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An Integrated Experimental and Computational System for the Thermal Characterization of Complex Three-Dimensional Submicron Electronic Devices

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ABSTRACT

The work presents the creation of an analysis engine and experimental system capable of fully characterizing the thermal behavior of complex three-dimensional active submicron electronic devices. First, the transient surface temperature field of pulsed devices is non-invasively measured with submicron spatial resolution. Next, the thermal conductivity of each thin-film layer composing the device is measured and a numerical model is built using these values. The temperature distribution map is then used as input for an ultrafast inverse computational solution to fully characterize the thermal behavior of complex three-dimensional devices. By bringing together measurement and computation, it becomes possible for the first time to non-invasively extract the transient three-dimensional thermal behavior of nanoscale embedded features that cannot otherwise be accessed. The power of the method is demonstrated by verifying that it can extract details of interest of specially constructed micro-resistors.

INTRODUCTION

The determination of temperature fields is crucial for the design, reliability analysis, and predictions of performance of microelectronic devices. As a result, there is an increased need for methods to determine the temperature of features at the submicron level [1, 2]. Computational

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approaches can provide insight into the internal thermal behavior of such complex devices, but can be limited by the inherent necessity of modeling the heat sources, which in the case of self-heating microelectronic devices, are the result of electrical fields whose exact shapes and locations are difficult to specify with reasonable certainty. Moreover, such devices can actually experience irreversible changes in thermo-physical properties and/or geometries that cannot be otherwise predicted from theory or monitored. Experimental approaches can also be helpful in determining thermal behavior, but require either physical access or a visual path to the region of interest. Contact methods, for example, present the difficulties of having to access features of interest with an external probe, or in the case of embedded features, fabricate a measuring probe into the device, and then having to isolate and exclude the influence of the probe itself. Non-contact methods, on the other hand, can provide surface temperature profiles, but in and of themselves cannot impart information on internal behavior. In other words, these methods provide a two-dimensional perspective on what otherwise is, in the case of stacked complex devices, an intricate three-dimensional thermal behavior.

However, by combining an experimental method capable of mapping the surface temperature of a complex device with spatial and temporal accuracy together with a computational engine capable of rapidly and accurately resolving the geometric and material complexities of a full three-dimensional microelectronic device, it becomes possible to use the independent information from the experimental measurements to mitigate the lack of knowledge in the source model parameters, which directly affect the usefulness of the computational results. This article introduces a proof of concept of a coupled computational-experimental approach that uses a measured two-dimensional surface temperature mapping to help obtain a fully three-dimensional thermal characterization of an active micro-device.

METHODOLOGY

The overall approach combines computational and experimental methods previously developed by the authors. The transient two-dimensional surface temperature is measured by the use of the thermoreflectance thermography system [3], while the three-dimensional thermal behavior of multi-layered integrated circuits (with embedded features) is inferred by solving the inverse heat transfer problem with the self-adaptive ultra-fast numerical technique [4, 5]. To minimize the number of uncertainty sources that the inverse method must deal with, the thermo-physical properties of the various thin layers are measured independently with the Transient

Thermo-Reflectance technique [6-8]. In what follows are the details of each of these three methods.

Thermo-Reflectance Thermography System

The experimental temperature mapping system is based on the thermoreflectance (TR) method, where the change in the surface temperature is measured by detecting the change in the reflectivity of the sample. Since the change in reflectivity (i.e., thermo-reflectance coefficient, C_{th}) is of the order of 10^{-4}-10^{-5} K^{-1} for most electronic materials, the system had to be designed, built, and fine-tuned to achieve the levels of uncertainty that are required for the success of the measurements presented here. The C_{th} is extremely sensitive to the wavelength of the laser and varies strongly from one material to another. Hence, in order to maximize the signal to noise ratio, we modulated the probing laser light and used a lock-in amplifier to extract the useful signal.

The measurement methodology requires two steps. First, the coefficient of thermal reflectance is determined for each of the surface materials to be scanned (calibration). Second, the changes in the surface reflectivity as a function of changes in temperature are measured at each point of interest with submicron spatial resolution and better than microsecond temporal resolution. The resulting reflectivity waveforms are combined to obtain a transient temperature field over the scanned area.

A schematic of the proposed TTRG is shown in Fig. 1. The probing beam reflects from the heated surface back along the optical path to the sensitive area of a photodiode. The intensity of the reflected light depends on the reflectivity (temperature) of the

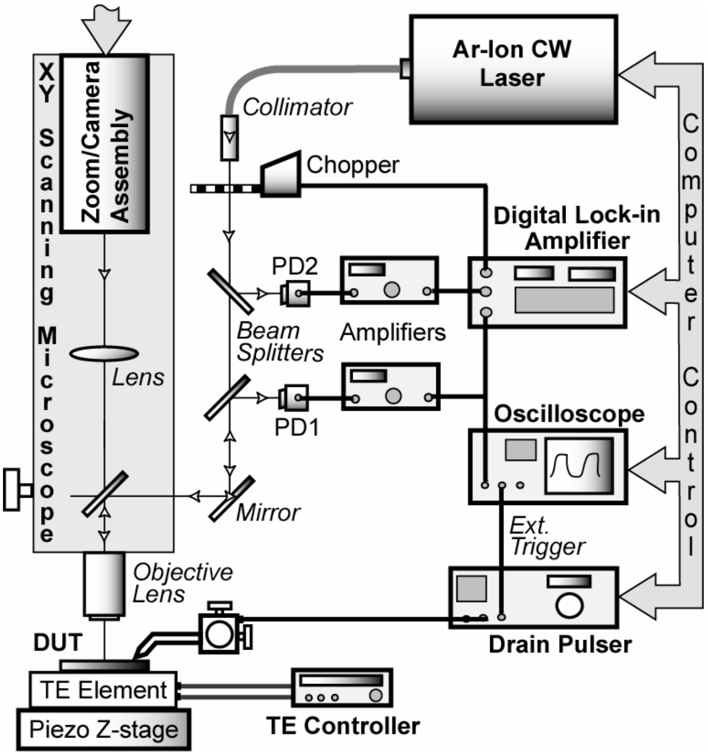

Fig. 1 Surface temperature mapping system

sample's surface. To overcome the inherently low signal to noise ratio, the activation voltage of the device is modulated, resulting in a modulated photodetector signal that can more easily yield the useful signal from the raw photodetector signal output. The photodetector signal, containing the change in surface reflectivity caused by the temperature variations of the DUT, is acquired with a lock-in amplifier (or an oscilloscope) and scaled according to the calibrated data. The limitations of the lock-in and oscilloscope will be discussed.

The calibration approach consists of determining the relationship between the changes in reflectance and surface temperature. The change in reflectance will be measured by a differential scheme involving two identical PDs in order to minimize the influence of fluctuations in the energy output of the probing laser. The sample temperature will be controlled by a thermoelectric (TE) element and measured with a thermocouple. The calibration must be performed for each of the materials on the surface of each device where a mapping of the temperature is carried out. The temperature field of the desired area of the activated device can be mapped by repeating the procedure at multiple physical locations, which is achieved by precisely moving the probing head with submicron resolution.

Computational Engine

The numerical engine is capable of simulating the transient thermal behavior of active multi-layered devices whose dimensions vary over several orders of magnitude and where the thermophysical properties of the materials used are not isotropic. The thermal modeling engine is used to for solving the required inverse heat transfer problem. The measured experimental surface temperature data will be used as input. Since the heat transfer problem is parabolic in nature, a unique temperature field can be computed in the entire structure by solving the corresponding heat transfer problem.

The novel approach begins by solving the corresponding steady-state problem by the use of a grid nesting technique. The nesting technique defines a template that is then used to solve the transient problem in a multiple grid fashion. The advantage to solving with multiple grids in time is that the majority of the problem domain can be resolved in time at lower nest levels (with a coarser grid), while the finer grid resolution is reserved for the parts of the problem that demand the finer resolutions in space and time.

Since the physical dimensions of the various materials used in modeling high performance electronic devices vary greatly, a uniform mesh that resolves all of the details in three

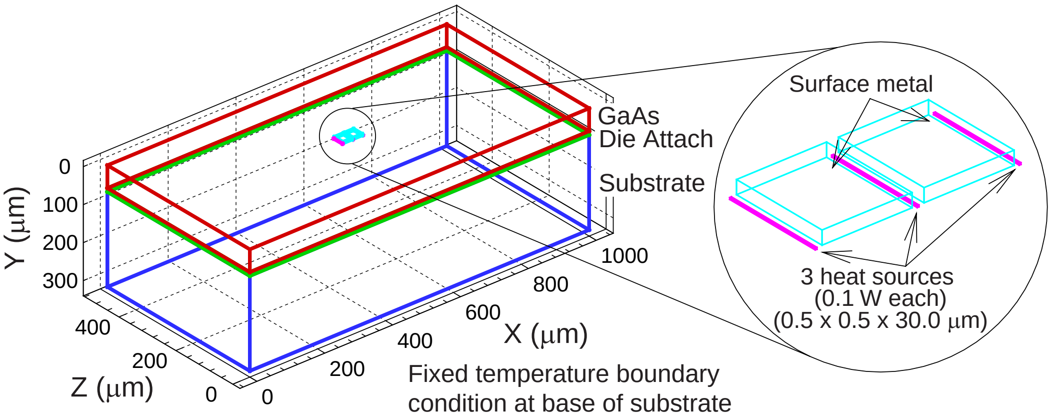

Fig. 2 Schematic of a representative complex IC problem

dimensions results in a prohibitively large computational grid. A common method for dealing with dimensional variation is to skew the mesh and concentrate more grid points in areas where higher resolutions are needed. The shortcoming of using a biased-mesh approach to resolve the geometry is that the problem geometry, and not the temperature gradients, will end up dictating the meshing. The meshing strategy used in the development of the novel numerical technique [4] was set on ensuring that the method is (i) automatic and adaptive, (ii) independent of user expertise, and (iii) independent of materials (including air), geometry features, embedded vias, and heat source locations. The approach makes it possible to start with the full 3D geometry of a real device in all of its complexity, and then uses a physics-based automatic error predictor to focus the entire available computational power on only those regions that require further refinement in order to achieve the level of acceptable error prescribed by the analyst [5]. The new approach allows for the addition of the difficult problem geometry associated with top surface features of an IC over a large area, and then letting the error prediction technique decide if the regions need further refinement. The strength (and novelty) of the method is that it uses effective thermal properties that are consistent with the local grid spacing at the particular grid level in use. As a result, dealing with air, embedded vias, and ultra-thin multi-layered structures requires no special treatment

For complex computationally demanding problems, such is the case of complex electronic ICs one of which being presented in Fig. 2, the approach affords a *two order of magnitude increase* in speed over conventional methods. The benefits are even more significant if one considers the facts that, in conventional methods, (i) significant effort must be expended by an experienced analyst on mesh generation and optimization; (ii) several mesh iterations are normally required to ensure that features of interest are well resolved; and (iii) several solutions with increasing resolution are required to ensure that grid convergence is achieved. When the most complex case is solved on the newest personal computers, the simulation time is further reduced into the minutes.

Thermal Properties Measurements System - Transient Thermoreflectance (TTR)

Since it has been proven [9] that the thermal properties of thin-films varies from that of bulk materials it is necessary for the numerical simulation to input the real value of the thermal conductivity for all of the materials composing the system under study. The transient thermoreflectance measurement system is used to determine the real properties of the thin-film materials to be used in the numerical simulation.

The schematic in Fig. 3 depicts the heating and probing spots produced by a typical TTR system. The source of energy in the TTR method is provided by a pulsed laser with a short pulse duration. During each pulse, a given volume below the sample surface heats up to a temperature level above ambient due to the laser light energy absorbed into the sample. The heating area is a function of the laser aperture and the optics of the system. The depth of the volumetric heating, on the other hand, is determined by the optical penetration depth, which is a function of laser wavelength and surface material properties. After each laser pulse, the sample begins to cool down to its initial temperature. During this process, the probing CW laser light reflected from the sample surface at the heating spot center is collected on an ultra-fast photodetector that reads the instantaneous surface reflectivity. The changes in surface reflectivity are linearly proportional to the changes in surface temperature, within a wide but finite temperature range [10,11]. The specific system in the NETS Laboratory at SMU (http://engr.smu.edu/netsl) uses an Nd:YAG pulsed heating laser whose

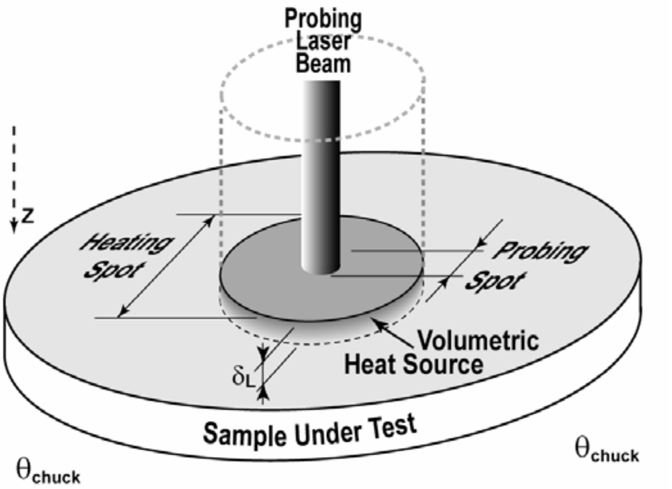

Fig. 3 Schematic of the heating and probing spots on a sample for a typical TTR system

wavelength is 532 nm, pulse width is 6.1 ns, and maximum pulse energy is 0.5 mJ. The CW probing laser is an He-Ne with a 633 nm wavelength.

RESULTS

By the use of the integrated approach presented above we are able to solve the inverse conduction problem associated with a complex, multi-layered, deep submicron IC in order to infer the thermal behavior of the embedded features that cannot be otherwise achieved. To prove the concept, we begin by applying it to a simple device type for which the heat source shape is controllable and well defined. The inverse solution will focus on determining a single unknown, namely the depth of the heat source from the device surface. Therefore, we constructed a series of Aluminum micro-resistors, embedded in a layer of silicon dioxide at different depths from the surface. The actual depth of each device is measured independently with an ellipsometer and a stylus profiler. The geometry of the resistor is shown schematically in Fig. 4. A gold pad is deposited on top of the oxide layer to enable probing of the surface temperature (the oxide layer is transparent to the wavelength of the probing light irradiation).

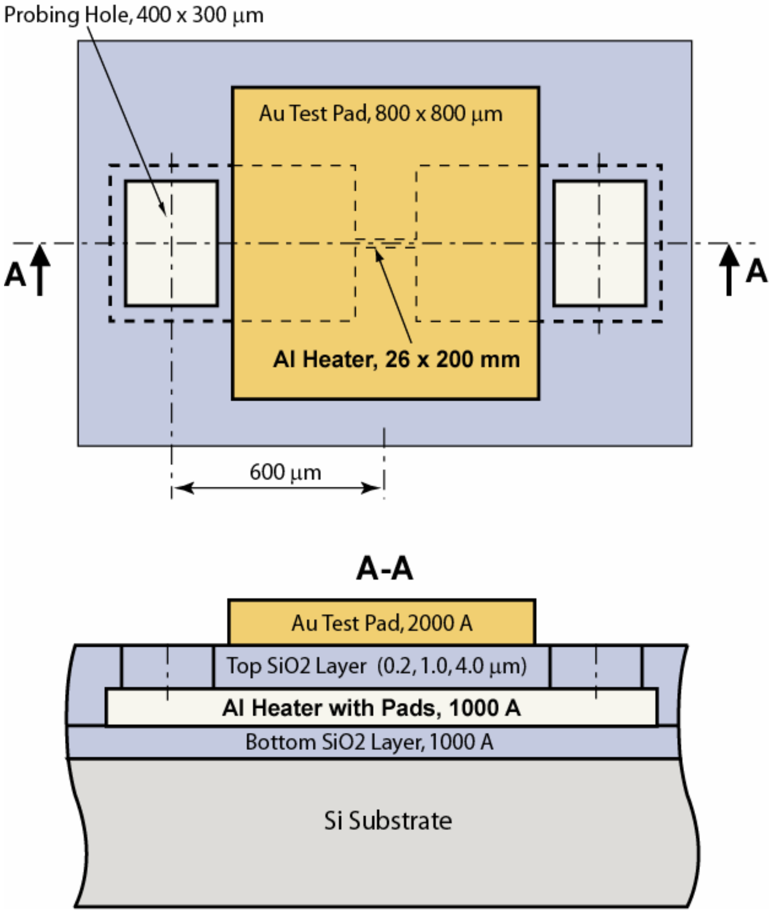

Fig. 4 Geometry of the scanned micro-resistor

The integrated experimental-computational approach will then be used to infer the depth of the heater by first scanning the surface temperature and then using the numerical simulation to solve the inverse problem for the unknown depth. Because in this case the problem involves only one unknown, the method will use a single-parameter optimization approach that minimizes the RMS error between the measured and computed surface temperature fields. The validity and power of the method will thus be demonstrated by comparing the depth values inferred from applying the coupled technique with those measured by the ellipsometer and profiler. The determination of the correct heat source depth yields the correct, complete, three-dimensional temperature field.

For existing devices, the highly resolved and accurate picture of the 3D temperature field would provide the ability to detect hot spots, diagnose performance, and assess reliability. In design and manufacturing of new devices, the new tool has the potential to provide a rapid approach for analyzing the thermal behavior of complex stacked structures, identify regions of excessive heat densities, and ultimately contribute to improved thermal designs, better device reliability, and shorter design cycle time. In the long-term, this tool can also be integrated with existing electrical characterization tools to provide the ability to design devices while concurrently comprehending electrical and thermal issues. The outcome of this work will contribute to dealing with the critical aspects facing the electronics industry and that are brought about by continued miniaturization, introduction of novel materials, and never-ceasing demand for higher performance.

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