MINIMIZATION PROCEDURES FOR THERMAL PARAMETERS IDENTIFICATION: FROM THE EXPERIMENT TO THE PHYSICAL MODEL

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ABSTRACT The thermal conductivity measurement of materials as thin films or nanostructured devices is still a challenging task. It is generally required to make the experiment suitable with the system to be characterized, avoiding thus the use of commercial apparatus than can only deal with “classical” configurations. In addition, the characterization of the thermal properties has to be performed within a large temperature range in order to highlight the most significant features of the materials with regards to its final application. We will illustrate our talk by considering phase change chalcogenide alloys, as GeTe or GeSbTe, that are used nowadays as the core material of non-volatile memories devices. Those alloys present a phase change between amorphous and crystalline state at a specific glass temperature. The huge electrical resistivity change observed between those two states is used to store a bit.

As a first step, we will illustrate how the inverse methods can be implemented in order to identify the thermal properties of such materials. Different contact and contactless experimental techniques have been developed in order to deal with such materials and devices. We will present the experimental methods we have used in our team: the modulated photothermal radiometry, the periodic pulse photothermal radiometry, the time domain thermoreflectance, the 3-omega and the scanning thermal microscopy. A model of the heat transfer within each experimental configuration has been developed and an inverse procedure has been implemented in order to identify the thermal parameters of interest. In this talk we will focus mainly on thermal conductivity and thermal resistance at interfaces.

Several models can be used in order to explain the identified thermal properties, ranging from first principal methods (ab- initio, DFT), molecular dynamics and models based on the phonon density of states using the expression of the phonon scattering relaxation time associated to each type of scattering (phonon-phonon, phonon-defects, phonon-electron, ballistic regime, ...). This later approach has led to the so-called Callaway, Callaway-Holland, Slack or Klemens models for instance. Those models are still widely used since they provide fast and reliable analysis of the thermal conductivity in a large range of temperature from 1K to the melting temperature. In this keynote, we will present the identification approach of the parameters involves within the relaxation time functions based on a complete sensitivity analysis and different minimization techniques.