

Prototype 11:

Modelling Tool for SThM Tip and Sample Interactions

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Scanning thermal microscopy (SThM) is a key technique for probing thermal transfer at the submicron-scale. SThM maps the sample topography and acquires a thermal image that is representative either from the sample temperature or local thermal conductance. However, the thermal image is usually only qualitative and it is not straightforward to deduce quantitative data from it. This is due to the fact that many parameters play a role in the tip-sample heat exchange which is further complicated by the complex shape of the thermal probe and the multiple heat flow paths. Until now each SThM user has been developing his/her own method to analyze results, requiring a significant amount of time and lacks consistency.

In order to ease the analysis of the data, we have developed a free online software tool that allows computing the tip-sample thermal exchange in ambient conditions under certain hypotheses such as flatness of the sample. The tool is based on the COMSOL software [1] that solves heat transfer in the diffusive regime through a Finite Element Method (FEM) and that is well-known in academia and industry. The online tool is hosted and maintained at the University of Lancaster (ULANC), where a server performs the calculations with key SThM parameters entered remotely by the user. Various computations can be performed in the same time. The principle is based on the fact that only few kinds of thermal probes are available and that it is therefore possible to gather a library of key configurations that will be helpful for all SThM users.

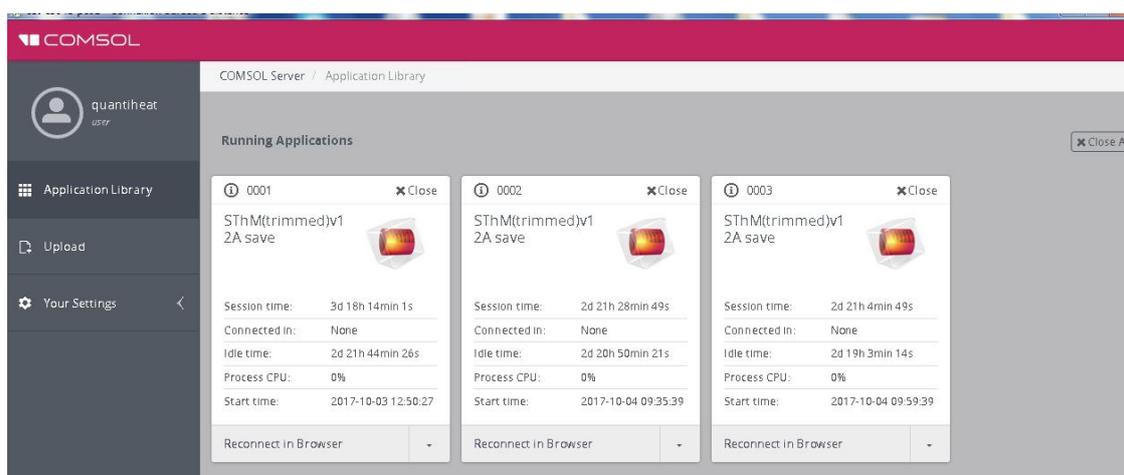


Figure 1. Main window of the online tool once the user is logged. User's computations are listed.

How to access and use the online simulation tool?

The web address is <https://simqheat.lancs.ac.uk/>. A login and a password are then required to enter into the system. A list of possible computations for various configurations appears on the screen in addition to the list of current computations performed by the server (see Fig. 1). Once the user has selected the configuration of choice, a window with the parameters that the tool allows to select – only a limited amount are manageable – appears on the screen as shown on Fig. 2. Bulk samples and thin-film-on-sample are typical geometries considered, as they encompass many of the situations of interest in a simplified way. Once the user has entered the parameters (a list of materials is already available), the computation takes place. In the easiest cases it lasts few seconds before the temperature field in the system starts to be displayed. The key quantities that are given by the software are the average and maximal temperatures of the thermal sensor, the maximum temperature of the sample, and the tip-sample heat flux exchanged. These quantities allow determining the thermal conductance from the probe to the sample, which is measured experimentally.

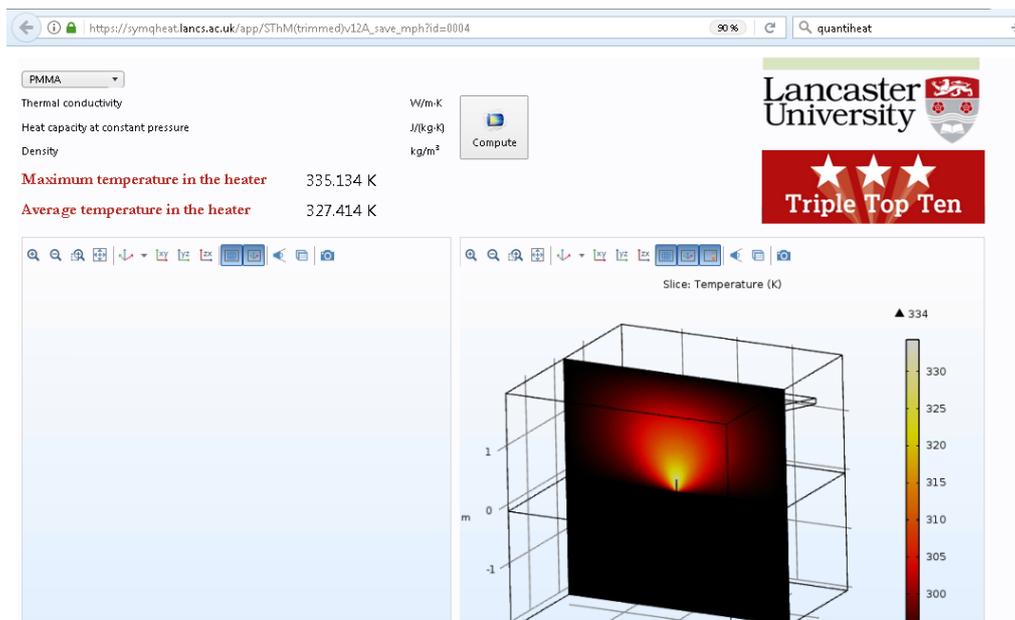


Figure 2. Example of computation in the online tool. Computed data appear in red. The temperature field is represented at right around the vertical tip.

Heat transfer at the tip-sample contact

At first sight, the COMSOL software allows only to consider diffusive heat conduction, while it is now well-established that heat transfer at nanoscale can be much more complicated. Indeed, heat can flow from the tip to the sample through the mechanical contact, with a contact radius often difficult to determine and small enough to lead to ballistic constrictions, through a meniscus of water lying around the mechanical contact or through air, with a transfer that can be partly ballistic. In addition, thermal boundary resistances (TBC) at the contacts between materials can be significant, especially if

roughness is large. Radiation is fortunately often less significant if the measurements are performed in ambient conditions, but the all the other mechanism cannot be simulated rigorously by diffusive laws.

In order to cope with these issues, many ways are possible and have been developed with the Quantiheat project. For instance, the constriction resistance [2,3] including some ballistic term [4] through a Wexler formalism can be included in the boundary resistance between the tip and the sample. The ballistic limitation to the heat transfer through air can be included by keeping the probe away from the mechanical contact at a distance representative of ballistic heat transfer through air [5,6]: only the air conductance is therefore computed in the 3D FEM simulation. A way to include the meniscus and the contact in an analytical way is to consider a heat sink with a determined conductance associated to the meniscus and mechanical contact [7]. All these methods have been reported in publications and can be used as guides for the use of the associated configurations in COMSOL tools.

It is important to note that the COMSOL tools have been developed for flat samples with limited roughness only. While the user can use these tools to improve its understanding of rough samples, the tools have not been developed for this purpose.

Thermal probes available

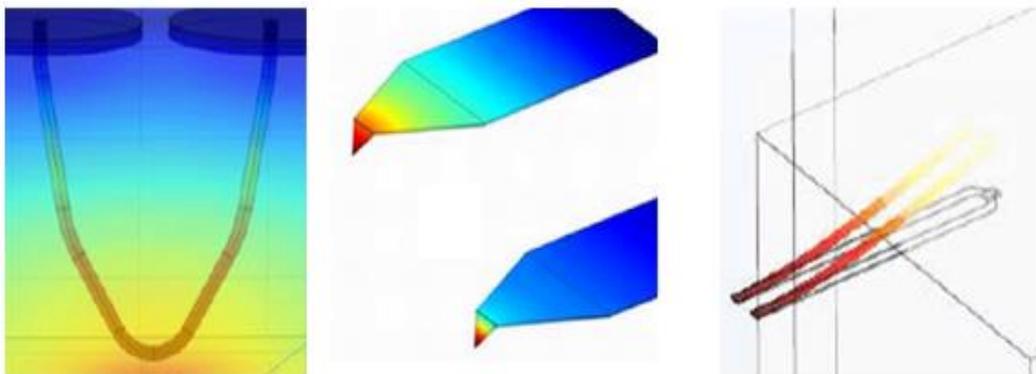


Figure 3. *Thermal probes simulated by FEM within Quantiheat: Wollaston probe (URCA), Palladium probe (ULANC), Doped silicon probe (CNRS-CETHIL). The temperature fields inside the probes are represented for the two first cases (both out of contact and in contact for the Palladium one), while the Thermomechanical deformation is shown for the third one.*

Key configurations with the three main types of scanning thermal probes currently used in the world, i.e. the Wollaston probe, the palladium probe (from Quantiheat partner KNT) and the doped silicon probe, will be available on the online tool. Configurations will be progressively uploaded in the system, by keeping almost identical graphical user interface. The partners devoted to these tasks are ULANC, CNRS-CETHIL and University of Reims-Champagne Ardennes (URCA). The expertise of the Czech Metrology Institute (CMI) is also necessary.

If some external contributor proposes to add additional simulation setup associated with another type of probe it will be positively valued. However, only a limited number of such proposals can be accepted.



Note that the same online tool can be used for computation of heat conduction within nanomaterials involving partially-ballistic transport. This is the object of a separate Application Note¹.

References

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- [6] A.M. Massoud, J.-M. Bluet, P.-O. Chapuis, *Air contribution in calibrated scanning thermal microscopy*, in press (2017)
- [87] A. Pic, S. Gallois-Garreignot, V. Fiori, P.O. Chapuis, *Microelectronics thin films and boundaries characterized by local electro-thermal measurements*, Proceedings of THERMINIC 23 (Thermal Investigation of ICs and Systems), Amsterdam (Netherlands), September 27th-29th, 2017.
- [9] Quantiheat consortium Application Note, *Simulation tool for heat transfer within nanomaterials* (2017)

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¹ Prototype 12: Simulation Tool for Heat Transfer in Nanomaterials