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A Hybrid Modelling Approach for Parameter Estimation of Analytical Reflection Models in the Failure Analysis Process of Semiconductors*

Simon Kamm, Kanuj Sharma, Nasser Jazdi and Michael Weyrich

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Abstract—**Electronic devices are one of the key factors for recent advances in smart production systems or automotive. Reliability and robustness are key issues. To further increase this reliability, occurring failures in an electronic device has to be investigated in post-production failure analysis processes. One recent technique to detect and locate failures in electronic components is Time-Domain Reflectometry. This method offers the chance to detect several kinds of failures (e.g. a hard or soft failure) and localize the failure nondestructively. In theory, this can be determined following defined physical formulas. Nevertheless, the received signals are not perfect and mixed with noise from the measurement device or disturbed by nonoptimal material properties. In addition, complex architectures of devices are hard to model based on analytical models. Thus, these models solely are not sufficient for the failure analysis process. For this reason, a hybrid modeling approach is proposed, using a Machine Learning model in combination with physical models to detect and characterize the failure and its exact position. The Machine Learning model will be trained with simulated Time-Domain Reflectometry data.**

I. Introduction

Electronic Components consisting of e.g. microelectromechanical systems (MEMS) are a key factor for the deployment of new functionalities. Recent examples are smart production or driver assistant functions in the automotive domain. These advanced functionalities are solely possible with the help of newly developed electronics. To ensure functionality over the expected lifecycle of a product, the reliability of an electronic device is an essential factor [1]. To improve the quality and reliability of an electronic device, occurring failures in an electronic component needs to be analyzed. The gained insights can be fed back to the development process. This makes the failure analysis a base to optimize the development and production of an electronic device. Based on this, the failure analysis tries to improve the quality of industrial production and with it the overall product quality [2].

The failure analysis process of electronic devices is becoming more and more complex due to new product demands like miniaturization or integration of more functionality into reduced volumes. Therefore conventional nondestructively defect inspection techniques as Time-Domain Reflectometry (TDR), Scanning Acoustic Microscopy (SAM) or X-Ray were adapted to the needs of novel concepts in microelectronics technologies [2]. Knowledge is available for these techniques as well as for the microelectronic technologies in the form of experts or physical models. However, manual failure analysis is costly and time-consuming due to the few amounts of experts, the increasing complexity of the systems and the amount of generated data. For these reasons, new automated and intelligent approaches for failure analysis are required.

Machine Learning algorithms are widely applied to handle complex data. These algorithms consume training data to model the observed input-output behavior in a data-driven approach and have shown impressive results in various domains (e.g. Natural Language Processing [3] or Image Recognition [4]). Due to data-driven learning, these models are considered as “black-box” whose outputs are not comprehensible. The performance of the models is depending on the choice, availability and distribution of training data. In contrast, existing physical models (white-box) were developed over a long period and represent extensive existing knowledge. These models are interpretable and need no training data to model the system. However, these models are not capable of modeling every arbitrary complex and nonlinear system with sufficient accuracy. Combining both, the data-driven and physical models, into a hybrid model shall use the advantages of both approaches and lead in the end to an improved model with higher accuracy, shorter training time, fewer required data as well as more interpretable results [5]. These coupled approaches have different names in literature and vary in their realization (e.g. hybrid models [6], Grey-Box models [7], physics-informed deep learning or neural networks [5], [8]). Overall, all approaches try to use existing knowledge as well as available data to improve the final model performance. In the following, we will refer to the term “hybrid model” for this approach.

In this paper, a new hybrid modeling approach for the parameter estimation of an analytical reflection method in the failure analysis process of semiconductors will be introduced.

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Simon Kamm, M. Sc. Is scientific staff member at the Institute of Industrial Automation and Software Engineering at University of Stuttgart, Stuttgart, 70569 Germany (corresponding author, phone +49 711-685 67293; fax +49 711-685-67302; e-mail: simon.kamm@ias.uni-stuttgart.de).

Kanuj Sharma, M. Sc. Is scientific staff member at the Institute of Robust Power Semiconductor Systems at University of Stuttgart (e-mail: Kanuj.sharma@ilh.uni-stuttgart.de).

Dr.-Ing. Nasser Jazdi, IEEE Senior Member, is deputy head of the Institute of Industrial Automation and Software Engineering at University of Stuttgart (e-mail: Nasser.jazdi@ias.uni-stuttgart.de).

Prof. Dr.-Ing. Dr. h. c. Michael Weyrich is head of the Institute of Industrial Automation and Software Engineering at University of Stuttgart (e-mail: michael.weyrich@ias.uni-stuttgart.de).

The novel approach outperforms existing techniques in the failure analysis on TDR data by bringing additional benefits from using existing knowledge and data-driven models. The used nondestructive testing method is TDR, where data is generated with the help of a simulation. The simulation data serves for training a machine learning model, in which the output is used to automatically characterize a failure based on the observed reflected wave with physical equations. Simulation data is used to generate a suitable amount of data for a first evaluation. Reproducing this with real measurements requires more time and cost for the preparation of the Device under test (DuT). A simplified example of a microstrip line with 150 mm length is used as DuT. The microstrip line from the simulation is shown in Fig. 1. It can have several conditions, e.g. "good", "open" or "short". "Open" and "short" represent hard failures at the microstrip line. Additional soft failures can occur, with small impedance changes to the characteristic load impedance. These soft failures give a first insight into a possible future hard failure. Thus, the final model shall be able to detect a soft and hard failure.

The remaining paper is structured as follows: Section 2 provides an overview and short discussion about the basics and related work of TDR, Machine Learning and the usage of Machine Learning for TDR analysis. In Section 3, the problem is described and the developed approach is introduced. The experimental setup is given in section 4 with the corresponding experimental data and model evaluation. In the final section 5, a conclusion is drawn and an outlook for future research is given.

II. Basics and Related Work

A. Time-Domain Reflectometry

TDR can be used to determine non-destructively an interconnection failure on e.g. a MEMS. With the obtained data localizing and analyzing the failure is possible [9]. The basic technique of TDR is reflectometry, which works on the same principle as radar or lidar. An injected signal is reflected by impedance discontinuities at the DuT. Based on the received reflectometry signatures, conclusions about the DuT can be drawn. In case of a failure, the location of it can be determined, too [10, 11]. In comparison to traditional test methods based on electrical resistance monitoring, TDR can distinguish between different failure modes and can additionally detect degradation before a hard failure (e.g. an open at a transmission line) occurs [12].

The TDR measurement (e.g. Fig. 3) shows the reflected signal $V_{reflected}$. With that measured signal and the injected signal $V_{incident}$, the reflection coefficient Γ can be obtained, which gives a direct look at the DUT's characteristics. The reflection coefficient is defined by (1) with Z_L denoting the impedance of the DuT and Z_0 the characteristic impedance of the circuit.

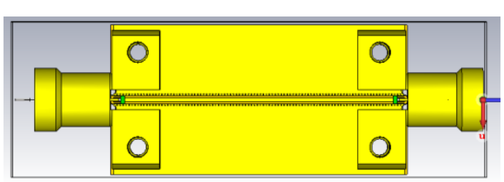

Figure 1. DuT – Microstrip line of 150 mm length

$$\Gamma = \frac{V_{reflected}}{V_{incident}} = \frac{Z_L - Z_0}{Z_L + Z_0} \tag{1}$$

The reflection coefficient for an open circuit ($Z_L = \infty$) is 1 and the reflection coefficient of a short circuit ($Z_L = 0$) is -1. By obtaining the reflection coefficient Γ and knowing the characteristic impedance of the circuit Z_0, the impedance Z_L of the DuT can be determined by (2).

$$Z_L = Z_0 \frac{1 + \Gamma}{1 - \Gamma} \tag{2}$$

Assuming Z_0 is real and noncomplex, a resistive mismatch can be detected and the degree of this mismatch can be calculated easily with the help of (2). With the propagation velocity v_p, the distance D of the failure and thus the location of it can be calculated as given in (3). The transit time from the monitoring point to the reflection point and back again is given as T. The velocity of propagation has to be determined previously from measurement and is depending on the transmission line properties.

$$D = v_p \frac{T}{2} \tag{3}$$

The reflections are behaving differently depending on the specific setup of the load impedance. A series R-L e.g. behaves differently from a parallel R-C combination (R as resistive, L as inductive and C as capacitive part). Based on these deviations, a soft failure of the DuT can be detected and characterized for complex load impedances, too. However, the detection capability of a soft failure is depending on the noise of the transmission line. When the noise covers the reflection signature of the soft failure, it cannot be detected. The TDR method is in general not only capable of detecting a hard failure like open or short but also can detect, characterize and localize a soft failure.

B. Machine Learning

Machine learning is a data-driven approach, where a processing rule is learned based on observed training data. Conventional machine learning algorithms use extracted features and perform the desired task (e.g. regression or classification) based on them. The features are extracted based on defined rules, e.g. from a domain expert or based on mathematical formulas. However, widely used machine learning approaches nowadays are deep learning algorithms. A deep learning model (e.g. a deep neural network (DNN)) learns and performs feature extraction in combination with the desired task (e.g. classification or regression). The trained network can then perform a mapping f of a given input vector $\underline{x}$ to the output $\underline{y}$ based on the learned network parameters $\underline{\theta_f}$ as given in (4).

$$\underline{y} = f(\underline{x}; \underline{\theta_f}) \tag{4}$$

By choosing suitable hyperparameters for the network (number of layers, neurons, activation functions), even a simple multi-layer perceptron can approximate an arbitrary continuous mapping. This property of neural networks enables them to be a universal function approximation [13]. By that, neural networks are capable of modeling, detecting and recognizing unknown patterns and complex relations in the data. This empowers deep learning methods for the failure analysis of electronic devices, where highly complex relations between a measurement signal and a failure exist.

Nevertheless, there are still open challenges for deep learning-based approaches [14]. Learning a suitable mapping function f requires a large amount of training data to on the one hand ensure sufficient accuracy and on the other hand avoid overfitting of the model to few training samples. Here comes a challenge, since in failure analysis, training data for defects is often rare, since damaged products and data of it are limited. Besides, deep learning models are black-box models, where no knowledge about the data processing in the black-box is available. The data is processed based on the learned function $f(\underline{x};\underline{\theta}_f)$, which makes the result of the network neither understandable nor interpretable [15]. In case of the wrong behavior of the model, this property makes it hard to find the error inside it. Furthermore, there is not one way to build a DNN, but it is partially a try-and-error game since the underlying theory of some relations within a DNN is not clear yet [14]. Therefore, a lot of time has to be spent optimizing and choosing the correct parameters of the network. Examples are the number of layers or the number of nodes per layer. Moreover, there exist further hyperparameters such as the learning rate, dropout rate, etc. which have to be optimized with specific knowledge and understanding of the training process. Overall, training a deep learning model is a complex, time-consuming and computationally expensive task.

C. Related Work

Different works have been published to show the effective usage of TDR for failure analysis. In [9] the authors demonstrated the application of TDR for advanced integrated circuits (IC) packages, where isolation of soft failures is required. They showed that TDR can be used in the failure analysis flow to locate and analyze the failure and the application was proved in six different use cases. Smail et al. [10] proposed a multi-layer perceptron-based method for reconstructing a wiring network. Another work ([12]) showed, that the TDR reflection coefficient can be used to detect soft failures and thus identify nondestructively interconnect failure mechanisms. Huang et al. [16] proposed an idea to apply deep learning algorithms to predict the TDR impedance for high-speed differential vias. This can be used in the design phase to predict the impedance of a high-speed differential via based on given design parameters. In [17] an intelligent approach for the diagnosis of wiring networks based on TDR is proposed. They use an artificial neural network for the classification of failure branches in a wiring network. A simple and fast localization and characterization algorithm is used to enable real-time diagnosis. However, just hard failures (open and short) are treated there. Overall, the different approaches tackle different parts of signal analysis based on TDR data.

Although multiple approaches exist for using machine learning to perform intelligent signal analysis, there are still open fields to discover. For example, none of the introduced approaches showed the capability of detecting, locating and characterizing soft failures with the help of machine learning-based signal analysis of the TDR data. Therefore, we will propose a new approach for the detection, localization and characterization of hard and soft failures for a DuT with TDR data. The soft failures not only contain resistive and thus real components but can also contain capacitive and inductive (i.e. complex) components. The final model should be able to characterize this kind of failure. Therefore not only data-driven methods are used, but also available analytical knowledge about the reflection behavior shall be used to form a hybrid modeling approach for the parameter estimation of analytical reflection models. This modeling approach shall enable advanced failure analysis of semiconductors.

III. Problem Description and Approach

In this chapter first, the investigated use case is described and the corresponding problem statement is derived for this use case. Based upon this, the proposed modeling approach is then introduced.

A. Problem Description

A simple microstrip line is used as DuT (Fig. 1) and the corresponding data is generated via simulation. The microstrip line can have different soft or hard failures or be in a "good" state. Hard failures are open and short. A pure resistance (R) or any combination of R with C or L (parallel or series R-L and R-C) represents the soft failures. This results in five possible soft failures, two hard failures and the normal state. For simplicity, the point of failure is not varied and is at 150 mm at the end of the microstrip line. The variation of failure points can easily be done in simulation and will be part of future work. The characteristic impedance Z_0 is 50 Ohms. The incident signal is a step function with $V_{incident}$ being 0.5 Volt. The rise time t_r of the step is varied in the range of 0 and 50 ps with 1 ps steps. For the soft failures the resistor was set to R=75 Ω, the capacitor to C=1pF and the inductor to L=1nH. The resulting scenarios are given in Table 1. The desired model shall be able to detect and locate a failure and classify it into the failure categories. The corresponding values for R, C and L and the location of failure shall then be estimated. Although the location of failures is the same in this paper, for further scenarios this is relevant.

B. Modelling Approach

To solve the previously introduced problem while using the existing knowledge (e.g. (1), (2) or (3)) in combination with a machine learning-based classification, we propose a hybrid modeling approach. The proposed model will use existing knowledge, which we denote as function g, which maps some input $\underline{x}$ to an output $\underline{y}$ based on selected parameters $\underline{\theta}_g$ as described in (5).

$$\underline{y} = g(\underline{x};\underline{\theta}_g) \quad (5)$$

TABLE I. Overview of Considered Scenarios

Failure type	**Normal**	**Hard Failure**		**Soft Failure**				
Setup	Good	Open	Short	R	RL	RC	RpL	RpC
Description	No failure	Open end	Short end	Only R	Series R and L	Series R and C	Parallel R and L	Parallel R and C

To combine knowledge-driven models with data-driven models, different approaches exist. By combining these models, new data-efficient physics-informed models shall be developed [8]. The combination of the knowledge-driven model g and the data-driven model f can in general be done in two ways: superposition or composition [6, 7]. Superposition combines the models in an additive way, where for example g is used to estimate the mean prediction and f models the residual nonlinear error or noise, as stated in (6).

$$\underline{y} = g(\underline{x}; \underline{\theta}_g) + f(\underline{x}; \underline{\theta}_f) \tag{6}$$

Besides, the combination or coupling of the two models can be realized via composition. One model's output serves as input for the other model. This is described by (7).

$$\underline{y} = g(f(\underline{x}; \underline{\theta}_f); \underline{\theta}_g) \tag{7}$$

In the described example, the output of the data-driven model f serves as one of the inputs for the knowledge-driven model g. The data-driven model can e.g. model non-linear dependencies to estimate a parameter based on observation. This parameter can be used in g by an analytical formula to calculate the desired final output $\underline{y}$. This can also be realized in an inverted fashion, where the output of g is used as input for f.

In this work, the composition is used as a coupling approach. Based on that, the overall approach for TDR data is built, which is shown in Fig. 2. The proposed approach consists of three parts and will be explained in the following. It starts with a new **TDR measurement** $\underline{x}$, which shall be analyzed.

The first part performs **anomaly detection with failure localization**. Within that part, anomalous data shall be detected and the failure shall be localized. Therefore, first, *baselining* is performed. This step allows removing unintended effects from the measurement setup. In this paper, a simple approach is used. A previous performed and stored "good" measurement $\underline{x}_0$ is subtracted from the measurement to gain a baseline measurement $\underline{x}_B$ by (8). In more complicated setups this step can also be realized with the help of machine learning algorithms to detect and remove unintended signatures from the measurement embedding.

$$\underline{x}_B = \underline{x} - \underline{x}_0 \tag{8}$$

The baseline data is then checked for anomalous patterns in the *thresholding* step. When a threshold t is reached, the measurement is seen as "anomalous", while it is declared "good" when it is below. Comparison can be done in different ways. The approach, which is used in this paper, is to define a time window of length w and calculate a mean squared error (MSE) of each window as given in (9). The MSE of each window is then compared to t.

$$MSE_{window} = \frac{1}{w}\sum_{i=1}^{w} x_{B,i}^2 = \frac{1}{w}\sum_{i=1}^{w}(x_i - x_{0,i})^2 \tag{9}$$

Based on the detected "anomalous" windows the *Region of Interest (RoI)* is extracted. In this step, the possible faults are extracted and localized. The exact location of the failure is determined. Around this identified failure location, the RoI is determined resulting in one "failure" vector $\underline{x}_f$ per possible failure for the parameter estimation.

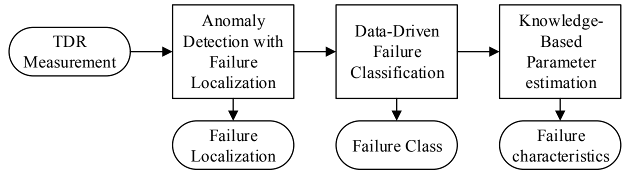

Figure 2. Proposed approach for the hybrid modelling

After the localization of and detection of an anomaly, the anomalous measurement $\underline{x}$ is fed into a **data-driven classifier** for *failure classification*, which maps the input to a categorical output, as given in (4). The possible categories in our scenario are obtained from Table 1 with seven possible failure categories $C_j, j \in [0,6]$ (two hard failures and five soft failures). Multiple models can realize the classifier. In this work, a convolutional neural network (CNN) is used for the time-series classification, since they have already shown good results for this task [18].

A classified hard failure is finally classified, while a soft failure has to be further analyzed in **the knowledge-based parameter estimation** to determine the severity and kind of failure. In this step, the corresponding parameters R, L and C are estimated using the known analytical equations $g(\underline{x}_f, C; \underline{\theta})$ (observed from [19]). To select the correct analytical equation, the output C of the black-box classifier of the previous part is needed to estimate the parameters correctly.

With these previously described steps, the failure can be localized, classified and characterized. For soft failures, the severity of the soft failure can be estimated via the hybrid model. The procedure is given as pseudocode in Algorithm 1.

IV. Experimental Setup

To evaluate the first prototypical implementation of the novel approach, different setups as given in Table 1 have been considered for a microstrip line: Two hard failures as well as five different soft failures located at the end of the microstrip line. A simple scenario is chosen to understand the weaknesses of the approach and have a good data understanding.

Algorithm 1 Hybrid Modelling for Failure Localization, Classification and Characterization

Input Measurement data $\underline{x}$
Output Failure Category C, Failure Location d, Failure Parameters $\underline{\theta}_{failure}$
$\underline{x}_B \leftarrow \underline{x} - \underline{x}_0$
if $MSE_{window} < t$
  $\underline{y} \leftarrow$"good"
else
  $anomaly_{idx} \leftarrow idx \text{ where } MSE_{window} > t$
  $\underline{x}_f \leftarrow \underline{x}(anomaly_{idx})$
  $d \leftarrow v_p \frac{T(\underline{x}_f)}{2}$
  $C \leftarrow f(\underline{x}; \underline{\theta}_{CNN})$
  $\underline{\theta}_{failure} \leftarrow g(\underline{x}_f, C; \underline{\theta}_g)$
END

A. Experimental Data

The experimental data in this paper comes from a simple microstrip line of length 150 mm. The propagation velocity is assumed to be the speed of light. The data is generated via simulation in ADS (Advanced Design System). The time step within the simulation is 100 fs with a simulation time of 5 ns. Different failures (Table 1) are simulated, which are all located at the end of the microstrip line. Different rise times t_r are used within the range 0 to 50 ps with 1 ps steps, resulting in 51 simulation curves per setup. Fig. 3 shows exemplarily the simulated data for a good, open and short setup with a rise time of 10 ps.

B. Model Evaluation

The approach is evaluated based on the previously described data. Within the approach (Fig. 2), different parameters have to be set. These parameters contain the threshold t and the window length w. In addition to those, the CNN has separate hyperparameters, e.g. the number of layers, number of neurons per layer, learning rate. For brevity, we just name the corresponding values. The values are chosen experimentally with t=0.005 and w=1000.

The CNN for failure classification consists of five convolutional blocks followed by two fully connected layers (with 128 and 7 neurons respectively). The input layer has 50.000 neurons to capture the input signal with its time steps. Each convolutional block consists of a 1d-convolutional layer, a 1d-MaxPooling layer and a dropout layer. The pooling size is 4 and the dropout rate is 0.25. The 1d-convolutional layers have filter sizes of 64, 32, 16, 8, 4 and kernel sizes of 5, 5, 3, 3 and 3. For all hidden layers (five convolutional and one fully connected) a rectifier linear unit is used as the activation function. The output layer with seven neurons uses the softmax activation function. We train the model with categorical cross-entropy loss and the Adam optimizer with a learning rate of 0.001, 50 epochs and a batch size of 16. We split the available data by a ratio of 70/10/20 % into training, validation and test data resulting in 252/42/84 measurements.

For the parameter estimation, a least-squares estimator is used. The least-squares estimator uses the trust-region reflective algorithm [20] to minimize the cost function $J(\underline{\theta})$ given in (10).

$$\min_{\underline{\theta}_g} J(\underline{\theta}_g) = \min_{\underline{\theta}_g} \sum_{n=1}^{N} \left[y_n - g\left(x_{f,n}; \underline{\theta}_g\right)\right]^2 \qquad (10)$$

In the following, the obtained results from the classification module and the parameter estimation method are shown. For the data-driven classification module, an exemplary training and validation loss, as well as the corresponding accuracy over number of epochs, is shown in Fig. 4. K-fold cross-validation (with k=10) is performed with a random selection of training, validation and test data to evaluate the model's mean performance and its variance. For the CNN as classification module, a mean training accuracy of 79.63% and mean validation accuracy of 86.67% is achieved. The accuracy on new unseen test data is given in Table 2 with 86.15%. Table 2 shows additionally the obtained accuracies and standard deviations (std) for the further tasks, namely failure localization and characterization.

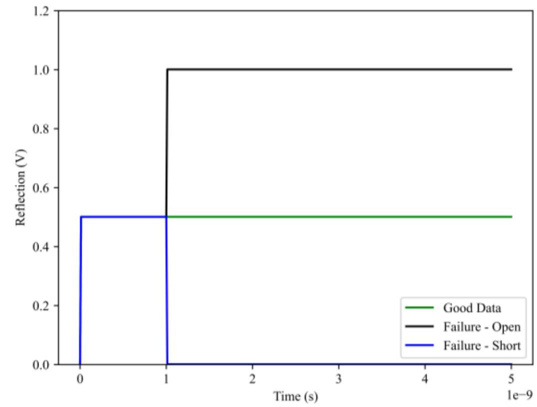

Figure 3. Exemplary data for a good (green) measurement , an open (black) and a short (blue) failure with a rise time of 10 ps

Localization is performed by identifying anomalous windows in the data. A failure in TDR data is typically not just resulting in one anomalous window but in multiple consecutive anomalous windows. By identifying the first window and the start of the anomalous behavior in it, the location can be calculated with the help of (3). The final result is given in Table 2. We obtain a mean deviation in the failure localization of 1.31%, which gives the localization accuracy of 1.96 mm in the investigated scenarios. The anomalous behavior can be detected correctly in 100% of the cases.

The parameter estimation is performed as described previously. Based on the classified failure, the corresponding formula is used to estimate the parameters with (10), where $\underline{y}$ is real extracted failure behavior $\underline{x}_f$ and $g\left(\underline{t}_f; \underline{\theta}_g\right)$ is the modelled physical equation with the time $\underline{t}_f$ and the related parameters $\underline{\theta}_g$. To evaluate the performance of this approach, we assume perfectly classified failures (100% accuracy) and perform the parameter estimation for the given scenarios. The overall metric is given as a deviation of the estimated parameter relative to the correct parameter values over all scenarios and parameters in percent. The result is given in Table 2 with 13.61% mean deviation. However, this metric varies heavily for the different parameters, which have to be estimated. The mean deviation for the resistance parameter is 4.51% (in absolute values 75±3.38 Ω), for the capacitance parameter 14.38% (1±0.14 pF) and the inductive parameter

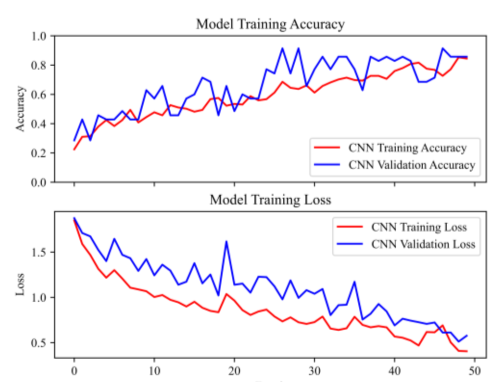

Figure 4. Training progress classification model (CNN)

TABLE II. FINAL ACCURACY AND DEVIATION OF THE MODELS ON TEST DATA

RoI Extraction (Failure localization)	**Failure Classification**	**Parameter Estimation (Failure characterization)**
Mean and std of deviation in %	***Mean Accuracy and std. in %***	***Mean and std of deviation in %***
0.46±0.96	86.15±9.04	13.61±14.92

31.05% (1±0.31nH). The inductive parameter seems to be the most challenging one to estimate.

Overall, the introduced approach can use the given data and available knowledge to identify, classify and characterize the failure within the DuT. Previously introduced existing approaches are not able to perform these steps for soft failures, which shows the additional benefit of the novel approach. Thus, comparison can only be performed for hard failures. The most recent approach in [17] achieves a mean deviation of 0.165% for the failure localization is given with their approach. The novel approach in this paper achieves a mean deviation of 0.77% for failure localization on hard failures. The novel approach as well as the approach in [17] achieve a classification accuracy of 100% for hard failures. In addition to this comparison, the novel approach can handle soft failures, which is not fulfilled from existing approaches. The approach delivers promising results across the different tasks also for soft failures. Nevertheless, the different steps within the approach have to be refined and optimized further.

V. CONCLUSION AND OUTLOOK

To handle the increasing complexity of failure analysis for electronic devices, a new hybrid modeling approach is introduced, which uses data-driven and knowledge-based methods to obtain an advanced failure analysis:

- Existing approaches for TDR are compared. They showed the need for an advanced approach for the intelligent analysis of the failure for complex devices.
- A new hybrid approach for the localization, classification and characterization of a failure is introduced.
- The presented approach is realized for a first use case, where different hard and soft failures on a microstrip line are simulated for TDR signals.
- The hybrid modeling approach can identify a failure. In case of a failure, it is located and classified. When a soft failure exists, this failure is characterized and the corresponding parameters of the soft failures are estimated.

Future work will take a deeper look into the different steps of the hybrid modeling approach. Further approaches, as well as data processing techniques, shall be investigated and evaluated for the different steps. Additionally, the approach will be transferred on measurement data to evaluate the performance there as well as with other DuTs. Measurements are planned with SiC transistors. Further, the approach shall also be transferred to other failure analysis techniques (e.g. SAM data) to prove the generalization capabilities.

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