x} N_0 f \tag{15}$$

If the two mediums air and silicon exist in the FEM region, i.e. two different dielectric constant ε_1 and ε_2 (for the present formulation these are denoted by ε_{12}) and if only air exists in the BEM region which is represented by ε_3 then the saddle point formulation of the problem for all:

$$(w, v, \psi) \in \tilde{H}^{1/2} \times H^1_{D,0}(\Omega_{12}) \times \tilde{H}^{-1/2}(\Gamma_3)$$

$$2a\varepsilon_{12}(u_{12},v)+\varepsilon_3\langle Wu_3,u\rangle_{\Gamma_T}+\varepsilon_3\big\langle (I+K')\varphi,v\big\rangle_{\Gamma_T}=2(f,v)_{\Omega_{12}}+2\langle t_0,v\rangle_{\Gamma_N\cap\Gamma_2}-\langle N_1 f,v\rangle_{\Gamma_T} \tag{16}$$

$$\varepsilon_3\langle Wu_3,w\rangle_{\Gamma_3\cap\Gamma_N}+\varepsilon_3\big\langle (I+K')\varphi,w\big\rangle_{\Gamma_3\cap\Gamma_N}=2(t_0,w)_{\Gamma_3\cap\Gamma_N}-\langle N_1 f,w\rangle_{\Gamma_3\cap\Gamma_N} \tag{17}$$

$$\varepsilon_3\langle (I+K)u_3,\Psi\rangle_{\Gamma_3}-\varepsilon_3\langle V\varphi,\Psi\rangle_{\Gamma_3}=\langle N_0 f,\Psi\rangle_{\Gamma_3} \tag{18}$$

where H is the Sobolev spaces (Adams and Fournier, 2006). If the bases are introduced as span $\{v_1,\ldots,v_F\}=X_F$, span $\{w_1,\ldots,w_F\}=X_B$ and span $\{\psi_1,\ldots,\psi_F\}=Y_B$, the basis function of X_F and X_B are supposed to be ordered such that:

$$\text{span}\{v_1,\ldots,v_F\}=X_F\cap H^1_{D,0}(\Omega_2)$$

$$\text{span}\{w_1,\ldots,w_F\}=X_B\cap H^{1/2}(\Gamma_3).$$

If the coefficients of u_{12} and u_3 are denoted by u and the coefficients of ϕ are denoted by ϕ again then this system is equivalent to the original differential equation that can be used for discretisation. This system corresponds to a matrix system which can be written as $\mathbf{AX}=\mathbf{b}$ where $\mathbf{A}$ is the following matrix:

$$\mathbf{A}=\begin{pmatrix} \mathrm{M} & B^T & 0 & 0 & 0\\ B & \mathbf{F}_{NN} & \mathbf{F}_{NC} & 0 & 0\\ 0 & \mathbf{F}_{CN} & \mathbf{F}_{CC}+W_{CC} & W_{CN} & (K^{\mathrm{T}}+I)_C\\ 0 & 0 & W_{NC} & W_{NN} & (K^{\mathrm{T}}+I)_N\\ 0 & 0 & (K+I)_C & (K+I)_N & -V \end{pmatrix},$$

$$\mathbf{X}=\begin{pmatrix} u_1\\ u_2\\ u_T\\ u_3\\ \varphi \end{pmatrix} \text{ and } \mathbf{b}=\begin{pmatrix} b_1\\ b_2\\ b_T\\ b_3\\ b_\varphi \end{pmatrix}. \tag{19}$$

The subscript C means contribution from the coupling nodes and N means contribution from the non-coupling nodes. Finally, the blocks W, V, $K+I$ and $K^{\mathrm{T}}+I$ provide the coupling between two ansatz spaces $\mathbf{X}_F$ and $\mathbf{X}_B$. Here, u_1 is the potential near the tip, u_2 and u_3 are the nodal potentials inside the FE domain and on the boundary of the BE domain, respectively, u_T are the nodal potentials on the FE-BE coupling interface and ϕ are the normal components of the electric field distribution on the boundary of the BE domain. The vector $\mathbf{b}$ includes the corresponding boundary conditions and the charge distribution. As the matrix in equation (19) is not positive definite, a specific algorithm such as the MINRES algorithm is required for the solution.

A typical potential and electric field distribution considering moving object are shown in Figures 5 and 6, respectively. In the present model some charges are injected inside the silicon chip. The medium outside the measuring object is air, i.e. there exists

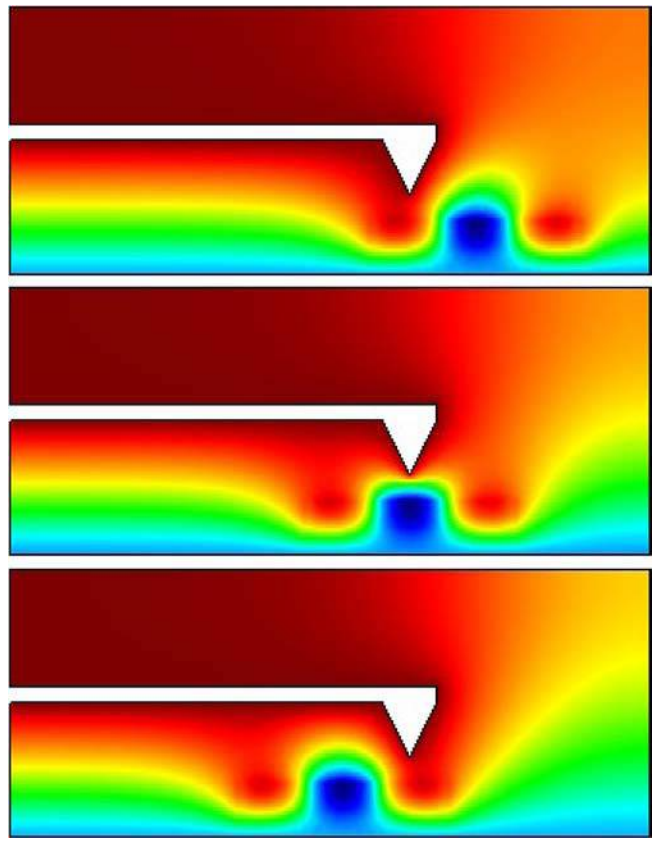

Figure 5.
Potential distribution considering moving object

different charges and different dielectric constants in the simulation region. As these charges will cause potential inside the surface, they will produce remarkable effects on the simulation result. Usually, the highest value of electric field occurs at the peak of the tip which plays the dominant role for the cantilever deflection. But, it may be the case due to the different values of surface charge density; the highest values of the electric field may not appear at the peak of the tip but may be at the corner of the material surfaces. Since the sample is moving, there must be a deviation of electric field at the peak of the tip. By utilizing these deviations of the electric field the EFM will plot the charge distribution on the moving sample.

Since the scanning process of the EFM is dynamic, one has to deal with a moving sample and moving boundaries. As a result the finite element mesh needs to be updated at each time step. To solve this problem one can recall the mesh generator at each time step. But it will be time consuming and not so convenient. The approach presented here for mesh updating is based on an arbitrary Lagrangian-Eulerian (ALE) algorithm (Stoker, 1999; Donea *et al.*, 2004). In this algorithm the mesh is assumed to be a massless elastic. As the present ALE does not include any time derivative so there is no need to any modification of the governing equations and the ALE simply reduces to a mesh updating program.

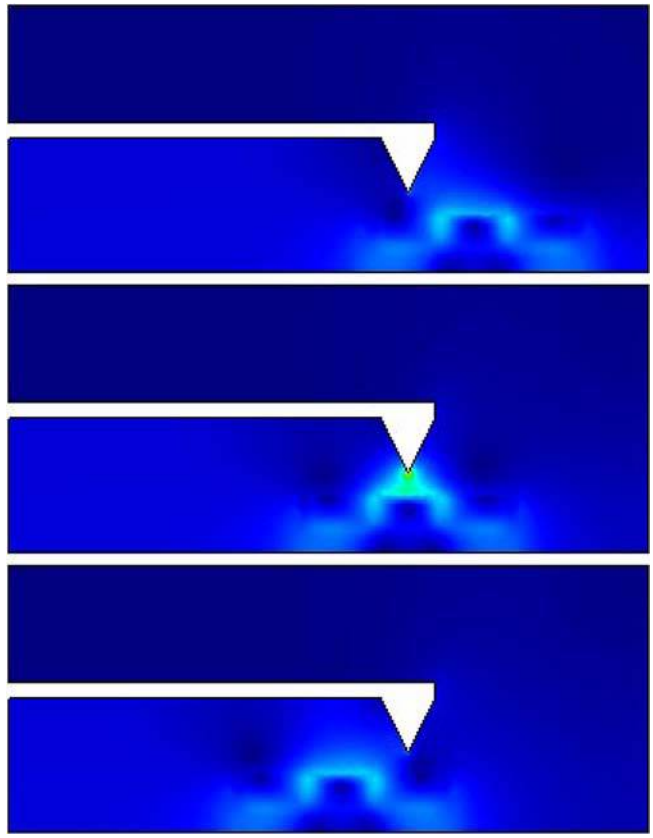

Figure 6.
Figure 6 Electric field distribution considering moving object

Conclusion

A hybrid numerical approach for the simulation of EFM is presented considering charge inside the sample and different dielectric constants. Since the different problems occur at the different places of the simulation regions, different numerical methods are applied to overcome these problems and later all the methods are coupled with each other. Here, the simulation is performed using FEM-BEM coupling. As the high values of electric field occur at the peak of the tip, it is necessary to calculate these high values of electric field more efficiently. Since the sample moves at each time step, the mesh of the FEM region needs to be updated at each time step. In the present case the mesh is updated using an elegant mesh updating algorithm ALE.

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