Prototype 13:

SThM Image Processing Tool

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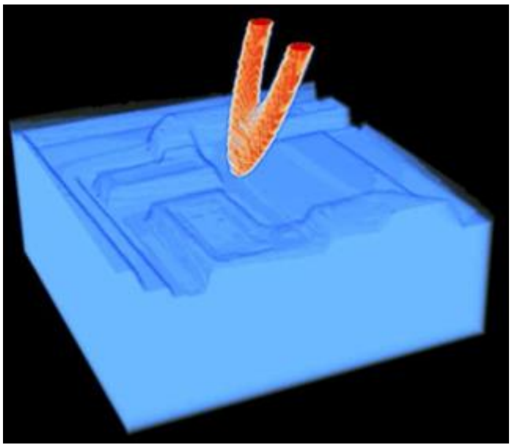
Scanning Thermal Microscopy images are often being affected by local changes in the probe-sample geometry configuration related to sample topography, either related to features on the sample (surface structures edges) or to sample roughness. This makes the evaluation of sample thermal properties much harder and user often cannot be sure if the contrast observed on the image is related to thermal conductivity variations or to topography effects. Here a numerical tool designed for fast compensation of topography artefacts developed within Quantiheat project is presented [1]. It uses Finite Difference Method implemented on graphics cards to solve the diffusive heat transfer on realistic probe sample geometry.



Key Benefits

- *Virtual thermal image with one to one correspondence of the measured SThM image.*
- *Software is compatible to many data formats and data processing operations via its integration to Gwyddion open source software.*
- *Most of the samples can be modelled using the client-server approach, which is the easiest way of using the solver; however, there is also an alternative in manually creating the input files for the solver, then the variability is even bigger.*

Software description

The key goal is to obtain a virtual SThM image for some probe and sample surface model. For this, several steps are needed, all covered by the software. There are two separate software tools used for the process, working in a client-server regime, so the following description lists also the tasks distribution between them.

- on the client, sample topography is loaded within Gwyddion open source software [2] and local thermal conductivity is assigned to the surface; using masks we can also use multiple materials or add more layers, which in total gives many possibilities on how to setup the problem.

- on the client, probe is modeled either in Gwyddion or on basis of some surface data representing probe apex.

- regular voxel based mesh is constructed from both probe and sample, still on the client side.

- the server gets the meshes, list of all the positions which probe should follow on the surface and computation parameters. The calculation is performed on NVIDIA graphics cards (with CUDA technology), solving Poisson equation for the heat flow between probe and sample. At each step probe is moved to the appropriate position on the surface and steady heat flow is calculated. This gives one pixel of the final image. Then, next point is computed. When the points are close enough, many of the data can be recycled during computation, which speeds up the process significantly.

- the client obtains regularly updates from the server, so that the results can be presented to the user and stored together with the source data (sample topography and probe topography).

The computational engine that runs on the server can be also run locally, the only reason for client-server separation is to enable this computing technology to people that have no access to the high-performance graphics cards.

Applications

Two examples of the applications are given below, both related to samples developed within the Quantiheat project.

First, a rough silicon surface SThM measurment and simulation is presented in Figure 3. This was created using the following steps (all the data processing was done in Gwyddion):

(1) Probe apex shape is determined using the blind tip estimation algorithm. To do this the surface needs to have enough topographic features like sharp spikes, which is the case of the used surface. In our case it was possible; the estimated probe had radius of 96 nm in fast scan axis direction and 68 nm in slow scan axis direction.
(2) Surface reconstruction is performed in order to reduce the probe-sample convolution effect. The resulting surface is shown in Fig. 3C together with the estimated probe.

(3) Reconstructed surface is used to form the mesh, probe is modeled using the results obtained in step 1.

(4) Surface and probe conductivity is set to have silicon material properties, with thin native SiO_2 layer on the top of the surface (2 nm).

(5) Virtual SThM image is computed pixel by pixel using the Finite Difference Method, shown in Fig. 3D.

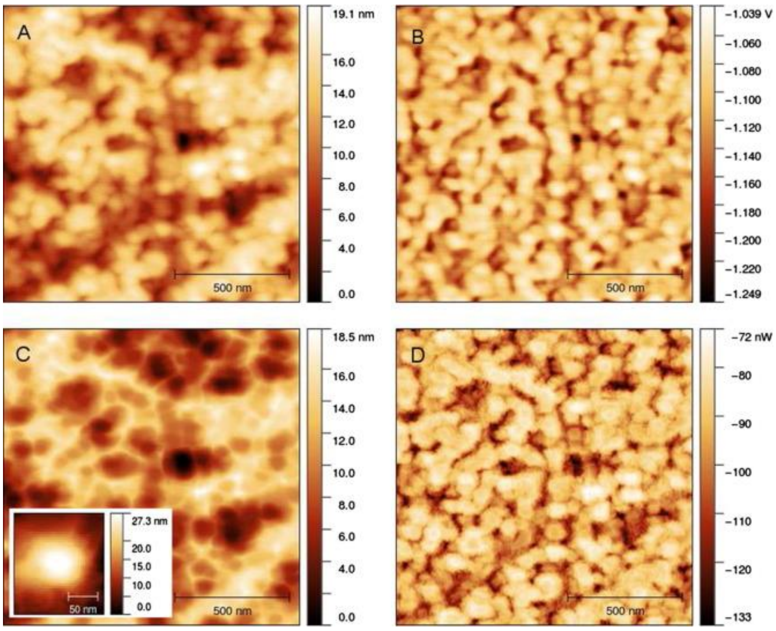


Figure 1: Roughness simulation: (A) rough surface, (B) thermal signal, (C) surface after reconstruction (with estimated probe in inset), (D) simulation result. (reprinted from [1]).

In Figure 4, a simulation of a virtual SthM image on calibration sample developed by Glasgow University is shown. Here the simulation procedure was much easier as the probe could be modeled as a simple paraboloid (we don't need to get the edges simulated that correctly). Substrate was assigned to have the silicon thermal conductivity, while all the steps had conductivity of silicon dioxide. Note that the voxel size was too small to correctly represent the first step. As the Finite Difference Method works with non-adaptive mesh, there is always some tradeoff between the mesh size and computation time (and memory needs).

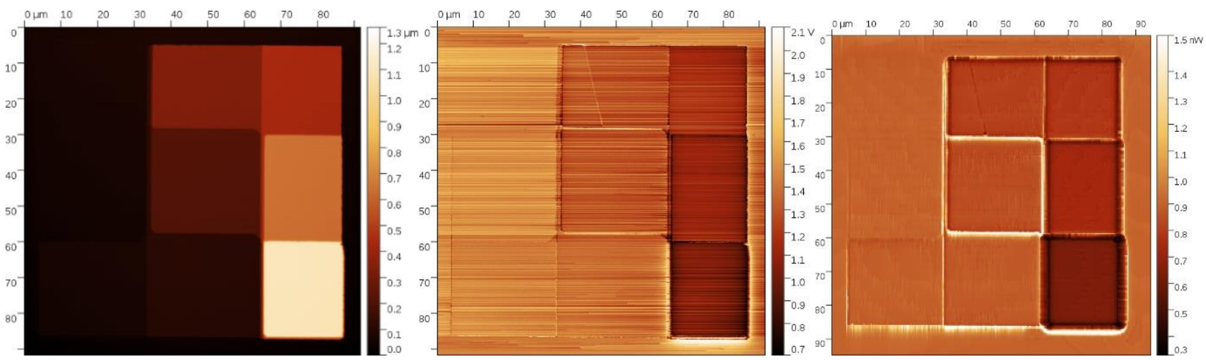


Figure 2: (A) sample topography, (B) SThM thermal conductivity contrast and (C) modeled virtual SThM image.

The time necessary for computation of a single problem (one probe position) is around 2–4 s. Even if this means a speedup of about 400 compared to a Finite Element Method solution (via SfePy software), it is still not ideal. If we want to calculate 100x100 pixels virtual SThM image, it still takes about eight hours on a single graphics card. With four cards available on our computer it can be two hours as the problem scales linearly with number of graphics cards. To simplify the selection of areas of interest user can compute first a coarser image or pick only some critical parts to be calculated and then the full calculation can be started. Further speedup of the computational engine is also planned in the future by better memory management on the graphics card. It should be also noted that the heat transfer model is diffusive, so the smaller the scale of problem is the further it can be from physical reality.

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