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Numerical techniques for the reduction of thermal conductivity measurements at nanoscale

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Nanostructuring offers the opportunity to increase the figure of merit of materials for thermoelectric applications, through the reduction of their thermal conductivity. The development of innovative anostructured materials for thermoelectric applications requires the improvement of techniques and rocedures for the reliable measurement of the thermal conductivity on a nanometric scale. Techniques for the measurement of thermal conductivity require heaters and temperature sensors (thermoresistors or thermocouples) whose width cannot be very small with respect to that of the nanostructures to be characterized. Conventional data analysis assumes that they are negligible, and can thus lead to misleading results. We propose to analyse the experimental measurements by means of finite element (FEM) modelling, taking into account the thermal and electrical transport both in the heaters/sensors and in the material to be characterized.

We present a numerical method for the characterization of thermal conductivity at the nanoscale with the 3ω□technique[1]. This method has been applied to the analysis of experimental data for a device based on silicon nanomembranes, whose SEM image is shown in Fig. 1: a metal strip is fabricated on the suspended silicon structure, and is biased with a sinusoidal current; the amplitude and phase of the third harmonic of the voltage drop is measured in a four-probe configuration, through a lock-in amplifier. The key challenge of the 3ω□technique is toevelop suitable models for relating this third harmonic amplitude with the thermal conductivity of the structures under test. Analytical models have been developed in the past[2], assuming that: 1) the room temperature value of the heater resistance can be used for calculating the dissipated power; 2) the width of the heater is negligible with respect to the size of the structure to be measured; 3) the nanostructures are good electrical insulators. All these assumptions can lead to misleading results at the nanoscale. Our numerical technique consists in detecting the exact size both of the nanostructures and of the metal strip (heater) from SEM images; the thickness of the Si structures and of the metal heater is estimated from AFM images. This information is used to define a 3D model of the whole device (nanostructures and heater), for which we generate a discretization grid (see Fig. 2). Then, the electrical and thermal transport is simulated (within this 3D model) by means of the finite-element (FEM) technique, considering the thermal conductivity as a fitting parameter (see Fig. 3). An excellent fitting of the data can be obtained, overcoming the limits of conventional modelling (see Fig. 4). An automated procedure (Python code) for SEM photo survey, grid generation, and FEM simulation has been developed to achieve an acceptable throughput in the processing of experimental data.

We applied this method also to material deposited on top of suspended Si_3N_4 membranes (see Fig. 5). A metal heater has been considered in the middle of the nanomembrane, and the thermoelectric transport equations have been numerically solved for the thermal characterization of the material. Comparison with analytical models[1] will be reported.

Some materials cannot be deposited on suspended nanomembranes, but need to be supported on a semi-insulating substrate. In this case, conventional thermal conductivity techniques can be easily applied only to the measurement of the thermal conductivity in the perpendicular direction with respect to the film plane. Our numerical method can be applied also for the measurement of the thermal conductivity in the film plane, parallel to the supporting substrate. To this end, two metal strips, deposited on the supported film, must be considered. The distance, width and thickness of the two metal strips can be designed so that the thermal conductivity in the film plane is prevalent. Our FEM fitting procedure allows reliable data analysis for the thermal characterization of films deposited on a supporting semi- insulating substrate.

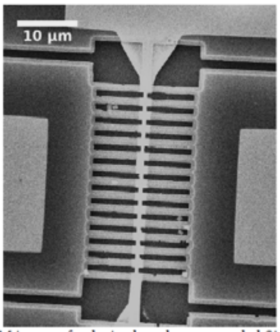

Fig. 1. SEM image of a device based on suspended Si nanomembranes, with a metal track (heater) fabricated in the middle

Fig. 2. A 3D model of the device of Fig. 1. Lenghts and widths have been determined from the SEM photo, thicknesses have been determined by means of AFM imaging.

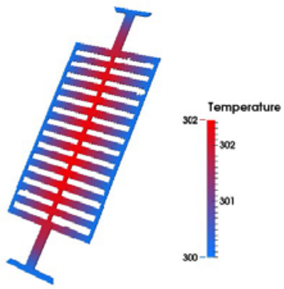

Fig. 3. Thermoelectric transport equations are solved by means of the Finite Element technique, considering the 3D model of the device (see Fig. 2). A current is imposed in the metal heater.

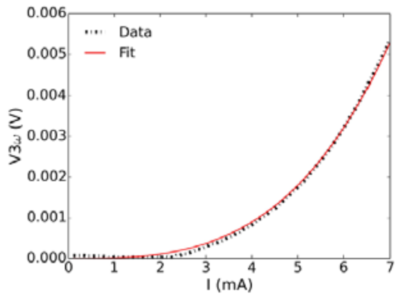

Fig. 4. The thermal conductivity is obtained by fitting the experimental data.

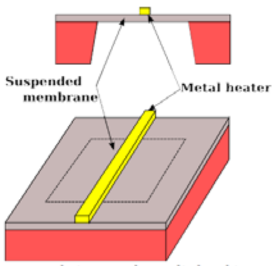

Fig. 5. The same technique can be applied to thin suspended nanomembranes, with a metal heater fabricated in the middle

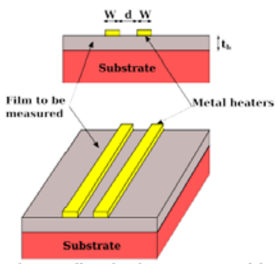

Fig. 6. Two heaters allow the characterization of the thermal properties of films on substrates. The width the separation of the metal tracks must be made small enugh to guarantee that thermal transport through the substrate will be negligible.

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