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Simulation of the Set Tip-Cantilever in a Non-Contact Atomic Force Microscope

C. J. Camargo[1], C. Garzón[1], S. Sadewasser[2], J. A. Plaza[3], H. Campanella[3], T. Rada[1]

[1]*Fundación Universidad del Norte, Barranquilla, Colombia*
[2]*Hahn-Meitner Institut, Berlín, Alemania*
[3]*Centro Nacional de Microelectrónica, Barcelona, España*

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Resumen

El microscopio de fuerza atómica ha sido empleado para detectar con resolución atómica el potencial de contacto de una superficie; sin embargo, la incidencia de los parámetros geométricos en la resolución lateral aún no ha sido estudiada a fondo. En el presente trabajo se desarrolla un modelo de simulación por el método de elementos finitos en el software ANSYS®, con el cual se analiza la interacción electrostática del sistema por medio de la simulación de fuerza y capacitancia del sistema. El modelo ha sido validado a partir de investigaciones realizadas y los resultados obtenidos concuerdan con lo desarrollado hasta el momento. Finalmente, se ha planteado un nuevo método de análisis comparativo de resolución lateral para geometrías arbitrarias donde se mantiene fijo el radio de punta

Palabras claves: Fuerzas electrostáticas, método de elementos finitos, microscopio de fuerza atómica, potencial de contacto, resolución lateral.

Abstract

Atomic force microscope has been widely used to detect surface contact potential with atomic resolution; however, incidence of geometric parameters on lateral resolution has not been studied deeply yet. In this paper, we develope a simulation model in ANSYS® using Finite Element Theory to analyze electrostatic interaction of the system through the simulation of the force and the capacitance of the system. The model has been validated based on previous models and the results obtained are coherent with them. Finally, we have found a comparative method of lateral resolution for random geometries with constant tip radii.

Key Words: Atomic force microscope, contact potential, electrostatic forces, finite element method, lateral resolution.

1. Introduction

The development of new electronic devices depends on the techniques and the technologies of fabrication implemented, but also on the previous study of the materials to build them. For this reason, it is important to have the tools that allow to do a deep and precise theorical study of these materials.

The chances to study surfaces in a nanometric scale has obvious consequences for nanotechnology, which is undoubtedly one of the areas that in some years will produce an enormous impact in echonomy, industries and society; with this research, the computational optimization of parameters for measurement is achieved through the modification of microscopy techniques or in the physical characteristics of the measurement tools.

Additionally, the research done is a base for the modelling of more complex situations, closer to what is experimentally done in microscopy, for example, the inclusion of the tip oscillation and the application of AC voltage to detect electrostatic forces.

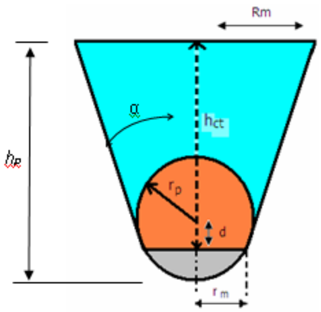

Fig.1 Graphical description of variables

2. Building the Simulation Model

A. Geometry of the system:

The system can be divided in three main components: the tip, the cantilever and the sample, where the last two are a rectangular prism and a plane, this is why their construction is simple; on the contrary, the tip requires a more complex process to build it, which is explained below.

The tip has been built using the concept of the junction of a truncated cone and a sphere, located on its end. In order to achieve a uniform junction between them and not to have deformations, the building process is done in the point where the tangent to the sphere curvature presents a slope equal to the one of the truncated cone (see Fig.1).

The manipulated variables of the tip are: α: half angle of aperture of the cone, r_T: radii of the tip, h_T: height of the tip and *d*: vertical distance between the origin of the sphere and the lower base of the truncated cone.

With regard to the axial symmetry of the tip, the analysis was simplified treating the problem as a bidimensional one and the half of the transversial area of the designed tip is rotated over the *y* axis obtaining the volume of this.

Likewise, the conducting sample is modeled as a node plane distant from the tip *d* nm. The electric potential is asigned to these nodes according to the particular situation simulated.

B. Meshing process:

In ANSYS®, the mesh implemented in the system is the product of the results obtained during the validation of the simulation model. This division of the volumes was made with a mesh that persues the achievement of some factors, such as:

- The area of most interaction and variation of the electric field must have a finer mesh than the areas where this interaction is not that strong. Consequently, the mesh around the end of the tip presents elements in a ratio 1:1000 in size with respect to the elements that sorround the upper part of the tip.
- The mesh must be homogenously fine around the tip; in order to assure that this would happen, the bidimensional mesh of the tip was created first and the rotated over its axis.
- All the area that has a boundary condition, must be meshed proportionally to the degree of incidence in the outcome. This way, the surface of the tip, the sample and latter the lowest area of the cantilever, is divided with elements with a similar size of the one of the adjacent elements.

C. Validation of the model:

In order to validate the accuracy of the model, a previous work similar to the system made was used. Belaidi, et al. [1] showed a model in which the geometry of the tip is also conic, with an spheric ending and the numeric analysis is performed using the finite element method.

The simulated conditions are matched in order to compare and test the designed system. Moreover, the presence of the cantilever was not considered because Belaidi, et al., did not either; besides, the parameters that allow to give the tip shape and the boundary conditions are stablished in the same values, which are: $\alpha=10^{o}$, $h_t=10\mu m$, $R_t=10nm$, $d=5nm$, $V_{tip}=1V$, $V_{sample}=0V$.

Furthermore, to match the precision of Belaidi's, et al. model, the calculated force must be 6.73e-11N and to improve it the results should be in the range of 5.55e-11N - 6.73e-11 N, where the lower limit is given by an analitical model introduced by them. The resulting force with the final model was 5.992e-11N, which improves the numerical simulations and is close to the force obtained analitically; this is how the model was validated and so is considered accurate to make any electrostatic analysis of a tip/cantilever system as long as it has the same electric characteristics of the model and the same concept of tip.

3. Results and Discussion.

The relation found between the values of the lateral resolution for variations in the geometry of the sensor, are in agreement with previous works in this area.

According to Jacobs, et al. [2], for a smaller aperture angle a better lateral resolution is obtained; for this reason the more the aperture of the cone is, the walls of it will be closer to the sample producing and increased capacitance of the cone; consequently, the tip becomes more sensitive to lateral forces, which affects negatively not only the resolution but also the precision in the measurment of the contact potencial difference (CPD).

On the contrary, Colchero, et al. [3], points out that for a good resolution the tip must mantain a small aperture angle, based on the reduction of the area of "high range" interaction, where the electrostatic forces are classified.

This, also supports the outcomes for changes in the width and the size of the cantilever, where its increment represents more sensitivity of the tip due to lateral forces and less interaction of the ending of the tip with respect to the sensor; this have been mentioned before by Koley, et al. [4], who states that less area of the cantilever included implies more precision in the reading of the CPD.

About the incidence of the tip height, other authors have mentioned that the highest is better and this improves the reading of the CPD, because the cantilever is more distant from the sample decreasing its effect in the measurement [4]; however, Belaidi et al. [5] affirm that an increased in the height is limited by the increment on the sensitivity of the lateral forces. According to our results, it is found that there is no explicit relation between the tip height and the lateral resolution; still, this is not completely true (details about it will be presented in a latter work).

Moreover, according to the research of Sommerhalter, et al. [6], it can be seen that when the distance between sample and tip is increased, the precision and the resolution are worse; the reason for this is that at longer distances the interaction between the tip apex and sample decreases drastically, being the cantilever the more important element in the measurements [3].

Likewise, the capacitance of the system was simulated at different tip – sample distances in order to graph $\partial C/\partial z$; then a regression was made with the points and with the equation that models the changes, the gradient was obtained (See Fig.2 and Fig.3). The importance of the simulation of the gradient of capacitance is that this is proporcional to the electrostatic force of the system, for this reason its performance shows how the lateral resolution is if its analyzed correctly.

Based on these results, a new method that allows the comparison of the lateral resolution for several sensors with arbitrary geometry keeping the tip radii constant has been designed. This method is based on the study of the capacitance of the whole system: tip/cantilever-sample and not as an approximation of this, assuming that the capacitance of the tip is parallel to the capacitance of the cantilever [7].

In addition, the model is not divided in several parts (ending of the tip, conical area and cantilever) but is considered as a whole, which avoids distorsions in the results due to approximations in the coupling of the parts and does not take in consideration the interaction of the electric field of each of the components. The method will be formally described in a latter work.

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References

[1] S. Belaidi, et al. "Finite Element simulations of the resolution in electrostatic force microscopy". Appl. Phys. A 66, 239 (1998).

[2] H.O. Jacobs, et al. "Surface potencial mapping: A qualitative material contrast in SPM". Ultramicroscopy, J. Appl. Phys. 69 , 1168 (1997).

[3] J. Colchero, A. Gil and A.M. Baró. "Resolution enhancement and improved data interpretation in electrostatic force microscopy". Phys. Rev. B 64, 245403 (2001).

[4] G. Koley, M.G. Spencer, H.R. Bhangale. "Cantilever effects on the measurement of electrostatic potentials by scanning Kelvin probe microscopy". Appl. Phys. Lett. 79 (4), 545 (2001).

[5] S. Belaidi, P. Girard, G. Leveque. "Electrostatic forces acting on the tip in atomic force microscopy: Modelization and comparison with analytical expressions". J. Appl. Phys. 81 (3), 1023 (1997).

[6] Ch. Sommerhalter, et al. "Kelvin probe force microscopy in ultra high vacuum using amplitude modulation detection of the electrostatic forces". Appl. Surf. Sci. 157, 263 (2000).

[7] T. Hochwitz, et al. "Capacitive effects on quantitative dopant profiling with scanned electrostatic force microscopes". J. Vac. Sci. Technol. B 14 (1), 457 (1996).

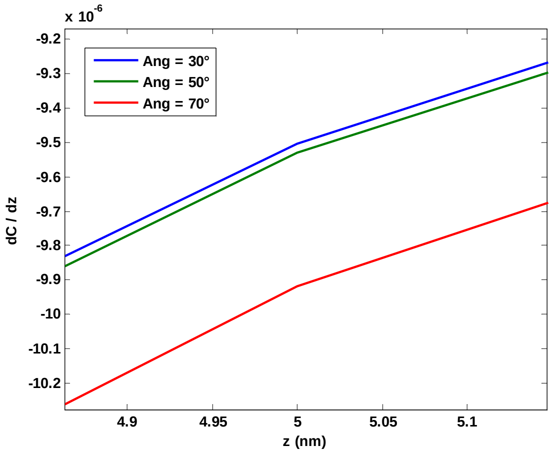

Fig.2 Capacitance gradient results. Variation of aperture cone

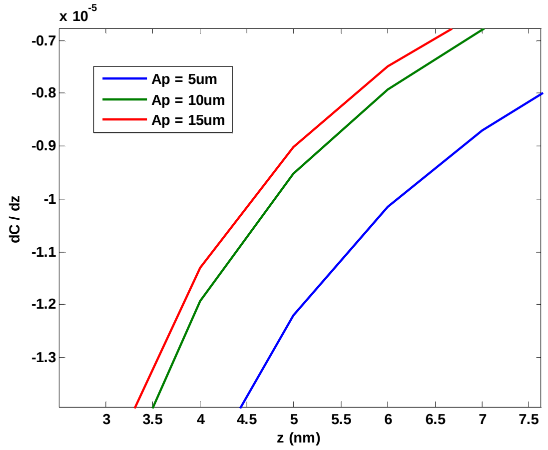

Fig.3 Capacitance gradient results. Variation of tip height.