A Three Dimensional FEM-BEM Approach for the Simulation of Magnetic Force Microscopes

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Abstract — A hybrid numerical model for the simulation of Magnetic Force Microscopes (MFM) is presented. Furthermore, to describe the mechanical behavior of the MFM cantilever different kinds of force calculation methods are considered and compared to each other with respect to the total force as well as to the force distributions.

1. INTRODUCTION

In recent years a rapid miniaturization of integrated devices and data storage media is noticeable. In this regard, high resolution measurement techniques have been developed, which fulfill the increasing requirements for device error analysis. One of these highly sensitive measuring instruments is the Magnetic Force Microscope (MFM), which reveals the magnetic properties of an arbitrary sample. During the measurement process a micro-mechanical cantilever, which holds a magnetic coated tip underneath, is moved over a magnetic field inducing sample surface. Due to the magnetic interactions attractive or repulsing forces act on the cantilever and cause a deflection, which can be detected by a reflected laser beam focused onto a photodetector. Thereby it is possible to image the magnetic domain structures and hence to draw conclusions about the sample magnetizations or currents. Due to different error sources, as for instance a tip asymmetry or a heterogeneous tip coating as well as occurring difficulties in the investigation of soft magnetic sample materials, it is useful to support the laboratory measurements with theoretical considerations.

The simulation of such a microscope can be divided into two parts, the electromagnetic and the mechanical behavior of the magnetized tip and the cantilever. In this work a three dimensional numerical MFM model is presented, which deals with the description of the electromagnetic behavior. Due to the immense differences in size between the single components inside the microscope, which are most extensive between the apex radius of the magnetic coated tip and the length of the cantilever (10 nm versus 200 µm), the FEM cannot conveniently be applied for the discretization of the whole considered calculation domain. Therefore, for this multiscale problem the considered domain is enclosed with boundary elements. This FEM-BEM coupling is necessary for a precise and efficient calculation of the magnetic interaction fields.

In order to simulate an overall MFM scanning process and the involved cantilever deflection, it is essential to compute the resulting forces acting on the cantilever. For this purpose different kinds of force calculation methods, i.e., equivalent sources methods, the Maxwell stress tensor and the virtual work principle are implemented and compared with each other. Each of these methods is applicable for the total force calculation of a body. However, in the case of permanent magnetic materials the local force distributions strongly differ from each other [1], which has an impact on the material deformation [1, 2]. Hence, considering a following structural analysis of the cantilever deflection, appropriate physical local forces on the magnetic coated tip are required. For this reason, the virtual work principle is furthermore implemented in such a manner as reported in [3] in order to obtain the applicable local interaction forces between the tip and the magnetic inducing sample.

2. HYBRID NUMERICAL MODEL

For the simulation of a magnetic force microscope different kinds of field sources and effects have to be considered. Beside the tip magnetization, sample currents as well as sample magnetizations are possible sources for the magnetic interaction between the sample material and the microscope tip. Furthermore, the sample material under investigation could be nonlinear or even features a hysteresis. Another difficulty is the above mentioned difference in size of the calculation domain. In order to overcome all these requirements the considered domain is decomposed into two parts
\[\Omega = \Omega_F \cup \Omega_B\ (\text{Fig. 1(a)}).\] Therefore, the model problem is defined as follows:

\[
\nabla \times \left( \frac{1}{\mu} \left( \nabla \times \vec{A} \right) \right) - \nabla \times \frac{\mu_0}{\mu} \vec{M} - \vec{J} = 0 \quad \text{in } \Omega_F
\]

\[
\nabla^2 \vec{A} = 0 \quad \text{in } \Omega_B,
\]

with the boundary conditions \(\vec{A} = \text{continuous}, \frac{\partial \vec{A}}{\partial n} = -\frac{\partial \vec{A}}{\partial n} \bigg|_{\Gamma_{FB}}\) on \(\Gamma_{FB}\) and \(\vec{A} = 0\) on \(\Gamma_{B,\infty}\), whereas \(\vec{A}\) is the magnetic vector potential, \(\vec{J}\) is the current density, \(\vec{M}\) is the material magnetization, \(\mu\) is the material permeability and \(\mu_0\) is the permeability of free space. The minus sign at the second boundary condition on \(\Gamma_{FB}\) results from the orientation of the normal vector at the interface. In \(\Omega_F\) the following weak formulation can be obtained by adding the Coulomb gauge in such a manner:

\[
\int_{\Omega_F} \left[ \left( \frac{1}{\mu} \nabla \times \vec{A} \right) \left( \nabla \times \vec{\omega} \right) + \frac{1}{\mu} \left( \nabla \cdot \vec{A} \right) \left( \nabla \cdot \vec{\omega} \right) \right] d\Omega_F - \int_{\Gamma_{FB}} \left[ \vec{\omega} \times \left( \frac{1}{\mu} \nabla \times \vec{A} \right) - \left( \frac{1}{\mu} \nabla \cdot \vec{A} \right) \vec{\omega} \right] d\Gamma_{FB}
\]

\[
= \int_{\Omega_F} \left[ \frac{\mu_0}{\mu} \vec{M} \left( \nabla \times \vec{\omega} \right) + \vec{\omega} \vec{J} \right] d\Omega_F - \int_{\Gamma_{FB}} \vec{\omega} \times \frac{\mu_0}{\mu} \vec{M} d\Gamma_{FB},
\]

where \(\vec{\omega}\) is the vector weighting function.

Now consider \(\Omega_B\), where (2) has to be solved. In this regard, the method of weighted residuals is applied to (2) and the generalized Gauss’s theorem is used:

\[
\int_{\Omega_B} \nabla^2 \vec{A} d\Omega_B + \int_{\Gamma_{FB}} \vec{\omega} \vec{Q} d\Gamma_{FB} - \int_{\Gamma_{FB}} \vec{A} \frac{\partial \vec{\omega}}{\partial n} d\Gamma_{FB} = 0,
\]

where \(\vec{Q}\) is the normal derivative of \(\vec{A}\). The weighting function \(\omega\) can be hereby replaced by the fundamental solution of the Laplacian in 3D, which is given by

\[
u^*(\vec{r}, \vec{r'}) = \frac{1}{4\pi} \frac{1}{|\vec{r} - \vec{r'}|}.
\]

With (5) and \(q^* = \frac{\partial \nu^*}{\partial \vec{n}}\), (4) leads to the following expression [5]

\[
c(\vec{r}) \vec{A}(\vec{r}) - \int_{\Gamma_{FB}} u^*(\vec{r}, \vec{r'}) \vec{Q} d\Gamma_{FB} + \int_{\Gamma_{FB}} q^*(\vec{r}, \vec{r'}) \vec{A} d\Gamma_{FB} = 0,
\]

where the function \(c(\vec{r})\) contains the interior solid angle at \(\vec{r}\).
Discretizing $\Omega_F$ with finite elements and $\Gamma_{FB}$ with boundary elements and expressing the vector potential in (3) and (6) with applicable shape functions, the coupled system of equations can be written in a sorted matrix form \[6\] as:

\[
\begin{pmatrix}
F_{\Omega \Omega} & F_{\Omega \Gamma} & 0 & A_\Omega \\
F_{\Gamma \Omega} & F_{\Gamma \Gamma} & T & A_\Gamma \\
0 & [K] & & Q_\Gamma \\
0 & [V] & &
\end{pmatrix}
\begin{pmatrix}
\vec{A}_\Omega \\
A_\Gamma \\
Q_\Gamma
\end{pmatrix}
= \begin{pmatrix}
\vec{b} \\
0 \\
0
\end{pmatrix},
\]

where the matrices $[F_{\Omega \Omega}]$, $[F_{\Omega \Gamma}]$, $[F_{\Gamma \Omega}]$, $[F_{\Gamma \Gamma}]$ consist of values of the FEM-approach, $[T]$ is the boundary matrix, $[K]$ is the double layer potential and $[V]$ the single layer potential. The subscript $\Omega$ represents the contributions of the elements inside $\Omega_F$ while the subscript $\Gamma$ stands for the contributions of the elements which are bounded on $\Gamma_{FB}$. $A_\Omega$ is the solution vector of the magnetic vector potential in $\Omega_F$, whereas $A_\Gamma$ and $Q_\Gamma$ are the Dirichlet and the Neumann data on the boundary. Furthermore, $\vec{b}$ contains the values which correspond to the right hand side of (3).

3. FORCE CALCULATION

In order to describe the mechanical part of the MFM, the magnetic interaction forces between the magnetic coated tip and the field inducing sample have to be considered. In this regard, different force calculation methods are implemented and compared to each other with respect to the total force solution as well as to the solution of the force distribution on the magnetic coated tip.

3.1. Maxwell Stress Tensor

Considering the classical approach for the Maxwell stress tensor (MST), the ferromagnetic material in the region of interest could be replaced by a distribution of currents in such a manner that the external field is not altered [7]. Based on this consideration the occurring magnetic force can be computed by an integration of the divergence of the MST $\vec{T}$ over a domain $\Omega$, which can be transformed to an integral over the enclosing surface by applying Gauss’s law

\[
\vec{F} = \int_\Omega \nabla \cdot \vec{T} \, d\Omega = \int_{\Gamma} \vec{T} \cdot d\Gamma.
\]

Depending on the position of the enclosing integration surface, the force calculation with the MST yields to results with good accuracy. However, this method is difficult to implement and has a high computational cost.

3.2. Virtual Work Principle

The virtual work principle (VW) is based on the energy law and the principle of a virtual displacement of the considered body [8]. The total magnetic force can be calculated by the derivation of the magnetic energy or co-energy, while keeping the flux or current constant. For a permanent magnet the energy formulation can be expressed by using the abbreviation $\langle \vec{x}, \vec{y} \rangle := (\vec{x} - \vec{y}) \cdot (\vec{x} - \vec{y})$ as

\[
W = \frac{1}{2\mu_0} \int_\Omega \langle \vec{B}, \vec{B}_r \rangle \, d\Omega,
\]

where $\vec{B}_r$ is the remanent induction. A derivation of the energy $W$ in one direction $i$ leads to the corresponding force $F_i$ in this direction. In a finite element approach the domain $\Omega_F$ is divided into a set of subdomains. A local displacement of a node $k$ results in a variation of the energy in all elements surrounding this node. This leads to a nodal force which can be obtained by solving (10) at the elements $e$ corresponding to a node $k$ in a direction $i$

\[
F_{ik} = - \sum_e \left[ \int_{\Omega_e} \frac{(\vec{B} - \vec{B}_r)}{\mu_0} \frac{\partial \mathcal{J}}{\partial s_i} \vec{B} |\mathcal{J}| \, d\Omega_e - \int_{\Omega_e} \frac{\langle \vec{B}, \vec{B}_r \rangle \delta |\mathcal{J}|}{2\mu_0} \frac{\partial |\mathcal{J}|}{\partial s_i} \, d\Omega_e \right],
\]

where $\mathcal{J}$ is the Jacobian and $|\mathcal{J}|$ is the determinant of the Jacobian matrix. The total force is then given by a summation of the local forces at all nodes (in the following named as VW1).

Another approach (in the following named as VW2), first introduced in [3], suggests that in a theoretical consideration the total force solution can be decomposed into two different parts,
the intrinsic and the interaction forces. The former are the obtained forces of a single permanent magnet in air without other ambient influences. Thereby, the considered energy is the stored energy of the permanent magnet due to the magnetization process, but this energy is incorrectly described in (9). By contrast, the interaction forces arise from an external magnetic field. Unlike the intrinsic energy, the occurring interaction energy is well expressed with (9), while a linear rigid model can be assumed for the permanent magnet. For the interaction force evaluation the intrinsic forces of the permanent magnet have to be withdrawn from the forces obtained by (9) and (10), respectively. Concerning this matter (11) has to be solved

\[ F_{i,\text{interaction}} = F_i - F_{i,\text{intrinsic}} = \frac{\delta W_{\text{interaction}}}{\delta s_i} = \frac{\delta}{\delta s_i} \left[ \frac{1}{2\mu_0} \int_{\Omega} \left( \langle \vec{B}, \vec{B}_r \rangle - \langle \vec{B}_{\text{air}}, \vec{B}_r \rangle \right) d\Omega \right], \]  

(11)

where \( \vec{B}_{\text{air}} \) is the magnetic induction of the single magnet in air. The force calculation methods based on the Virtual Work Principle are relatively easy to implement and show a good relation between computational cost and the grade of accuracy.

### 3.3. Equivalent Magnetic Sources

Another proposal to calculate the occurring forces on a permanent magnet is to express the magnetizations as equivalent magnetic currents (EMS1) or equivalent magnetic charges (EMS2). As it was previously shown, for example in [9], the permanent magnet can be therefore replaced by a volume current density \( \vec{J}_v = \nabla \times \vec{M} \) and a surface current density \( \vec{J}_s = -\vec{n} \times \vec{M} \) or by a volume charge density \( \rho_v = -\mu_0 \nabla \cdot \vec{M} \) and a surface charge density \( \rho_s = \mu_0 (\vec{n} \cdot \vec{M}) \). If \( \vec{M} \) is constant, the volume current density or rather the volume charge density vanishes and the occurring force densities can be calculated with the following expressions

\[ \vec{f}_s = \vec{J}_s \times \vec{B}_s, \quad \vec{f}_s = \rho_s \vec{H}_s. \]

(12)

The force calculation methods based on equivalent sources are very straightforward. Compared to the above mentioned methods, the computational cost is low.

### 4. RESULTS AND DISCUSSION

For the simulation of the Magnetic Force Microscope a sample configuration with a span of \(-20 \mu m \leq x \leq 20 \mu m\) featuring alternating magnetic domains which hold a magnetization of \(557 kA/m\) is assumed (Fig. 1(b)). Furthermore, as a typical coating material of the cantilever tip a cobalt-chromium compound was chosen which has a magnetization of \(749 kA/m\) and is orthogonally directed with respect to the sample surface. With the mentioned field and force calculation methods a scanning process of this configuration was numerically investigated. In Fig. 2 the total lateral force (\(F_x\)) and normal force (\(F_y\)) are shown. It can be clearly seen that the presented force calculation methods are applicable to obtain the total magnetic force acting on the cantilever, especially for the normal component. But in order to include the mechanical behavior due to the occurring

![Figure 2](image_url)
forces, it is necessary to obtain an appropriate physical force distribution. In this regard, Fig. 3(a) displays our model in detail. The figure shows the micrometer scaled cantilever on the left side and the composition of the magnetic coated tip with the apex of the coating in a small distance on the right side. The illustrated curves in Fig. 3(b) represent the absolute value of the normal component of the force distribution on the outer surface of a vertical cut of the coating apex as a function of the apex angle at a cantilever position of $x = 16 \mu m$. Corresponding to these results, a three dimensional illustration on the half of the coating apex is given in Fig. 4. As it is shown, the force distribution of the five proposed methods strongly differ from each other and it is not completely clear which one is valid to use for a subsequent structural analysis. In [1] for example, it is suggested that reliable results for the deformation analysis can be achieved with the magnetic charge force density, whereas in [2], in which the numerical calculations of the assumed configuration are compared to experimental data, the method based on the energy principle is noted with the highest accuracy. However, when keeping in mind that for a MFM only the few atoms at the tip apex strongly interact with the sample material, the highest force density should be also located there. As it is shown in Fig. 4, it seems that at least the VW1 as well as both ESM approaches can be excluded with respect to the local physical behavior at the tip apex.

Figure 3: Model of the coated tip (a) and the force distribution of the normal force component (absolute value) on the outer surface of a vertical cut of the coating apex at a cantilever position of $x = 16 \mu m$.

Figure 4: Comparison between the five different force distributions ($\vec{f}_n$).

5. CONCLUSION

A hybrid numerical approach for the simulation of a Magnetic Force Microscope was presented. In order to include a subsequent structural analysis different kinds of force calculation methods were implemented and compared to each other. In the case of the total magnetic force all different methods agree well to each other, while the force distribution strongly differ. However, with respect to the physical behavior it seems that the VW1 and both ESM approaches could be excluded.
REFERENCES


