Analysis of time-resolved thermal responses in Lock-In thermography by independent component analysis (ICA) for a 3D-spatial separation of weak thermal sources and defects

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Abstract

Lock-In Thermography is an established non-destructively operating method for the analysis of failures in microelectronic devices. In recent years a major improvement was achieved allowing the acquisition of the time-resolved temperature responses of weak thermal spots that enhances defect localization in 3D stacked semiconductor architectures. The assessment of a defect’s depth based on the numerical estimation of the delay between excitation and thermal response by analyzing the value of the lock-in phase is often prone to thermal noise and parasitic effects. In sample structures that contain partial or full transparency for the infrared signal between the origin and the sample surface, the interference of the direct (radiated) and the conducted signal component largely falsifies the phase value on which the classical depth estimation relies. In the present study blind source separation based on independent component analysis of the thermal signals was successfully applied to separate interfering signal components arising from direct thermal radiation and conduction for a precise estimation of the defect depth.

Introduction

In microelectronics the ongoing trend aims at increasing functionality and performance while reducing the components spatial dimensions. With this trend continuing efficient and precise methods for identifying and localizing potential defects for the guidance of subsequent high-resolution failure analysis remain of major interest and thus, require continuous development and adjustment to the arising challenges [1]. In this respect, non-destructively operating defect localization techniques are specifically desired in the beginning of the failure analysis workflow. Furthermore, the resulting structural complexity of 3D integrated devices demands the need for localization of electrical and structural defects in all 3 dimensions.

Lock-in Thermography (LIT) is a powerful non-destructive technique for the localization of electrically resistive defects by tracing the accompanying dissipation-caused thermal signals [2, 3]. In recent years several improvements have been achieved utilizing the temporally resolved thermal response (TRTR) to the electrical excitation of a sample to improve the 3D defect localization based on the analysis of the propagation-related delay and to increase the signal-to-noise ratio (SNR) for enhancing the methods precision [4, 5, 6]. However, the technique remains challenged by interfering thermal signatures especially in 2.5D- and 3D-die architectures if they contain layers with partial or full IR-transparency as this causes interference of the radiated and the conducted thermal components. In addition, analytical approaches for separating interfering signals of adjacent thermal sources often reach their limit due to the influence of noise and parasitic effects e.g. edge reflections within the sample. Solutions for both restrictions are proposed in the present study.

In digital signal processing, the objective of separation of source signals from a mixture of interfering signals without the knowledge of information of the mixing process is known as blind source separation (BBS) [7]. In general, this is an underdetermined problem, for which several approaches are available to determine a set of possible solutions. The field of unsupervised machine learning provides several methods e.g. principal component analysis (PCA) or independent component analysis (ICA) that aim to discover common patterns and features from a set of input data [8, 9]. The current paper presents the application of independent component analysis (ICA) for source separation of temporally resolved lock-in thermography (TRTR) measurement data, aiming at the localization and identification of thermally active spots which are originated at subsurface defects in packaged microelectronic devices.

Materials and Methods

TRTR

Recently, 3D defect localization by LIT [2] was extended by acquiring and analyzing the time-resolved temperature response [5, 6]. The TRTR represents the temporal sequence of the emitted thermal signal which is induced by periodic electrical excitation of the sample under test and is recorded at the sample surface for each pixel in the thermogram. The signal emitted by a thermal source propagates through the sample by
unidirectional conduction and radiation until it reaches the surface of the sample from where it radiates off towards the camera. A schematic of the LIT setup with illustration of the TRTR analysis upon square wave excitation is shown in Figure 1. Transient thermal signals from each detector pixel are acquired and averaged over all performed lock-in periods. Furthermore, the resulting transient signal is processed to conduct a spectral decomposition for the extraction of the amplitudes and phase values at all frequencies of interest. In square wave excitation energy is contained at the excitation frequency and its harmonics which can be employed for computing the phase versus frequency characteristics and subsequently the sources depths underneath the samples surface. Given by the one-dimensional thermal wave propagation, the square root characteristics of the phase shift ($\phi$) to frequency ($f_{\text{lock-in}}$) behavior is a common approximation for depth ($x$) localization in packed devices by their proportional relationship:

$$\phi \sim z \cdot \sqrt{f_{\text{lock-in}}} \quad (1)$$

Thermal conduction simultaneously occurs in all three spatial directions resulting in lateral spreading and thus, a broadening of the hot-spot at the samples surface, depending on the thermal properties of the involved materials and their geometrical dimensions. The time a thermal signal requires to propagate from its origin to the samples surface via conduction depends on the thermal properties of the crossed materials but also the depth inside the sample resulting in specifically altered shapes of the acquired TRTRs.

When the surficial hot-spots of thermal sources originated at different depths superimpose, the resulting thermal trace contains interfering signals of different origin which leads to falsified phase values and thus an erroneous depth localization.

ICA

For an accurate defect localization in the axial and lateral dimensions, separation of the thermal sources from their convolutive mixtures as provided by the recorded TRTR is necessary. BSS [7, 8] refers to a set of methods for reconstructing both the source signals and the mixing parameters from a set of independent observations. In previous publications, such techniques were employed for automated defect identification in pulsed thermography for non-destructive testing and evaluation [10]. The assumption that the emitted thermal source-signals captured in the TRTRs are statistically independent and non-Gaussian distributed, enables the application of a BSS method known as ICA [8, 9].

In a formal definition, the linear mixing model of an observed thermal signal $\tilde{x}(t) = [x_1(t), x_2(t), ..., x_m(t)]^T$ from $m$ observations at $t = 1$ to $T_{\text{end}}$ is defined as:

$$\tilde{x} = A\tilde{s} \quad (2)$$

where $A$ is the unknown mixing matrix and $\tilde{s}(t) = [x_1(t), x_2(t), ..., x_n(t)]^T$ is the vector of $n$ contained independent components. The intent of this method is to obtain a linear static transformation, referred to as the unmixing matrix, to convert the thermal signals into an optimal resulting vector of maximally statistically independent components by either minimizing the mutual information or maximization of the non-Gaussianity of the source signals. The model can then be rewritten as:

$$\tilde{s} = W\tilde{x} \quad (3)$$

where $W = A^{-1}$ is the unmixing matrix that is estimated through ICA using numerical pseudo inverse techniques [9] and $s$ the original set of components, contained in the source signals. It is necessary that the number of observations (sensors) ($n$) is equal to or greater than the number of sources ($m$): $n \geq m$. The independent source-signals can be the results of a non-linear process as only the mixing process is assumed to be linear.

In the present study, the Fast-ICA algorithm as described in [11] was employed for estimating the independent signal components and their corresponding unmixing matrices. The algorithm is based on a gradient method to separate the independent signal components by maximizing the non-Gaussianity through estimating the kurtosis of the sources after each iteration. Ordinarily, the data is centered by subtracting the mean from the original data and whitened by applying PCA before employing the Fast-ICA algorithm. The resulting data from the observation vector are uncorrelated and have unit variance.

The identification of the independent spatial or temporal components and their mixing coefficients in the TRTR sequence, using ICA enables the extraction of the spatiotemporal evolution of the thermal spreads of each thermal source by the mixing matrix. It should be noted that the estimated thermal source signals are the result of the interaction of induced heat generation by the source upon electrical excitation and the dynamic temperature response from the surrounding medium.

The time-resolved acquisition of the thermal responses provides a 3D tensor containing the 2D images at each equidistant time-step of the lock-in period. Typically, the number of the spatial increments in a recorded TRTR dataset is higher than in the

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Figure 1: Schematic of the LIT setup with illustration of the TRTR acquisition. In contrast to classical LIT, each electrical excitation period is stored and averaged frame-wise which results in averaged thermal signals at each imaging pixel.
Consequently, the performance of the applied method appears promising. The correlation between the estimated temporal signals and the source signals shows a coefficient larger than 0.98 which clearly indicates an ideal solution of a decomposition. Furthermore, the 2D correlation of the summed ICA weights with the simulated spots reaches a rather high value of 0.96.

**Case Study I**

The application of the above described method is evaluated in a case study investigating a stacked die device illustrated in Figure 3. The sample consists of four axially stacked Si-dies deposited resistors (STV) on top of each die. Top: Cross-sectional view of comparable device with marked STVs by red and blue arrows on top of chip 1 and chip 4. Bottom: Thermal emissivity image of sample surface with marked areas corresponding to STV-Top and STV-Bottom.

**Figure 2:** Example of the spatial ICA applied to a simulated dataset. A) Simulated spatial spots (spot 1 and spot 2) with their two extracted temporal sequences from the center of each spot. B) Observation dataset with 9 exemplary frames at specified time steps (left). Two extracted temporal signals from the observation data at the center of the spots (right). C) Spatially independent components from sICA decomposition (left) and the associated temporal signal from the mixing matrix (right).

temporal dimension causing the computational effort easily exceeding the limits of the hardware capacity. Consequently, the ICA mixing model is transposed and the algorithm estimates the spatially independent components with their associated time courses according to:

\[
\mathbf{s} = W_{\text{sICA}} \mathbf{x}
\]

(4)

This technique is also known as spatial ICA (sICA) [12].
with a thickness of ~50 µm and underfiller layers. The circuits of each die contained several test structures including deposited resistors (STV) for a localized temperature assessment. In the current study the STV structures were employed to act as defined heat sources at each level of the stacked die sample. Aiming at the localization of the thermal sources in all three spatial dimensions, especially in the depth, LIT combined with data acquisition in TRTR mode was performed using a commercial LIT system, ELITE System (Thermo Fisher Scientific Inc., Waltham, U.S.). Electrical excitation was conducted in a square wave (on/off) mode at a lock-in frequency of 1 Hz. The lowest STV-structure (STV-Bottom) and the uppermost STV-structure (STV-Top) were excited and measured successively for 30 min with an induced electrical power of 8 mW. The amplitude and phase values of the recorded TRTR data were extracted up to a frequency of 23 Hz. The challenge LIT-analysis faces with the present sample is that the Si-dies and the underfill are transparent in the infrared range (IR). In such cases a common approach would be to add an IR-opaque coating on the sample surface that blocks the direct IR radiation from the thermal sources to the camera. However, due to its considerable thermal mass with respect to the filigree Si-dies, such layer would influence the overall thermal properties of the sample. In a subsequent investigation the sample was coated by SiC particles (FEPA 1200: grain size nearly 3 µm) that were deposited as a thin layer on top of the device. For comparison, TRTR-data acquisition and analysis was repeated.

**Results and Discussion**

Figure 4 shows the emissivity image of the described sample at room temperature with the analyzed region of interest marked (ROI) in red. The right-hand side graph contains the results of the classical LIT analysis of the resistor structure at the bottom level, STV-Bottom. The peak amplitude coincides with the lateral location of the resistor structure, exhibiting a strong contrast to other structures in this graph. The absence of thermal spreading leads to the hypothesis that the spot is mainly dominated by IR radiation. This can also be concluded from the graphs in Figure 5. The evaluation of the phase vs. frequency trace obtained from the TRTR measurements is expected to exhibit a major increase in the phase for the resistor-structure of the lowest die (STV-Bottom) in opposite to the resistor on the uppermost die (STV-Top), corresponding to the longer propagation path. This, however, cannot be observed. On the contrary, the phase difference at higher frequencies is even decreasing which seem to contradict with the theoretical expectations. The results of the applied ICA-algorithm, are shown in Figure 6. Here, two independent components, that contain 95 % of the signal variance of the entire dataset, were extracted. In “component 1” of Figure 6, the mixing weights contain a large lateral spread of the thermal response of STV-Bottom. The corresponding time trace resembles a typical response of thermal waves in solid media with increasing attenuation occurring at higher lock-in frequencies, which results in a low-pass filtering of the thermal response. This is in contrast to component 2, where the lateral thermal spread of the spatial component is considerably lower. The related time course follows the electrical excitation signal during the measurement of LIT by TRTR. Cumulating the weighted “components 1” and “2” results in the lock-in amplitude and averaged TRTR signal as shown in the top graph of Figure 6. It reveals that the predominant part of the thermal response corresponds to the ICA “component 2” as it exhibits the largest mixing weights. Based on these observations, the conclusion can be drawn that “component 1” is caused by thermal conduction, while “component 2” represents the amount of energy that has propagated through the sample by IR-radiation. The phase vs. frequency curve of the time course of “component 1” is included in the chart in Figure 7 (red trace). In comparison to the initial phase value of “STV- Bottom”, a steeper slope of the phase values of “STV-Bottom ICA” versus “STV-Top” can be recognized. This fact may be related to the larger delay of the thermal wave arising from the longer propagating path for the thermal signal to reach the sample surface, where it radiates off.
Figure 6: ICA applied on TRTR dataset of driven STV-Bottom structure (lowest die). Top: Lock-in amplitude and averaged TRTR signal of ROI in Figure 2 recorded from TRTR measurement of STV-Bottom. Center: Result of the ICA algorithm with separated spatial component (mixing weight) and time trace of component 1. Bottom: Result of the ICA algorithm with separated spatial component (mixing weight) and time trace of component 2.

Towards the camera. In order to verify these observations, an additional TRTR measurement was performed after coating the sample with SiC particles to reduce the influence of IR radiation through the surface. The phase evaluation after coating provided in Figure 7 also reveals a steeper increase of the phase values of “STV-Bottom (coated)” (green trace) in comparison to the resistor structure “STV-Top” at the surface. However, the phase difference appears larger than expected and the standard deviations increase with increasing frequency.

There are two reasons that likely explain this behavior. Introducing an additional layer on top of the sample surface causes a longer delay of the thermal response, as it forces the directly radiated component to heat up the volume and meanwhile spread laterally. Coupled with the increased heat capacitance of the SiC-particle layer a higher phase deviation seems reasonable. Furthermore, the thermal response obtained through thermal conduction contains considerably higher noise amplitudes compared to the IR radiation, especially at higher frequencies, which likely results from attenuation effects occurring along the propagation path of the thermal signal.

Summary

The application of an ICA based analysis appears highly promising for separating interfering signal components originated at individual thermal sources and benefits towards the aim of a highly precise lateral and axial localization of defect-related thermal sources in 3D microelectronic devices. The case study presented in this paper is a representative example for decomposing signal artefacts from IR radiation in a TRTR dataset recorded by LIT to ensure accurate phase estimation. The results from the phase over frequency evaluation show excellent agreement with the theoretical expectations.

References


