# 52. IWK

Internationales Wissenschaftliches Kolloquium
International Scientific Colloquium

PROCCEDINGS | 10 - 13 September 2007

## FACULTY OF
## COMPUTER SCIENCE AND AUTOMATION

# 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.

Professor Peter Scharff
Rector, TU Ilmenau

Professor Christoph Ament
Head of Organisation

Table of Contents

C O N T E N T S

Page

## 6 Environmental Systems: Management and Optimisation

## 7 New Methods and Technologies for Medicine and Biology



## 8 Embedded System Design and Application

## 10 Mobile Communications

## 11 Education in Computer Science and Automation

52nd Internationales Wissenschaftliches Kolloquium
Technische Universität Ilmenau
10 – 13 September 2007

T. Machleidt / D. Kapusi / T. Langner / K.-H. Franke

# Application of nonlinear equalation for characterizing AFM tip shape

## Abstract

At present, many researchers are working on different tasks to turn tactile scanning microscopy (AFM) from a pure “Imaging tool” into a precision measuring instrument. Furthermore, the semiconductor industry requires larger and larger measuring ranges at a resolution below some nanometres.

If a metrological evaluation of the AFM data is to be carried out, the shape and the position of the AFM tip has to be known. Its characteristics are not static but changing dynamically due to physical effects (e.g. friction) and normal attrition. Procedures for the reconstruction of the tip on the basis of the AFM measurement data are necessary to evaluate these changes. Based on these procedures the evaluation of the AFM tip can be realized.

Proceeding on the determined tip shape, procedures for extensive interpretation and quantitative characterization of the tip geometry will be introduced. Several approaches will be presented, which realize the transformation of topological data into geometrical primitives. In contrast to other publications a non linear method was used. This way has the advantage that some constraints are included in the transformation. With this approach the results have a better stability and are more then useful.

## Motivation

Having a closer look to an upper-bound estimation for the tip provided by the blind reconstruction method [1] leads to a first, qualitative impression of its geometric properties. Since the investigating of the tip and reconstruction quality includes the task of comparing results originating from several measurements a quantitative characterization approach has to be found. Motivated by the idea of being able to prove various effects on the tip, e.g. wear or lateral and deformation forces, a solution should provide flexibility as well as robustness. The characterization results then can be used to

determine strategies for choosing parameters, which optimise the reconstruction process.
Secondly the tip radius is a gauge to assess the AFM tip. In several publications the tip radius was presented as a measurement parameter. However no information is given about how this parameter is to be determined. Commercial software modules – for example „Scanning Probe Image Processor“ (SPIP) – provide a method to assign the tip radius. But in practical tests an uncertainty was found.
This publication gives an instruction to assign the tip radius by using non linear methods.

## State of the art

In [2] methods to give a tip assessment for 2D and 3D analysis are presented. In the case of 2D parameters, the apex angle, the tip radius and the curvature are discussed. The second part of the publication deals with a strategy to calculate the 3D parameters of geometrical primitives (sphere, pyramid). The simulated annealing algorithm was used for solving the non-linear problem. The results look promising if an exact isolation of the apex and body points has been realized.

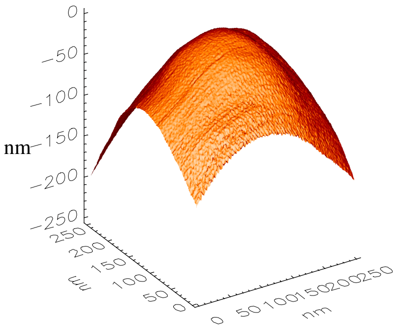


**Figure 1: Reconstructed AFM tip**

Figure 1 illustrates a reconstructed AFM tip shape. For the estimation of the tip radius the apex area has to be defined. This definition is essential for the correct tip radius calculating. Figure 2 illustrates the estimated tip radius

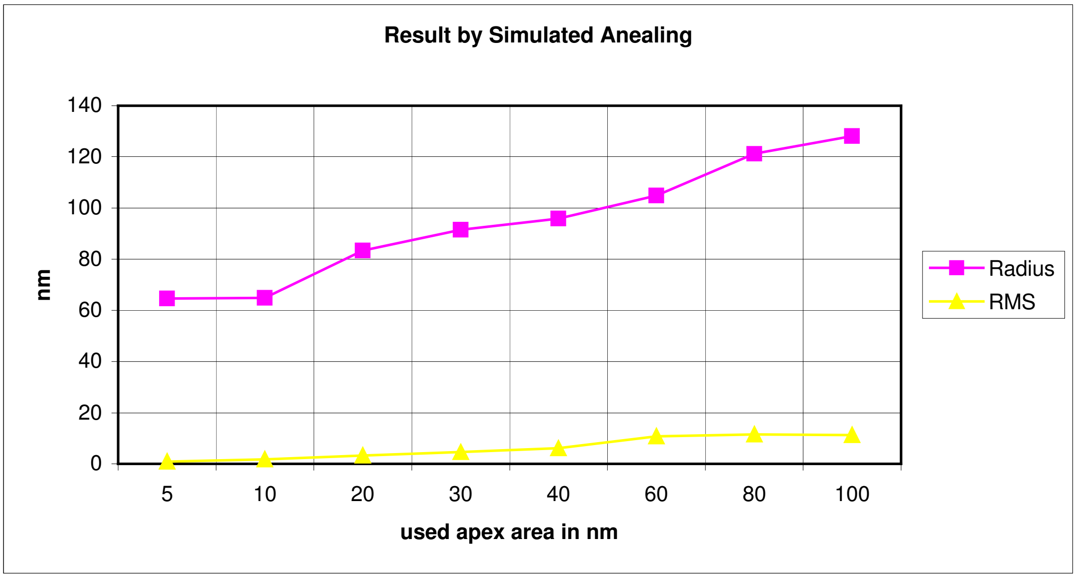


**Figure 2: Correlation of the used apex area and the calculated tip radius**

as a function of the used apex area. With the standard non-linear sphere fitting algorithm the influence of the tip body results in a wrong tip radius. In the fit error plot (Figure 3) the problem is demonstrated.

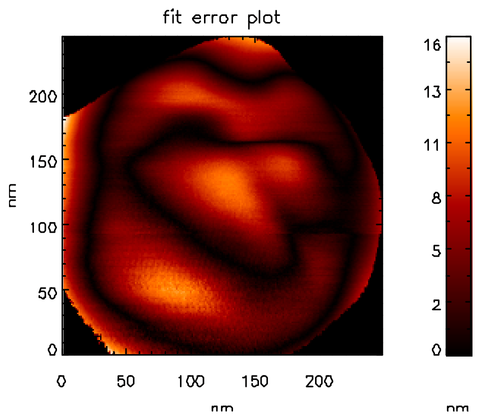


**Figure 3: Fit error plot by using standard non-linear fitting (apex area 100 nm)**

The same phenomena can also be found in commercial software modules. Scanning Probe Image Processor (SPIP) is a program to analyze AFM data. In the tip reconstruction module a calculation of the tip radius is included. The computed radius depends heavily on the fit range. So the user can compute different sphere parameters over a change of this parameter.

The "Zentrum für Bild- und Signalverarbeitung e.V." (ZBS) is versed by solving problems such as the calculation of geometric parameters of primitives from data points [3]. The methods are based on non-linear algorithms. In [4] the advantage of a correct geometric fitting is illustrated. This non-linear algorithm is qualified to solve the problems with the calculation of the AFM tip-radius. The integration of constraints in this algorithm gives a better stability. The fact, that these algorithms are concentrated in a commercial library [5] allows the integration in the assessment software for AFM tips and gives the basis for this publication.

## Methods to estimate the tip radius

The approximation of the tip radius is defined by a spherical fitting. Following the ZBS results a geometrical solving should be preferred. In this case a perpendicular distance was defined:

$$d_k = F(\vec{a}, \vec{x}_k)$$

The target function for fitting the sphere is given by:

$$Z(a_1, \dots, a_N) = \sum_{k=1}^{K} \left(F^{(k)}(\vec{a}, \vec{x}_k)\right)^2 \rightarrow \text{Minimum}$$

To solve this non-linear problem a Gauß-Newton-Algorithm or a Levenberg-Marquard-Algorithm can be used. As an abort criterion the root mean square, the change of the root mean square or a maximum of iterations is used.

With regard to estimating the AFM tip radius two methods are possible while observing certain constraints:

1. non-linear fitting with exponential weighting by using the distance to the apex
2. non-linear fitting with a static point (tip apex) on the fitting element

These variations are included in the fitting library created by the ZBS.

The first step to use the library was the integration in the Interactive Data Language (IDL), because the tip characterisation module was already developed in this language (Figure 4). This module was extended by two new methods for fitting the sphere.

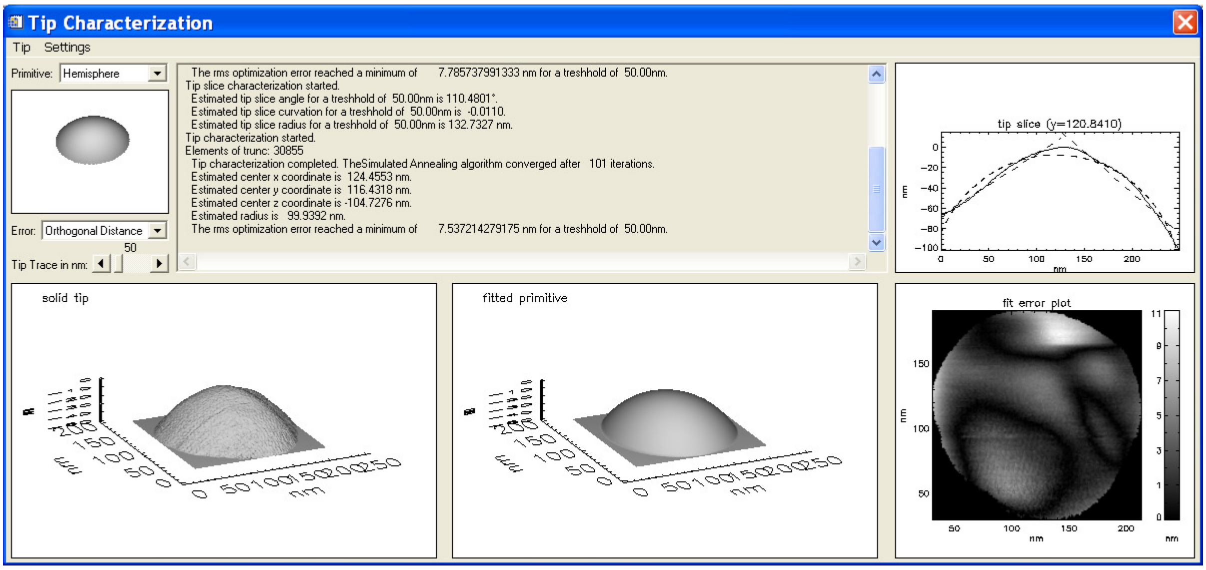


**Figure 4: Tip characterization module created in IDL**

Now the new method's can be tested just as in Figure 2. The results are illustrated in Figure 5 . It seems to be that the weighted version of the non-linear fitting comes with

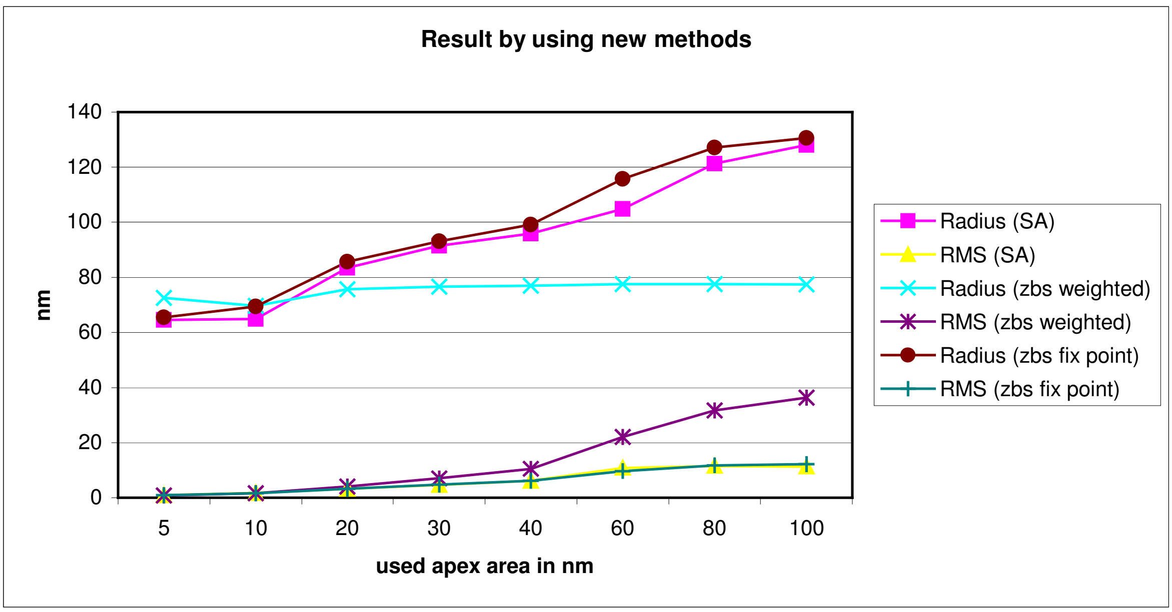


**Figure 5: Correlation of the used apex area and the calculated tip radius**

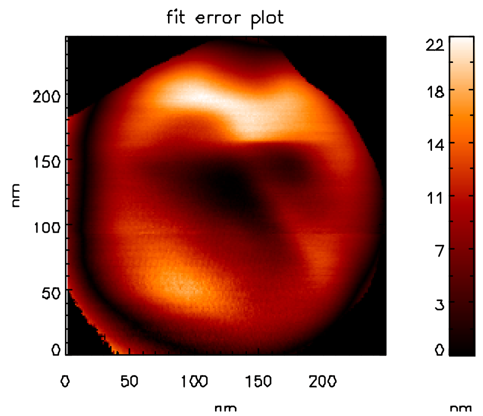


**Figure 6: Fit error plot by using non linear fitting with apex as fix point (apex area 100 nm)**

stable results of tip radius. Setting the apex point fix leads to the same bad results as the simulated annealing without constraints. The reason is illustrated in Figure 6. If an area of 100nm is used, the apex points and the points near the cut have a low rms. The number of points increases from 4599 (5 nm) to 63750 (100 nm) by using a bigger apex area. The non-linear algorithm searches for the best solution with a minimum rms. The influence of so many points in the cut area leads to a bigger sphere with a radius of 130 nm.

## Conclusion

The process of characterizing AFM tips by sphere fitting normally depends on the apex area points used. The calculated tip radius was greater when more points with a long distance to the apex were used. By utilizing the normal non-linear fitting the change of the tip radius is more than 100%. This effect can be solved by using a weighted non-linear fitting algorithm. The new method yields a constant tip radius. The algorithm was included in the AFM tip reconstruction module.

## Acknowlishments

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