Artefacts in Near-Field Optical Microscopy

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Abstract. In this article results of complete modelling of electromagnetic field distribution in a near-field scanning probe microscope (NSOM) are presented. It is shown, that using finite difference in time domain method the NSOM signal can be computed for real tip-sample geometry. The results of such a simulation can be used to predict presence and distribution of topography related artefacts in NSOM images.

Keywords: near-field scanning optical microscopy; artefacts;

1. Introduction
Near field scanning optical microscopy is a promising and still developed experimental technique that combines scanning probe methods resolution with imaging and analysis possibilities of optical microscopes [1].

As the complete electromagnetic field analysis in the near field area close to probe cannot be performed easily, near field scanning optical microscopy experiments are usually limited for imaging or detection of presence of different features in the sample, at one or more wavelengths. However, the optical information is not used for any local quantitative optical analysis in conventional experiments.

There are many approaches for extending the NSOM method towards quantitative optical analysis, using computational methods or special experimental devices [2, 3]. Theoretical models are usually limited to different model cases that are more or less related to the real experiments, namely due to the available computing resources and complexity of NSOM geometry. However, increase of the computational power of personal computers and further development of the electromagnetic field analysis methods offers new possibilities of solving these problems in the area of computational electromagnetics.

One of the largest problems in interpretation or further quantitative analysis of optical data obtained by means of NSOM is its relation to the local surface topography and real fiber geometry [4, 5]. This effect can be easily seen while imaging steep slopes or edges on the sample (here, it can be easily predicted) or while imaging surface exhibiting random roughness. Sometimes the topography artefacts can completely obscure the optical information contained in the data.

In this article we present results of complete electromagnetic modelling of the NSOM geometry, including its probe formed by fiber with small shielded aperture, tip-sample
configuration and far field result going to the photo-detector. All the material and geometrical parameters are related to concrete NSOM measurements and are therefore corresponding to the real situation. Two different materials are modelled and results are compared with the real measurements.

2. Experimental arrangement
For NSOM measurements, Aurora 2 NSOM instrument (Thermomicroscopes) was used. Standard metal shielded fiber tips with aperture between 80 - 100 nm were used for measurements. All the images were acquired in reflection mode.

As a sample, we used standard calibration grating (SiO$_2$) as a simple example of object forming topographical artefacts. Both clean grating and grating coated by thin gold film (designed for scanning tunnelling microscopy analysis) were measured using the NSOM instrument.

Atomic force microscope (AFM) measurements were performed by Explorer AFM (Thermomicroscopes) using standard non-contact tips and working in non-contact mode.

Geometry of used NSOM fiber tips was measured using scanning electron microscope Jeol JSM-6460.

3. Electromagnetic field modelling
For modelling the electromagnetic field we have used finite difference in time domain method (FDTD), which is probably most universal tool for computational electrodynamics. Within FDTD we simply solve Maxwell equations numerically in a leap-frog scheme (E and H components consecutively) with a proper placement of the field vector components in space and proper discretization. The years of development of the FDTD methods resulted on many methods for including different materials (metals, dielectrics, dispersive materials, nonlinear materials, etc.) and sources (planar sources, antennas). For further details, see e. g. Ref. [6].

We have used the following FDTD extensions:

- uniaxial perfectly matched layer (UPML) to allow waves to leave computational domain,
- conformal modelling of the material boundaries,
- near to far field transform (NFFF) for evaluation of the far field limit of the electromagnetic field distribution [7],
- computational domain stepping in one dimension to model structures elongated in one direction.

For modelling our NSOM geometry, we have used these two steps:

(i) optical fiber probe analysis based on geometry obtained using scanning electron microscope and data-sheet material properties of fiber; computed in space of $20\times3\times3$ wavelengths ($\lambda$), space discretization of $\lambda/20$, using stepping in one dimension and conformal modelling,

(ii) probe-surface geometry analysis using the probe apex fields computed in step 1 and AFM topography of the grating surface; computed in space of $4\times4\times4$ $\lambda$, space discretization $\lambda/40$, using NFFF computation of the far field limit

The second step geometry is illustrated by a cross-section presented in Fig. 1. Second step was repeated for all the predefined positions of tip above sample to obtain simulated NSOM profiles.

4. Results and discussion
In Fig 2. resulting electromagnetic field distributions (cross-sections of the computational space) for three different fiber tip positions are presented for both the uncoated and coated grating. Note that the colour scale is logarithmic for better visualisation. Within full computation, the
NSOM probe scans over surface keeping the minimum distance between body of probe and surface constant.

In Fig 3, the resulting NSOM profiles over the edge of coated grating depression are plotted. The far field limit computation was performed for 4 different points in the far field domain, where in principle the detector could be located. The points are located perpendicularly to orientation of grating. Therefore, four different profiles are obtained within computation: A and B that are located in direction parallel to the step, and C and D that are located perpendicularly to the step. The real NSOM geometry that was used for obtaining Figure 1 here corresponds to profiles ”D”. Profile obtained for real measurements on coated grating is plotted in Fig. 3 as well.

Note that the differences between A and B point (both parallel to step) are caused by a small angle tilt of sample relative to the NSOM head. The results for uncoated sample were very similar, however, the artefact strengths were slightly lower due to the optical properties and thickness of the film forming grating.

5. Conclusion
Finite difference in time domain calculation of propagation of electromagnetic field within real NSOM geometry can be efficiently used for modelling of the NSOM signals and prediction of topographic artefacts in optical data. It was shown, that involving the real parameters of NSOM instruments can be performed easily (from computational point of view) and can lead to results that refer to real experiments.

This method can be used also for other quantitative processing of near-field data or understanding process of creation of NSOM images. It can be run for different frequencies successively, or even at single run (with proper post-processing of far field data), which gives opportunities for near field spectroscopy experiments analysis too.

The method is still computationally very demanding (approximately 20 minutes of computation for one single point on Pentium D 3.4 Ghz), however, this drawback could be minimised using parallel computing approach.

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Figure 1. Geometry of the computational domain (cross-section).
Figure 2. Electromagnetic field intensity ($E_x$ component) at different positions of probe, A-C: metal coated grating, D-F: uncoated grating.
Figure 3. (left) electromagnetic field intensity profile while scanning across grating edge, 4 different NSOM detector positions, (right) real NSOM image of grating and profile over the edge of grating depression.