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Abstract
Purpose – The purpose of this paper is to introduce a method which allows the calculation of the interactions of tip and sample of a magnetic force microscope as a first step to increase the accuracy of this technique.

Design/methodology/approach – The emerging magnetic interactions between the cantilever tip and an arbitrary magnetized sample can be evaluated by the use of several numerical methods. For modelling this magnetically and mechanically coupled multiscale problem the finite element method is implemented.

Findings – The evaluated magnetic fields interact in such a manner that a constructive overlap at the tip apex occurs. This leads to attractive forces acting on the cantilever.

Research limitations/implications – In order to include the magneto-mechanical coupling, the implementation of a detailed force calculation is necessary. Furthermore, a hysteresis model is not yet considered.

Practical implications – Magnetic force microscopy is a very sensitive technique. For instance, ideally the end of the tip consists of only one atom, but this is not realizable. Measurement errors cannot be avoided. This approach is the first step in developing an opportunity to soften them.

Originality/value – One opportunity to verify real-time magnetic force microscope measurements is the comparison with theoretical considerations and calculations of the occurring magnetic distribution by using this technique. For this reason this paper deals with a new micromagnetic model to simulate the interactions between tip and sample of a scanning process of a magnetic force microscope.

Keywords Finite element analysis, Electromagnetism, Microscopes, Nanotechnology

Paper type Research paper

Introduction
Magnetic force microscopy (MFM) was developed in 1987 as a special application of scanning force microscopy (Martin and Wickramasinghe, 1987). Its resolution allows the detection of the magnetic properties of a sample surface on a nanometer scale. During the scanning process, a magnetized tip is moved over the sample surface (Figure 1). The orientation of the sample magnetization can be obtained by measuring the force acting on the tip. In addition to being a well known technique in material science for the investigation of magnetic properties, MFM allows the analysis of magnetic high-density storage media. In order to increase the resolution of MFM analyses and to facilitate an improved understanding of the micromagnetic behaviours in this technique, it is useful to develop theoretical models. To describe the procedure of a MFM analysis with numerical models we have to solve a magnetically and mechanically coupled multiscale problem. On the one hand, we have to compute

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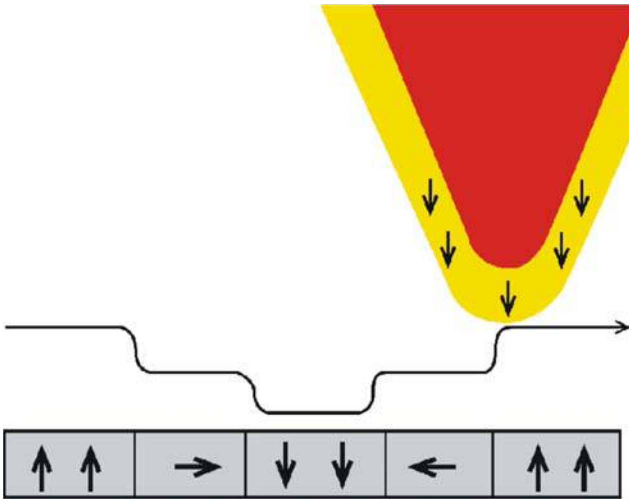


Figure 1.
Deflection of the cantilever due to several magnetic domains

magnetic fields and forces between tip and sample on a nanometer scale, on the other hand we have to deal with the macroscopic deflections of the cantilever.

Several concepts for modelling the magnetic interactions between tip and sample in MFM have been presented. One approach divides the magnetic coated or massive tip into cubic elements (Mansuripur, 1989). In further numerical models the magnetization distribution of the tip has been calculated by a 2D triangular structure (Oti, 1993) or using a 3D model (Tomlinson and Farley, 1997). These approaches are based on the Landau-Lifshitz-Gilbert equation.

In this paper, a more general approach is considered. In order to simulate a whole MFM process a mechanically and magnetically coupled multiscale problem must be solved. For instance, to analyze the deflections of the cantilever it is necessary to calculate the forces acting on the probe. For this reason a detailed computation of the occurring magnetic field strength is needed. Thus, we calculate the emerging magnetic interactions between the cantilever tip and an arbitrary magnetized sample with the finite element method (FEM). In the past, there are several discussions and comparisons about using different kinds of elements (Tsukerman, 1993; Mur, 1994). Especially, the well known edge elements have become very famous in the last two decades, because of providing a natural treatment of discontinuities. Hence, the approximation error at discontinuities is less than solving the problem with nodal elements (Tsukerman, 1993). Furthermore, the accuracy of the resulting field strength near protruding corners increases by using these elements (Mur, 1994). Anyhow, some studies have shown that edge elements are numerically less stable than nodal elements (Preis *et al.*, 1991) and they are known to be less efficient in storage requirement and computation time by having the same accuracy than nodal elements (Mur, 1994; Jiang, B-N., *et al.*, 1996). In addition some of the expressed problems, especially the discontinuities at almost flat material boundaries using nodal elements, can be softened by implementation of double layer nodes at these boundaries. For instance, one application is shown in (Yuan *et al.*, 1991). However, knowing the occurring numerical problems concerning nodal-based elements when dealing with the magnetic vector potential at protruding corners, for a first approach solving the above mentioned multiscale problem, we decided to discretize the treated area by first order nodal elements. In addition, the pyramidal tip of the MFM is assumed to consist of a hard ferromagnetic material, which is included by setting $\mu_r = 1$. Focusing on the computation of the magnetic flux density between tip and sample and the forces acting on the cantilever, the remained numerical discrepancies at the edges and corners of the sample caps are assumed not to have a large impact on our results. In order to account for the highly non-linear field distribution near the tip, we apply a relatively fine mesh there, while in the outer region a rougher mesh is sufficient. Furthermore, each element was allowed to carry a magnetization defined in three vector components. In setting up the system of equations, we chose the well known curl-curl equation and applied the method of weighted residuals. The results of the investigation are shown for an example with a CoCr-tip and an alternately magnetized AlNiCo-sample.

Formulations

The fundamental expressions for electromagnetic fields are the Maxwell equations. In a magnetostatic case, the first Maxwell equation becomes:

$$\nabla \times \mathbf{H} = \mathbf{J}. \tag{1}$$

Using the material expression:

$$\mathbf{H} = \frac{1}{\mu}\mathbf{B} + \frac{\mu_0}{\mu}\mathbf{M} \tag{2}$$

and the definition for the magnetic flux density:

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{3}$$

yield the well known curl-curl equation can be expressed as:

$$\nabla \times \frac{1}{\mu}(\nabla \times \mathbf{A}) = \nabla \times \frac{\mu_0}{\mu}\mathbf{M} + \mathbf{J}. \tag{4}$$

For the purpose of ensuring the uniqueness of the magnetic vector potential and making the solution of the coupled system of equations numerically stable (Preis *et al.*, 1991) the Coulomb gauge:

$$-\nabla \frac{1}{\mu}\nabla \mathbf{A} = 0 \tag{5}$$

is added to equation (4). Applying the method of weighted residuals to equation (4) and (5), the following formulation can be obtained:

$$\begin{aligned} &\iiint_\Omega \mathbf{N_a}\left[\nabla \times \left(\frac{1}{\mu}\nabla \times \mathbf{A}\right) - \nabla \times \frac{\mu_0}{\mu}\mathbf{M}\right]\mathrm{d}\Omega \\ &\quad - \iiint_\Omega \mathbf{N_a}\left(\nabla \frac{1}{\mu}\nabla \mathbf{A}\right)\mathrm{d}\Omega - \iiint_\Omega \mathbf{N_a}\mathbf{J}\mathrm{d}\Omega = 0, \end{aligned} \tag{6}$$

whereas the vector ω_a with $a = 1, 2, 3$ contains the weighting functions:

$$\mathbf{N}_1 = \begin{pmatrix} \mathrm{N}_1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{N}_2 = \begin{pmatrix} 0 \\ \mathrm{N}_2 \\ 0 \end{pmatrix}, \quad \mathbf{N}_3 = \begin{pmatrix} 0 \\ 0 \\ \mathrm{N}_3 \end{pmatrix}. \tag{7}$$

In order to derive the weak form of equation (6) we use a vector identity and apply the Gauss law. Furthermore, we assume $\mathbf{J} = 0$, because of nonexistent current densities in the considered regions:

$$\begin{aligned} &\iiint_\Omega \left[\left(\frac{1}{\mu} \nabla \times \mathbf{A} \right) (\nabla \times \mathbf{N_a}) + \frac{1}{\mu} \nabla \mathbf{A} \nabla \mathbf{N_a} \right] d\Omega \\ &\quad - \oiint_\Gamma \left[\mathbf{N_a} \times \left(\frac{1}{\mu} \nabla \times \mathbf{A} \right) - \mathbf{N_a} \left(\frac{1}{\mu} \nabla \mathbf{A} \right) \right] d\Gamma \\ &= \iiint_\Omega \frac{\mu_0}{\mu} \mathbf{M} (\nabla \times \mathbf{N_a}) d\Omega - \oiint_\Gamma \mathbf{N_a} \times \frac{\mu_0}{\mu} \mathbf{M} d\Gamma. \end{aligned} \tag{8}$$

Micromagnetic model

The 3D model used in this work consists of four different subspaces (Figure 2), where Ω_1 represents the space around the cantilever and sample. Γ_1 is the outer boundary surface. The subregion of the cantilever and the tip are represented by Ω_2 and Ω_3. The interface boundaries are Γ_2 and Γ_3, respectively. At last the subregion of the sample is described by Ω_4 and Γ_4.

Therefore, at the shown boundaries interface conditions must be satisfied. Derivable from electromagnetic theory, the continuity of the normal component of

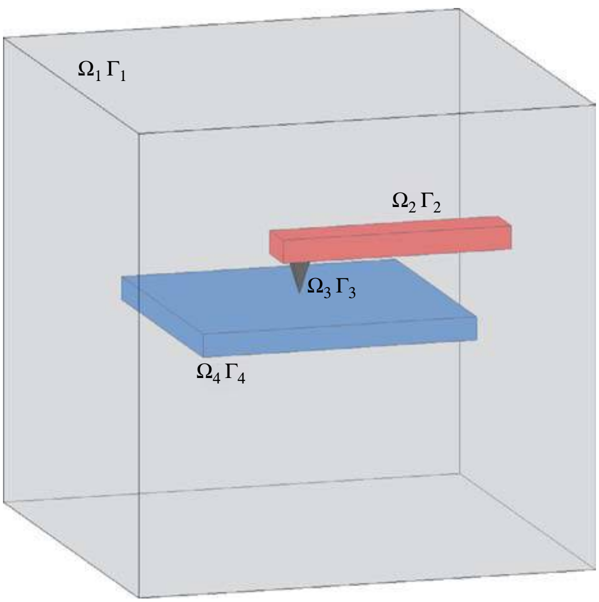


Figure 2.
The micromagnetic model of a magnetic force microscope

magnetic flux density **B** and the tangential component of magnetic field intensity **H** must be considered. By including the magnetic vector potential, the following two conditions must be met:

$$\mathbf{n}\cdot(\nabla\times\mathbf{A}_1)=\mathbf{n}\cdot(\nabla\times\mathbf{A}_2) \tag{9}$$

$$\mathbf{n}\times\frac{1}{\mu_1}\nabla\times\mathbf{A}_1=\mathbf{n}\times\frac{1}{\mu_2}\nabla\times\mathbf{A}_2, \tag{10}$$

in which **n** is the outward unit normal vector to the boundary. Thereby, the continuity of the normal component of the flux density **B** is implicit in the definition (3) (Chari *et al.*, 1981). Equation (10) is implemented by the boundary integral on the left hand side in equation (8).

For this micromagnetic model, several parameters are defined. One of them is the magnetization in the subregions Ω_3 and Ω_4. In the example at hand we assume a massive pyramidal tip. This tip consists of a cobalt-chromium compound, which is orthogonally magnetized with respect to the sample surface. Analogous to (Carl *et al.*, 2001), we set the value for the magnetization in negative y-direction to $M = 749$ kA/m. Furthermore, we assume such a hard ferromagnetic material, so that the permanent permeability of the pyramidal tip is approximately $\mu_r \approx 1$. Referring to (Spickermann, 2001), we chose an aluminum-nickel-cobalt compound for the sample material, which has a permanent permeability of approximately $\mu_r \approx 2.5$. In addition, the alternating magnetization of this material is set to $M = 557$ kA/m. These assumptions are shown in Figure 3.

The whole space around the tip and sample is filled with air. Therefore, the permeability in Ω_1 and Ω_2 is set to $\mu_r = 1$ and there is no magnetization in these areas. According to (Alhamadi *et al.*, 1991; Jiang, X., *et al.*, 1996), where the fields of permanent magnets have been calculated by transforming the magnetizations in the subregions to equivalent sheet currents, we consider each element in the magnetic area and assume a constant magnetization. In this case, we can neglect the volume integral on the right hand side of equation (8). Under these circumstances and observation of

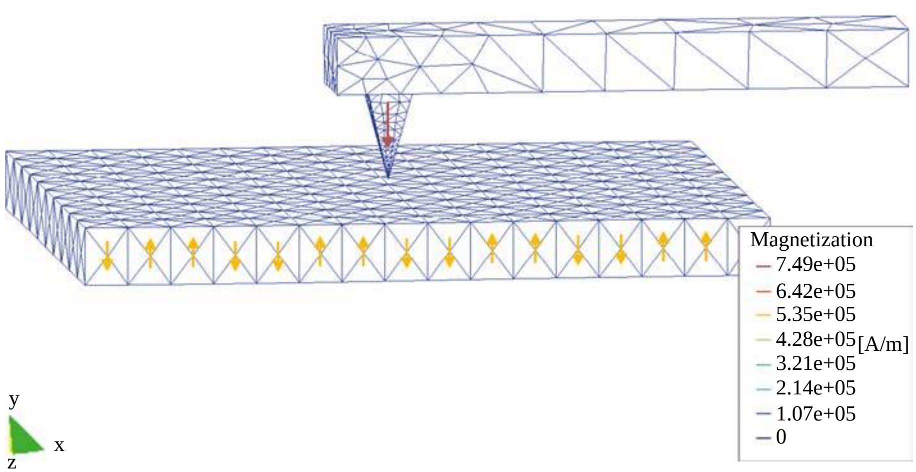


Figure 3.
Assumptions for the magnetization of the tip and sample for the micromagnetic model

equation (10) by using the normal unit vector we get the magnetic vector potential in the considered area. Applying the Galerkin method and solving the coupled system of equations, the occurring magnetic flux density can be found by equation (3).

Force calculation

In order to simulate the deformation of the cantilever, the occurring magnetic forces acting on the probe must be calculated. The source of the force is the interaction of the magnetic moments of tip and sample. Mainly, for a magnetic field problem there are three traditional methods to describe and calculate this phenomenon. The first one is the integration of the divergence of the Maxwell stress tensor $\mathbf{T}$ over a volume Ω:

$$\mathbf{F} = \iiint_\Omega \operatorname{div} \mathbf{T} d\Omega = \oint\!\!\!\oint_\Gamma \mathbf{T} d\Gamma, \tag{11}$$

which can be transformed to an integral over the enclosing surface by applying Gauss's law. However, previous works have shown that the force computed heavily depends on the integration surface enclosing the boundary surface under investigation (Ren, 1994). Furthermore, the solution of the force density is negatively affected by numerical errors.

A second method which has become very popular is the principle of virtual work. Thus, a variation of the magnetostatic energy δW_{mag} is a result of a virtual displacement $\delta_{\mathbf{r}}$ of a body due to a force $\mathbf{F}$:

$$\delta W_{\mathrm{mag}} = \boldsymbol{\delta}\mathbf{r} \cdot \mathbf{F}_{\mathrm{mag}}. \tag{12}$$

If the movable body is surrounded by air the basic equation for solving the total force in the r-direction becomes:

$$\mathbf{F}_{\mathrm{mag}} = -\sum_{e=1}^{n} \left(\iiint_\Omega \frac{\mathbf{B}}{\mu_0} \frac{\boldsymbol{\delta}\mathbf{B}}{\boldsymbol{\delta}\mathbf{r}} d\Omega + \iiint_\Omega \frac{\mathbf{B} \cdot \mathbf{B}}{2\mu_0} \frac{\delta(d\Omega)}{\boldsymbol{\delta}\mathbf{r}} \right),$$

where the index e describes the virtually distorted elements that adjoin to the movable body (Kaltenbacher, 2007). The third possibility to calculate the force is the equivalent sources method. This method is based on replacing the magnetization by an equivalent surface current density and using the well known Lorentz formula.

Results

For the presented model the emerging magnetic flux density was calculated. The solution of the absolute value of $\mathbf{B}$ is shown with contour lines in Figure 4. Apparent in the figure, the resulting magnetic fields interact in such a manner that a constructive overlap at the tip apex occurs. This leads to attractive forces acting on the cantilever. Another illustration is shown in Figure 5, where the magnetic flux density is represented by vectors. Owing to the vector illustration, the magnetic domains, which depend on the preconditioned alternating sample magnetizations, are identifiable. In addition, the intersections between these areas also can be seen. Furthermore, the maximum of magnetic flux density is clearly distinguished at the tip apex. To clarify the distribution of the magnetic flux density on the sample surface a one dimensional interpolation plot is shown in Figure 6.

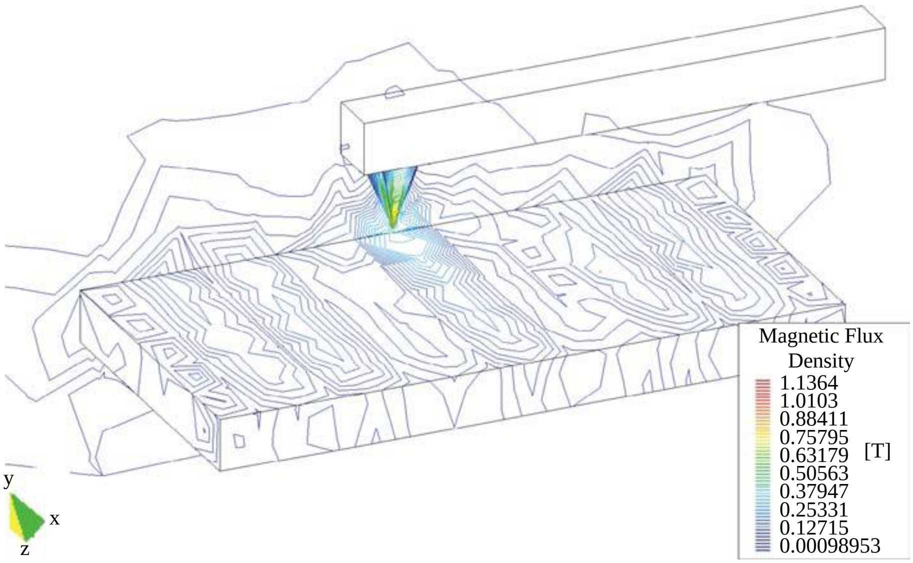


Figure 4.
The resulting absolute value of magnetic flux density of the 3D model, presented by contour lines

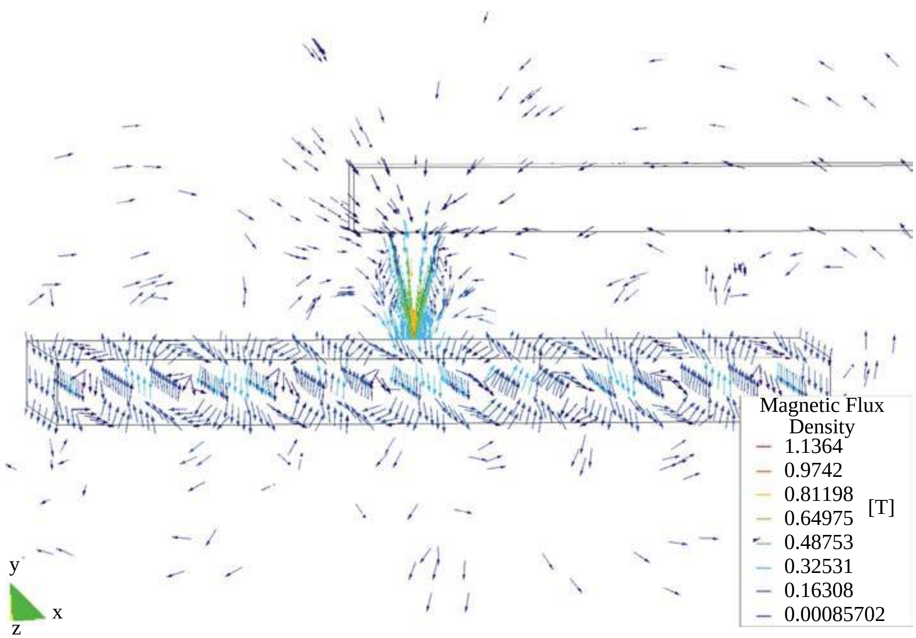
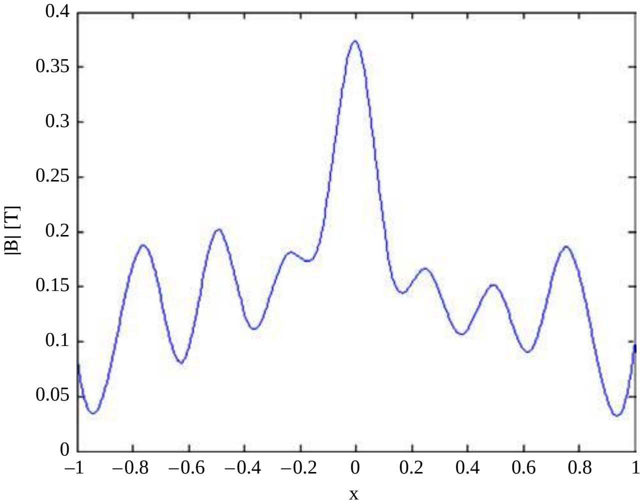


Figure 5.
The resulting magnetic flux density of the 3D model, presented by vectors

As we mentioned in the introduction of this paper, the accuracy of the results depends on the discretization of the considered regions. While the inner regions were modelled with a fine mesh, the outer area was modelled with an unstructured mesh. For this reason, the magnetic flux density under the tip apex is not exact symmetric.



Note: The limits – 1, 1 are the end caps of the sample. The value $x = 0$ represents the point at the tip axis

Figure 6. The magnetic flux density |**B**| on the sample surface in longitudinal x-direction

However, the interactions between tip and sample magnetizations can be easily seen. On the left and right side of the main peak at $x = 0$, the average of the absolute value of the magnetic flux density results in a sloping curve.

We compared our results with analytical considerations (Wadas and Hug, 1992). In this study, the orthogonal component of the magnetic stray field with respect to the sample surface was analytically calculated on tip axis exclusive of an influencing sample magnetization. Our results for this component in this region agree well with it.

Conclusions

In this paper, a micromagnetic model based on the FEM was presented. It allows the calculation of the magnetic interactions between the tip and an arbitrary sample for a magnetic force microscope. The considered subspaces were discretized by first order tetrahedral elements. The necessary interface and boundary conditions as well as the Coloumb gauge were noted. Additionally a short overview about different force calculation methods was given. Finally, an example with a massive magnetized CoCr-tip and an alternately magnetized AlNiCo sample was presented.

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