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COMPUTER SCIENCE MEETS AUTOMATION

VOLUME II

- Session 6 Environmental Systems: Management and Optimisation
- Session 7 New Methods and Technologies for Medicine and Biology
- Session 8 Embedded System Design and Application
- Session 9 Image Processing, Image Analysis and Computer Vision
- **Session 10 Mobile Communications**
- Session 11 Education in Computer Science and Automation



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Preface

Dear Participants,

Confronted with the ever-increasing complexity of technical processes and the growing demands on their efficiency, security and flexibility, the scientific world needs to establish new methods of engineering design and new methods of systems operation. The factors likely to affect the design of the smart systems of the future will doubtless include the following:

- As computational costs decrease, it will be possible to apply more complex algorithms, even in real time. These algorithms will take into account system nonlinearities or provide online optimisation of the system's performance.
- New fields of application will be addressed. Interest is now being expressed, beyond that in "classical" technical systems and processes, in environmental systems or medical and bioengineering applications.
- The boundaries between software and hardware design are being eroded. New design methods will include co-design of software and hardware and even of sensor and actuator components.
- Automation will not only replace human operators but will assist, support and supervise humans so that their work is safe and even more effective.
- Networked systems or swarms will be crucial, requiring improvement of the communication within them and study of how their behaviour can be made globally consistent.
- The issues of security and safety, not only during the operation of systems but also in the course of their design, will continue to increase in importance.

The title "Computer Science meets Automation", borne by the 52nd International Scientific Colloquium (IWK) at the Technische Universität Ilmenau, Germany, expresses the desire of scientists and engineers to rise to these challenges, cooperating closely on innovative methods in the two disciplines of computer science and automation.

The IWK has a long tradition going back as far as 1953. In the years before 1989, a major function of the colloquium was to bring together scientists from both sides of the Iron Curtain. Naturally, bonds were also deepened between the countries from the East. Today, the objective of the colloquium is still to bring researchers together. They come from the eastern and western member states of the European Union, and, indeed, from all over the world. All who wish to share their ideas on the points where "Computer Science meets Automation" are addressed by this colloquium at the Technische Universität Ilmenau.

All the University's Faculties have joined forces to ensure that nothing is left out. Control engineering, information science, cybernetics, communication technology and systems engineering – for all of these and their applications (ranging from biological systems to heavy engineering), the issues are being covered.

Together with all the organizers I should like to thank you for your contributions to the conference, ensuring, as they do, a most interesting colloquium programme of an interdisciplinary nature.

I am looking forward to an inspiring colloquium. It promises to be a fine platform for you to present your research, to address new concepts and to meet colleagues in Ilmenau.

In Sherte

Professor Peter Scharff Rector, TU Ilmenau

"L. Ummt

Professor Christoph Ament Head of Organisation

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E. Sparrer / T. Machleidt / R.Nestler / K.-H. Franke / M. Niebelschütz

Deconvolution of Atomic Force measurements in special modes – methodology and application

Abstract

The signal measured by Kelvin Force Microscopy is a convolution of an effective surface potential and a microscope intrinsic point spread function, which allows the restoration of the measured data by linear deconvolution. An analytical way is demonstrated by gaining the point spread function of the microscope. The linear shift invariant channel is introduced as a signal formation model and a wiener filter supported deconvolution algorithm is applied to the measured data.

Motivation

Since the early 1970ies semiconductor industry confirms the postulation of Gordon Moore known as Moores Law with remarkable continuity. Year by year the dimensions of semiconductor elements are shrinking. As per current International Technology Roadmap for Semiconductors [1] the size of 20nm is planed to be undershooting by the year 2017. Present, on light microscopy based, analysis systems are not capable to resolve these small dimensions, so new technologies have to be deployed. The well-known techniques of <u>a</u>tomic <u>force m</u>icroscopy (AFM) provide an opportunity to overcome this drawback. In this paper the AFM special mode of <u>K</u>elvin <u>Force</u> <u>M</u>icroscopy (KFM) is investigated. By A. Born and T. Heuer [2,3] the KFM resolution is estimated by 50nm to 100nm. Because common atomic force microscopes are capable of a higher resolution, the measured data seams blurred. Investigation of the signal formation process enables the restoration of KFM data.

Kelvin Force Microscopy

The KFM is a method to detect the surface potential of micro- and nanostructured samples using a common atomic force microscope. To detect the surface potential all

surface forces beside the electrostatic force must be eliminated. While the electrostatic force has a very long range compared to other surface forces, these forces are disposed by moving the cantilever tip to a height h of at least 100nm above the sample surface. Owing to the indirect dependence of the measured electrostatic force to the quadratic distance h² of the charged objects this distance must be kept constant to provide a proper measuring. Therefore a KFM measurement is done in two passes, which are demonstrated in Figure 1.



Figure 1 operating mode of the KFM in two passes a) determination of the sample topography b) measurement of the surface potential with constant altitude h

In the first pass the surface topography is detected by applying a standard AFM method. To provide a constant altitude h between tip and surface in the second pass the cantilever is driven at the desired distance h along the detected surface trajectory. During the measurement the cantilever is oscillated by applying a voltage U_{ac} between the cantilever and the sample surface, which is altering at the resonance frequency f_0 of the cantilever. According to H. O. Jacobs et. al [4] in case of resonance the acting electrostatic force at the cantilever tip can be expressed by equation (1)

$$F_{c,\omega_0}(x,y) = \frac{dC}{dz} \cdot \left(U_{dc} - \Phi(x,y) \right) \cdot U_{ac} \cdot \sin(2\pi f_0 t) \tag{1}$$

The controller of the KFM system adjusts an additional direct voltage U_{dc} until the acting force vanishes as described by equation (2)

$$0 = C'(x, y) \cdot (\Phi(x, y) - U_{dc}(x, y)), \text{ with } C' = \frac{dC}{dz}$$
(2)

The absolute value of the measured potential $\Phi_{dc} = U_{dc}$ is equal to the surface potential Φ at the point of measurement. The tip to surface capacity C can be described as a distributed capacity as described in Figure 2 and equation (3).



Figure 2 model of distributed capacity between tip and sample surface

$$C(x, y) = \iint_{i,j} C_{ij} (x - x_i, y - y_j) didj$$
(3)

Equation (2) solved for the measured potential Φ_{dc} and the capacity substituted by equation (3) results in the linear convolution integral displayed in equation (4)

$$\Phi_{dc}(x,y) = \iint_{i,j} \frac{C'_{ij}(x-x_i, y-y_j)}{C'(x,y)} \cdot \Phi(x,y) didj$$
(4)

The fraction described by the distributed capacity derivations C'_{ij}/C' can be realized as tip dependent <u>point spread function (PSF)</u> of the KFM system. Proofing the linear dependence of the measured signal Φ_{dc} to the actual surface potential Φ the linear shift invariant channel can be introduced as a model to describe the signal formation process. The linear shift invariant channel (Figure 3) consists of a linear shift invariant system and additive noise at the channels exit as described by Kreß and Irmer in [5].



Figure 3 the linear shift invariant channel

This model allows the restoration of the KFM data by a linear deconvolution. To deconvolve the data, the PSF of the KFM system must be known. Therefore a deduction based on the physical interrelations has been applied.

Estimation of the KFM systems PSF

In R. Königs dissertation [6] a method to calculate the electric field based on a hyperbolic coordinate system is presented. Utilization of this coordinate system allows a straightforward description of the electrostatic field lines between the charged tip apex and its mirror charge [7]. According to S. Gómez-Mõnivas et. al [8] only the apex of the KFM tip is responsible for the shape of the PSF and the apex can be well approximated by a hyperboloid. Estimating the apex shape by blind tip estimation [9] respectively measuring it at suitable standards the PSF can be derived by transforming the apex surface to polar coordinates and fitting a hyperbola as shown in equation (5) for every angle α .

$$u^{2} = C_{1}(\varphi)z + C_{2}(\varphi)z^{2}$$
(5)

By means of the parameters η_s , ξ and $r_{1,2}$ equation (6) the electrostatic force acting between a plane surface and the tip apex is given by equation (7).

$$\eta_{s}(\varphi) = \sqrt{\frac{1}{1 + C_{2}(\varphi)}}, \quad \xi(\varphi) = \frac{r_{1}(\varphi) + r_{2}(\varphi)}{2a(\varphi)}$$
with $r_{1,2}(\varphi) = \sqrt{a^{2}(\varphi) + u^{2}(\varphi)}$ and $a(\varphi) = \frac{C_{1}(\varphi)}{2C_{2}(\varphi) \cdot \eta_{s}(\varphi)}$
(6)

$$F_{el}(u,\varphi) = Q \cdot \frac{2\eta_s(\varphi)}{\ln\left(\frac{1+\eta_s(\varphi)}{1-\eta_s(\varphi)}\right)} \sqrt{\left(\xi^2(\varphi) - \eta^2(\varphi)\right)\left(1-\eta^2(\varphi)\right)} \frac{U_{Bias}}{h}$$
(7)

The PSF is finally calculated by a normalizing equation (7) to its integral. PSF estimations obtained by the method are shown in Figure 4.



Figure 4 PSF gained analytical deduction based on the physics of electrostatic fields

Deconvolution of the KFM data

To deconvolute the data an algorithm based on a PSF inversion and supported by a wiener filter as a regularization approach was implemented. In the measured KFM data and the deconvolved estimate of the actual surface potential is shown.



Figure 5 left: measured KFM data - right: deconvolved data

The red lines in Figure 5 represents the location of the plots to be seen in Figure 6



Figure 6 plot of the deconvoluted (blue) and measured (red) data along the marked line in Figure 4

Reasons for a wider basis of the deconvoluted peak and a lower potential to its right side shown in Figure 6, is the peaks topography. The KFM peak is caused by a deposited particle with three times extend than the average topography of the surrounding area. For this reason the formation of the peak can not be described by the linear channel model, which causes failures while applying it for deconvolution.

Conclusion

Assuming the surface of a sample as plane, the measured KFM data can be understood as a convolution of a microscope inherent transfer function with the actual potential distribution on the sample surface. Therefore the linear shift invariant channel can be introduced as model to describe the signal formation process. By analyzing the physical interrelations the transfer function can be determined and the measured KFM data can be deconvoluted. The restoration can be well done by a direct inversion of the transfer function supported by a wiener filter approach and the deconvolved data allow a better interpretation of the actual potential distribution.

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