MULTIPHYSICS SIMULATION OF A SCANNING MICROWAVE MICROSCOPE: A JOINT ELECTROMAGNETIC AND THERMAL ANALYSIS

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Abstract - *Scanning Microwave Microscopy is considered as one of the most promising techniques for quantitative determination of dielectric properties of material samples down to the nanoscale. Furthermore, the energy transferred to samples is negligible so the technique is considered as a non-destructive one.*

In this work, a COMSOL© multiphysics simulation of a Scanning Tunneling Microscope-aided Scanning Microwave Microscope is presented. In particular, the joint electromagnetic and heating transfer simulations are performed. Results about the maximum thermal gradient under typical testing conditions are presented. The results demonstrate that the technique is actually suitable for non-destructive analyses

INTRODUCTION

The recent progresses in nanoscience and nanotechnology require suitable instruments for quantifying material properties at almost an atomic scale. Scanning Probe Microscopy (SPM) techniques have increasingly developed during the last few decades [1].

The latter family of microscopes substantially differs from conventional optical microscopes that utilise visible light diffraction for operation; in that case of SPM a physical property is recorded by a probe placed in proximity to a sample. The physical interaction between the probe and the sample is then the identifying property of each microscope (*e.g.* an Atomic Force Microscope (AFM) works through recording the short-range interacting forces between few atoms of the probe and the sample underneath).

The Scanning Microwave Microscope (SMM) is part of this family since it works by recording the reflected electromagnetic field from the sample under study. The sensing probe in this case works as both an emitter and collector of the microwave field. It is possible to achieve a nanometric scale resolution since the tip is placed in extremely close proximity to the sample so that the interaction occurs within the so called *reactive near-field* region. The exponential decay of the interacting field is further sharpened by the shape of the probe, typically culminating in a very sharp apex.

For this reason, the most recent practical implementations of the SMM technique share a common probe with others SPM instrument (e.g. AFM, STM) that can ensure the working conditions required by the SMM technique (close proximity between tip and sample and nanometric size of probes). The already commercially available SMMs from Prime Nano or Keysight Technologies, for example, are both implemented within an AFM platform as an additional module [2]. The microwave signal is carried by an AFM tip to the sample under analysis.

In this paper we present numerical simulations of a Scanning Tunneling Microscope (STM)-aided SMM. In particular, the joint electromagnetic and heat transfer simulations are performed utilising COMSOL Multiphysics©. The different thermal behaviour of two typical sample substrates (HOPG and SiO_2) is shown, after a 5 minutes exposure to microwave energy. Furthermore, a bulk CuO sample is tested with the same method. This is for testing the *non-destructivity* of the technique during standard operating conditions. Monitoring the thermal evolution of the system is necessary for heating sensitive samples, like biological ones, or in case of complex environment, like in-liquid system measurements.

STM-AIDED SMM REALIZATION

Previous work has focused upon the practical implementation and application of the microscope which is analysed numerically in this paper [3]. In Fig.1, a schematic detailing interacting signals is shown. Although this particular kind of microscope is able to work across a wide range of microwave frequencies, we only report results related to a single frequency measurement. A typical working frequency (18.5 GHz) is then tested [4].

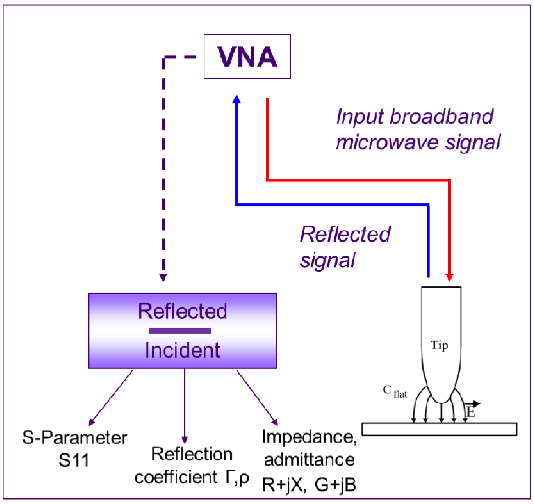

Fig 1. Scheme of the SMM working principle

NUMERICAL SIMULATION

The system is composed of a sample holder mounted on a piezoelectric device and on a motorized stage. This holder is supported by springs for minimising the effect of vibration.

From an electromagnetic point of view we choose to simplify the design and to simulate the effective size and material of the sample mounted on a simple cubic substrate made of aluminium which is the same material as the sample holder.

The microscope head design is the most critical part in terms of the microwave signal coupling. The signal is carried by a microwave cable from the Vector Network Analyser (VNA) to the microscope head, where it is connected by a truncated SubMiniature version A (SMA). The capacitive coupling to the tip section ensures the passage of the microwave signal only, without interferences from the STM DC signal.

The final design that has been simulated is reported in Fig. 2.

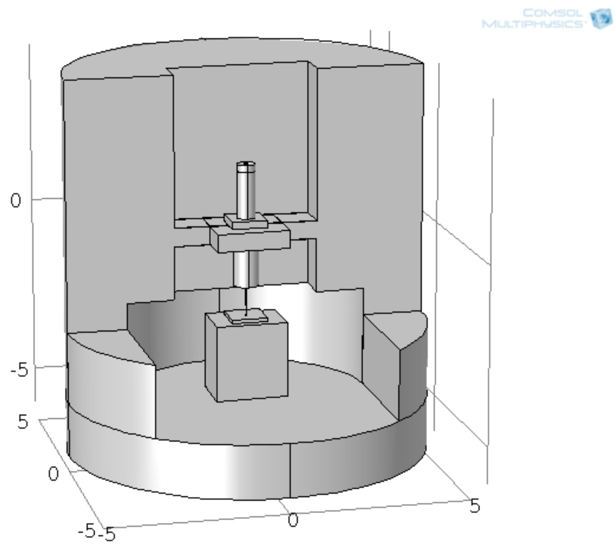

Fig 2. Simplified structure of the SMM used for simulations (scales are in cm)

In the first instance the entire structure of the microscope was simulated with the RF module of COMSOL Multiphysics© since this microscope design has never been tested before. It is then important to have full control of the field distribution in each part of the instrument and within the sample, in order to eventually improve the prototype design. The source is fixed far enough from the sample, in order to simulate the actual cabling system and a coaxial port is used in simulations in order to simulate the actual input power source coming from the port 1 of VNA.A full electromagnetic simulation of a 10cm-high structure, with a radiant tip curvature radius of 100nm, is an extremely complex problem for *mesh refinement. Therefore,* two spherical subdomains were created for limiting the simulation volume: the outer one (3cm radius) has then been partially surrounded by Scattering Boundary Conditions to a spherical wave with the centre placed on the tip. The inner one (100um radius) is used for mesh refinement around the apex of the tip, since it has been initially determined that the field is extremely concentrated in that volume as expected.

The Multiphysics node of the software has been exploited for calculating the temperature gradient due to microwave heating under the microscope tip during a conventional scan. For overestimating the effect of the heat transfer (in order to take into account non ideal behaviour of sample and instrument, as well as additional heating transfer phenomena) the input power is fixed at 1W, although the common operating power is typically only a few uW. Additionally, the scanning time for a single position is only a few seconds, while the effect of a concentrated radiation was examined for 5 consecutive minutes at a single point.

RESULTS

Different samples have been simulated, since the SMM analysis can be performed on a wide range of materials. In particular the joint electromagnetic and thermal behaviour of a SiO_2 substrate, a Highly-Ordered Pyrolytic Graphite (HOPG) sample and a CuO bulk sample have been tested. All data related to these materials are collected from past characterization works [5][6] or companies data sheet [7]. The first one can be considered as electrically insulating, the second one has anisotropic properties and the third one has a semiconducting behaviour at high temperature. They have been chosen for simulation a wide set of material properties, for making this study generic for the great majority of conventional samples under analysis.

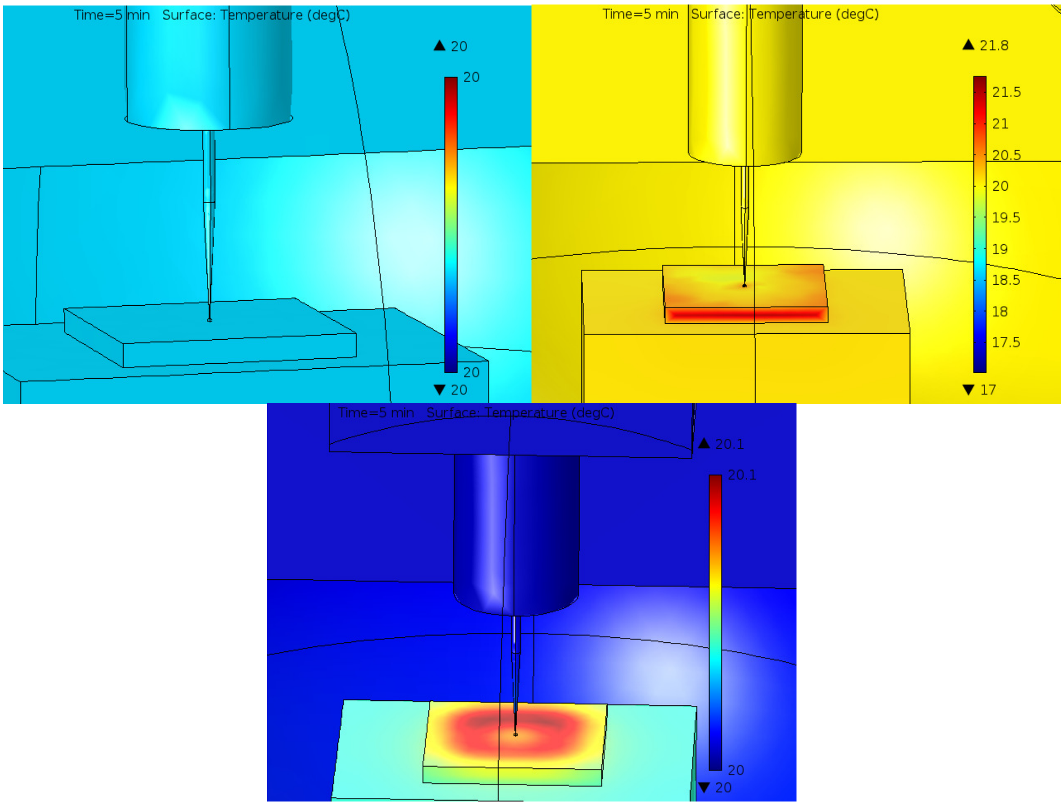

Fig 3. Thermal gradient result after 5 minutes exposure to a microscope input power of 1W on tested samples (from top right, counter clockwise: HOPG, SiO_2 and CuO)

In insulating SiO_2 substrates any current is induced by the microwave interacting field. The reactive energy from tip to sample is far enough to support any thermal gradient in the sample itself, even if we are considering an overestimating time of interaction and input power.

In HOPG, since the in-plane conductivity is high, there is a non-negligible real part of the interacting field that induces a current on the sample itself. Anyway, this is compensated by the thermal conductivity of the material, still high in the in-plane direction.

Finally, the bulk sample of CuO cannot support an appreciable thermal gradient, although its conductivity increases with the temperature. Anyway the starting kick-off energy from the microscope is not enough for supporting a non-linear behaviour and then an exponential increase of temperature on it.

CONCLUSION

In this work, a COMSOL© multiphysics simulation of a Scanning Tunneling Microscope-aided Scanning Microwave Microscope is presented. In particular, the joint electromagnetic and heating transfer simulations are performed. The different thermal behaviour of two typical samples substrate (HOPG and CuO) and of a bulk CuO sample is shown, after 5 minutes exposure to the microwave radiation.

The results demonstrate that the maximum thermal gradient on the samples under study is below 2 degrees (HOPG case), even with an input power of 1W (6 orders of magnitude higher than the typical power in use), making the technique suitable for *non-destructive* analyses and demonstrating that the microwave system does not cause heating of the sample to any extent; likely to change the physical or chemical properties.

Further work on the reported multiphysics model is ongoing for simulating the operating conditions reported in past works for obtaining reproducible etching phenomena by SMM on non-conventional samples [8].

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