Time Dependent Simulations of Thermoelectric Thin Films and Nanowires for Direct Determination of Their Efficiency with COMSOL Multiphysics®

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Abstract

Thermoelectric materials are one of the most promising materials for future and nowadays energy harvesting devices, as they can convert heat into electricity and vice-versa [1]. These devices are solid state, with no moving parts, and therefore silent, reliable, lightweight and durable. Thermoelectric materials are widely used for cooling electronic devices, but their applicability to energy harvesting is nowadays limited because of its low efficiency. The nano-structuration appears to be the way to improve this efficiency, since it has been proved theoretically that the reduction of the dimensionality of these materials involve an enhancement of their performance [2].

The efficiency of thermoelectric materials is related with the figure of merit, ZT. In order to characterize the quality of a thermoelectric nanostructured material one must measure its figure of merit, which can be done from indirect measurement of the individual properties of the sample or directly by applying the Harman method. In the Harman technique, ZT is determined based on the voltage developed across a thermoelectric material subjected to an AC current flow at high and low frequencies. The low frequency voltage incorporates both Ohmic and Peltier responses, while at high frequencies the Peltier component vanishes. The ZT is then calculated from the rate of voltages at low and high frequencies, ZT=Vs/Ve, where Vs is the Seebeck voltage generated by the sample and Ve is the pure electrical voltage drop across the sample .On the one hand, measuring the different properties of the material requires of different techniques, which takes a long time and many efforts. On the other hand, the Harman technique has been used successfully to measure in a straight forward way the ZT of thermoelectric bulk materials, but its extension to thin films or nanowires is still challenging. [3,4]

Our work deals with the determination of the parameters that affect the measurement of the ZT with the Harman technique and the best experimental conditions for this kind of measurements. For that purpose, time dependent simulations of thermoelectric thin films and nanowires under vacuum and atmospheric conditions have been carried out to determine the high and low frequency regimes of the Harman technique and the figure of merit of the nanostructures. Moreover, we have analyzed the influence of the presence of electrical contact resistances and

different types of substrates underneath the thin film. As no commercial software exist for thermoelectricity simulations, we used the PDE interface in COMSOL Multiphysics®, where we introduced the time dependent thermoelectric equations, in combination with the laminar Heat Transfer Module.

Reference

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Figures used in the abstract

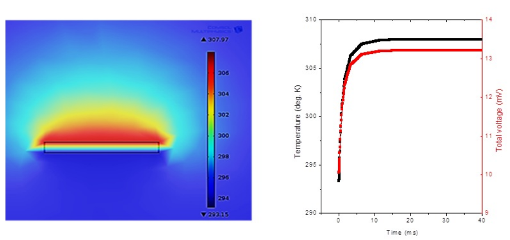

Figure 1: Left: Steady-state temperature distribution in a 60 µm Bi2Te3 under a 10mV pulse of 0.5 s length. Right: Temperature and voltage as function of time for same applied voltage pulse.