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Graphics cards based topography artefacts simulations in Scanning Thermal Microscopy

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ABSTRACT

We present an approach for simulation of topography related artefacts in local thermal conductivity measurements using Scanning Thermal Microscopy (SThM). Due to variations of the local probe-sample geometry while the SThM probe is scanning across the surface the probe-sample thermal resistance changes significantly which leads to distortions in the measured data. This effect causes large uncertainty in the local thermal conductivity measurements and belongs between most critical issues in the SThM when we want to make the technique quantitative. For a known probe and sample geometry the topography artefacts can be computed by solving the heat transfer in the SThM for different probe positions across the surface, which is however very slow and limited to single profiles only, if we use standard tools (like commercially available Finite Element Method solvers). Our approach is based on an assumption of diffusive heat transfer between the probe and the sample surface (and within them) and on the use of a Finite Difference solver that is optimized for the needs of a simulated SThM images computing. Using a graphics card we can achieve computation speed that is sufficient for a virtual SThM image generation on the order of few hours, which is already sufficient for practical use. We can therefore use the measured sample topography and convert it to a virtual SThM image – which can be then e.g. compared to real measurement or used for artefacts compensation. The possibility of performing fast simulations of topography artefacts is also useful when uncertainties of the SThM measurements are evaluated.

1. Introduction

Scanning Thermal Microscopy (SThM) is a special Scanning Probe Microscopy (SPM) technique dedicated to measurements of local temperature and heat transfer phenomena [1–3]. Such measurements are important namely in the field of microelectronics and in various nanotechnology fields where local power dissipation and heat generation plays some role. It offers far the best spatial resolution out of all the thermal techniques, however despite its long development, the uncertainty of the measured temperature or thermal conductivity is still very large on most of the devices, if the method is made traceable at all (which is typically not the case).

In most of the commercially available scanning thermal microscopes a local resistive heater and/or temperature sensor, either in a form of a microfabricated probe or a very thin wire bent to form a probe is used [4–6]. This probe is scanned across the surface in a standard contact mode (monitoring the repulsive forces via optical lever technique), therefore microscope provides at least two channels of simultaneously provided information – topography one and temperature related one. The inevitable presence of some surface structures and irregularities on the measured sample is also one of the big problems of the uncertainty evaluation as these lead to artefacts in all the thermal channels [7,8]. In case of local temperature measurements these can be prevented using null point technique in some of its variants [9] – evaluating the apparent temperature for zero flux between the probe and the sample. In case of measurement of local thermal conductivity the results are based on the non-zero heat flux, thus such approach cannot be done.

Topography artefacts in SThM are related to changes of the flux while there is a variance of the contact area of the probe depending on local sample geometry or while there is a variance of sample volume where heat can flow into different parts of the sample. If the probe is located e.g. on the edge of a flat sample surface, we can expect that the heat flow between the probe and the sample

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will be approximately twice lower compared to the situation when the probe is at the center of the sample. At the edge we have twice smaller probe-sample contact area and less material in probe vicinity where heat could flow to. On real samples the probe-sample area is varying rapidly both due to microscale objects that may accidentaly lay on surface and random roughness that is present nearly everywhere.

One possible way of treating the topography artefacts is to model them and to correct the measured data afterwards, or at least detect which parts of the data are influenced by the artefacts and which may contain other relevant information. The biggest problem in such simulations is that we need to perform pixel-by-pixel simulation of the probe-sample response, forming a virtual SThM image. The number of individual calculations of the probe-sample interaction is given by number of pixels of the final image, which usually means hundreds of thousands at least. For such number of individual calculations, most of the modeling tools are too slow.

In previous articles [7,10] we have implemented and compared various methods for calculation of a virtual SThM image that could be used for estimation or removal of the topography artefacts. Some of the methods tested were correct (at least under assumption of diffusive heat transfer), but slow, e.g. Finite Element Method. Some produced apparently nice results, but only qualitatively, being rather fast, e.g. Neural Network. Due to this tradeoff between physical correctness and speed we have used the simpler techniques like Neural networks so far, which are however limited to some class of surfaces and need very careful measurement and neural network training. Moreover, all the physical content is hidden in training of the neurons and the result is therefore not exact solution of some physical equation.

The next logical step is to make physically correct solution of the tip-sample heat transfer fast enough for practical purposes. We have developed a methodology and associated numerical tool that is focused on fast calculations of virtual SThM images. In contrast to general packages (e.g. any commercial FEM) it is almost single purpose software. This allowed us to optimize the calculation speed much further than what would be possible with an universal software. We have started with a very simple numerical approach based on Finite Difference Method (FDM) with regular equally spaced three dimensional mesh and we have optimized this for fast calculations of steady state heat transfer in slightly changing tip-sample configurations as the tip is scanning across the sample surface.

It should be noted that the presented approach is still not covering all the physical phenomena that would need to be taken into account for heat transfer in all the scales observed in SThM experiments. On the small scale, the heat flux through the air gap between the probe side and the sample surface is ballistic and should be modeled using another approach [11]. Also in the probe and in the sample itself, the heat flux is not necessarily diffusive (depending on material and its dimensions compared to mean free path of phonons). There is some meniscus formed by capillary condensation in the gap between the probe and the sample and some of the heat is transferred through the water layer [12,13]. On the other hand we believe that for larger probes, at presence of different surface contaminations, adsorbed water layer, etc., the heat flux is so complex that assumption of the simple diffusive heat transfer is still a good approximation for topography artefacts compensation. Moreover, some of the promising models for taking the ballistic heat transfer into the account, e.g. based on some flux lines evaluation would also benefit of the computed Poisson equation solution, so the developed model can be also used as a first step for building more complex and more physically correct model for these small scale calculations.

2. Numerical model

2.1. Finite difference method

Poisson's equation is one of important tools for calculating temperature fields. It is a parabolic differential equation in the form

$$\Delta T = f$$

where T denotes temperature, and f is a function defined on the manifold. The Poisson's equation has many applications not only in heat study, but also in other fields of physics, typically electrostatics, diffusion and others. Nevertheless, in our context, temperature field T is the unknown function which is to be calculated.

The most common method for solving the equation is based on discretization (tesselation) of the domain of interest into finite number of elements. It is important to study mutual interactions between the neighbouring elements.

At first, we will consider a special case of Poisson's equation, where there is zero on the right hand side:

$$\Delta T = 0$$

In this situation the temperature field is determined solely by boundary conditions. It can be viewed as a special case of heat equation

$$\frac{\partial T}{\partial t} - \alpha \Delta T = 0$$

when steady temperature field is required. At this assumption, any closed volume (i.e. volume element) must fulfill the condition of zero net heat energy exchange with its surrounding. The incoming heat flow must be equal to outcoming heat flow for each of the elements in the discretized volume. From this principle we can deduce a steady state for a rectangular grid.

The heat flows between a given element and all its neighbors, while each element has two neighbors in the direction of principal axis (x, y, z). We will describe the situation for two dimensional case (see Fig. 1), where each element has four neighbors.

The heat flow q, which is an important property in the calculation, is equal to the gradient of temperature multiplied by thermal conductivity k. This equation is known as the Fourier's law:

$$q = -k\nabla T$$

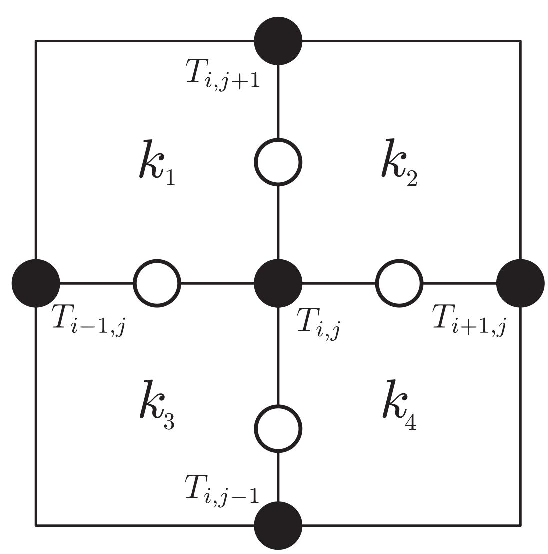

Fig. 1. A five-node stencil representing a node with temperature T_{ij} surrounded by four neighbouring nodes. The heat flows through areas of thermal conductivities $k_1, \ldots, k_4$.