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# <Training of the Language Model> <PikabERT>

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## **Abstract**

Infineon's Failure Analysis department examines the produced chips for errors in production and also deals with customer complaints. There are over 2,000 types of chips, which differ only minimally in layout. For the analysis, microscopes, lasers and X-Ray equipment is used. The department makes a very important contribution to the quality assurance of products at Infineon. If a product is not working properly, the resulting error code can be determined and the now called target product is sent to the failure analysis (FA) laboratory. Detection and localization of faults in semiconductors is a knowledge-intensive and tedious task. To increase the chances of success, an electrical engineer should be able to get all available information about the samples of similar past jobs. Various support systems used in Failure Analysis (FA), like databases, wikis, or file shares, often have this information stored as documents describing previous analysis reports of similar samples, best practices, specifications, customer reports, etc. However, accessing knowledge contained in these documents can be problematic, since in most cases, such support systems only provide rudimentary search functionality, like keyword matching. As a result, to find relevant information about jobs similar to the considered one, an engineer must query multiple systems, manually evaluate returned reports looking for similar characteristics, and asserting the value of each document for the current problem.

Modern Natural Language Processing methods (NLP) already showed their efficiency in various applications, including automatic translators, Recommender Systems or chatbots. Among these applications, text classification is one of the most promising to solve the FA search problem by automatically associating labels with a report denoting physical or electrical faults described in it, applied methods and tools, etc. The engineers can then use these labels to perform various tasks, like identifying similar jobs or getting statistics on possible faults, tools, or methods.

This is why one of the first applications of Artificial Intelligence (AI) tools at the FA laboratory of Infineon consisted on a classifier of the FA reports, using word2vec embeddings and clustering models, which satisfactory results.

With the apparition of more sophisticated tools in NLP during the last few years, the development of Transformer models until the publication of BERT, the results obtained by these models surpass anything utilized in previous times in almost every field where Transformers have been tested.

## **Zusammenfassung**

Die Fehleranalyseabteilung von Infineon untersucht die produzierten Chips auf Produktionsfehler und kümmert sich auch um Kundenreklamationen. Es existieren über 2.000 Chiptypen, die sich nur minimal im Layout unterscheiden. Für die Analyse werden Mikroskope, Laser und Röntgengeräte verwendet. Die Abteilung leistet einen sehr wichtigen Beitrag zur Qualitätssicherung der Produkte bei Infineon. Funktioniert ein Produkt nicht richtig, kann der resultierende Fehlercode ermittelt und an das FA-Labor gesendet werden. Das Erkennen und Lokalisieren von Fehlern in Halbleitern ist eine wissensintensive und langwierige Aufgabe. Um die Erfolgchancen zu erhöhen, sollte ein Elektroingenieur in der Lage sein, alle verfügbaren Informationen über ähnliche vergangene Jobs zu erhalten. Verschiedene Unterstützungssysteme, die in der Fehleranalyse (FA) verwendet werden, wie Datenbanken, Wikis oder Dateifreigaben, haben diese Informationen oft als Dokumente gespeichert, die frühere Analyseberichte ähnlicher Proben, Best Practices, Spezifikationen, Kundenberichte usw. beschreiben. Jedoch kann das Zugreifen auf das enthaltene Wissen in diesen Dokumenten problematisch sein, da solche Unterstützungssysteme in den meisten Fällen nur rudimentäre Suchfunktionen, wie z. B. Keyword-Matching, bereitstellen. Um relevante Informationen zu Jobs zu finden, die dem betrachteten ähnlich sind, muss ein Ingenieur daher mehrere Systeme abfragen, zurückgegebene Berichte manuell nach ähnlichen Merkmalen auswerten und den Wert jedes Dokuments für das aktuelle Problem bestätigen.

Moderne Methoden der Verarbeitung natürlicher Sprache (NLP) haben ihre Leistungsfähigkeit bereits in verschiedenen Anwendungen unter Beweis gestellt, darunter automatische Übersetzer, Recommender-Systeme oder Chatbots. Unter diesen Anwendungen ist die Textklassifizierung eine der vielversprechendsten, um das FA-Suchproblem zu lösen, indem Etiketten automatisch mit einem Bericht verknüpft werden, der darin beschriebene physikalische oder elektrische Fehler, angewandte Methoden und Werkzeuge usw. bezeichnet. Die Ingenieure können diese Etiketten dann zur Durchführung verwenden verschiedene Aufgaben, wie das Identifizieren ähnlicher Jobs oder das Abrufen von Statistiken über mögliche Fehler, Werkzeuge oder Methoden. Aus diesem Grund bestand eine der ersten Anwendungen von Tools für künstliche Intelligenz (KI) im FA-Labor von Infineon in einem Klassifikator der FA-Berichte unter Verwendung von word2vec-Einbettungen und Clustering-Modellen, die zufriedenstellende Ergebnisse lieferten.

Mit der Entstehung immer ausgefeilterer NLP-Tools in den letzten Jahren, der Entwicklung von Transformer-Modellen bis zur Veröffentlichung von BERT, übertreffen die Ergebnisse dieser Modelle alles, was in früheren Zeiten in fast allen Bereichen, in denen Transformers getestet wurden, verwendet wurde.

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# Table of Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Problem Definition . . . . .	1
1.1.1	Research Questions . . . . .	2
<b>2</b>	<b>Literature Review</b>	<b>3</b>
2.1	Natural Language Processing . . . . .	3
2.1.1	Tokenization . . . . .	3
2.2	Transformer . . . . .	4
2.3	Evolution of Language Models . . . . .	4
2.3.1	BERT . . . . .	4
2.3.2	Difference from BERT and word2Vec . . . . .	5
2.3.3	From BERT to SciBERT . . . . .	5
2.4	Masked Language Modelling . . . . .	5
2.5	Named Entity Recognition . . . . .	5
<b>3</b>	<b>Analysis</b>	<b>7</b>
3.1	BERT based Language Models . . . . .	7
3.2	Finding the Model Entrypoint . . . . .	7
<b>4</b>	<b>Data Collection</b>	<b>11</b>
4.1	Data Sources . . . . .	11
4.1.1	Failure Analysis Ontology and Reports . . . . .	11
4.1.2	S2ORC Dataset . . . . .	12
4.1.3	Infineon Dataset . . . . .	13
4.1.4	Additional Data . . . . .	13
4.2	Data Preprocessing . . . . .	13
4.2.1	Data Cleaning . . . . .	14
4.2.2	Dataset Formatting . . . . .	15

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<b>5 Experiments</b>	<b>17</b>
5.1 Tokenization of the dataset . . . . .	17
5.2 Training of the Tokenizer . . . . .	19
5.2.1 Extending the tokenizers vocabulary . . . . .	19
5.2.2 Pre-Training the tokenizer . . . . .	19
5.3 Training Process . . . . .	20
5.3.1 Moving the bias towards FA domain . . . . .	21
5.3.2 Trying different types of losses . . . . .	23
5.3.3 Changing the Masking Method . . . . .	25
<b>6 Results</b>	<b>29</b>
6.1 Performance Measures . . . . .	29
6.2 Discussion of Results . . . . .	29
<b>7 Conclusion</b>	<b>31</b>
7.1 Future Work . . . . .	31
<b>Bibliography</b>	<b>33</b>

# 1 Introduction

Infineon technologies Austria is one of the leading semiconductor companies worldwide. With around 4,820 employees, the company makes an important contribution to shaping the digital and networked future. Through the development of microelectronics and their constant improvement, Infineon enables efficient energy management, intelligent mobility and secure, seamless communication.

Introduction to failure analysis

Failure Analysis process?

Detection and localization of faults in semiconductors is a knowledge-intensive and tedious task. To increase the chances of success, an electrical engineer should be able to get all available information about the samples of similar past jobs. Various support systems used in Failure Analysis (FA), like databases, wikis, or file shares, often have this information stored as documents describing previous analysis reports of similar samples, best practices, specifications, customer reports, etc. However, accessing knowledge contained in these documents can be problematic, since in most cases, such support systems only provide rudimentary search functionality, like keyword matching. As a result, to find relevant information about jobs similar to the considered one, an engineer must query multiple systems, manually evaluate returned reports looking for similar characteristics, and asserting the value of each document for the current problem.

Modern Natural Language Processing methods (NLP) already showed their efficiency in various applications, including automatic translators, Recommender Systems or chatbots. Among these applications, text classification is one of the most promising to solve the FA search problem by automatically associating labels with a report denoting physical or electrical faults described in it, applied methods and tools, etc. The engineers can then use these labels to perform various tasks, like identifying similar jobs or getting statistics on possible faults, tools, or methods.

This is why one of the first applications of Artificial Intelligence (AI) tools at the FA laboratory of Infineon consisted on a classifier of the FA reports, using word2vec embeddings and clustering models, which satisfactory results.

goal of the project

## 1.1 Problem Definition

The goal of this project is to develop a FA report classifier with a BERT model. In order to do so, the task has been divided into two phases:

First, we have developed a Language Model based on the state-of-the-art model BERT. Therefore we had to consider our specific domain and select the most appropriate model for our domain. Since many successors of BERT have been developed but none of them aimed at the electrical domain, we had to select a model as close as possible to our field of study in order to achieve a satisfying performance later.

Second, we focused on defining the structure of the classifier, which consisted on the BERT network and additional classification layers. To test the results, we have defined a series of classification problems based on the FA reports.

Given the nature of this project the two phases were developed in parallel so the joint performance hasn't been tested yet.

### 1.1.1 Research Questions

This thesis will address the following research questions:

- What kind of BERT models already exist
- How well do they fit to the Infineon semiconductor domain
- What data to use for further training
- Evaluation of the resulting model

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#### general structure of the project

In order to fulfill this goal, an innovative language model trained on the semiconductor domain had to be developed. Therefore it was necessary to find an existing language model to use it as entry point and further train it on a domain specific dataset to achieve the desired results. This specific dataset had to be collected by myself and transformed into a shape which allows to train a BERT based language model.

#### Structure of the thesis

#### The following chapters

## 2 Literature Review

### 2.1 Natural Language Processing

Communication and the sharing of knowledge is an essential part of human society. History has shown that the best way to transmit knowledge is in writing. It is not difficult for a person to learn to read and to understand the context in texts. For computers, this task is much more difficult. Natural Language Processing (NLP) is a subfield of Artificial Intelligence (AI) which deals with teaching computers to understand and interpret human language and has emerged in 1940. The initial need of NLP was the translation from one language into another which was used during the second world war. Nowadays it is widely used in health care, spam detection, sentiment and cognitive analysis. NLP also provides computers with the ability to read text, hear speech, and communicate with humans. Every person had contact with a NLP device at least once in their life. The best example everyone might know are personal assistants like Siri or Alexa. These are applications which work with NLP and have learned to communicate with humans and nearly seem humanely.

Generally speaking, NLP breaks down language into shorter, more basic pieces, called tokens (words, periods, etc.) which get saved as vectorial representations. The technique of mapping words to real vectors is called word embedding. To understand the relationships of the tokens, the model gets trained by predicting some hidden part of the text using some other part of their surrounding text. One way to calculate the representations of the vectors is the method *Word2Vec*. Until BERT has emerged, Word2Vec was the most common technique to create word embeddings. It is a two-layer neural network which processes text and turns it into a numerical form that can be understood by deep neural networks. Given enough data, Word2vec can make highly accurate guesses about a word's meaning based on past appearances. Those guesses can be used to establish a word's association with other words. The difference between Word2Vec and BERT will be covered in Section 2.3.1.

#### 2.1.1 Tokenization

Texts cannot be processed by ML models directly. Tokenization is a method that transforms sequences of characters into a sequence of integers. As an example we can take the sentence:

"This is a cat."

A tokenization transforms this sentence into ['This', 'is', 'a', 'cat']. Punctuations will be removed. This step is important to help the model understanding the meaning of a text. The model can

- Count the number of words in the text
- Count the frequency of the word, that is, the number of times a particular word is present

In modern LMs, tokenizers are trained together with the model to identify the best possible transformations, which can happen on both word and sub-word levels. The set of obtained tokens determines the vocabulary of an LM. If a word appears in the vocabulary of LM, it can be represented as a vector in the target space. Otherwise, a word is split into parts until each of them can be mapped to a set of tokens from the vocabulary. In the worst case, a word is split into individual letters. Such splitting may significantly reduce the quality of word embeddings in the vector space, thus reducing the quality of features extracted for the classification layers of a network. Therefore, it is essential either to select an LM whose vocabulary provides good coverage of the main terms used in an application domain or to extend the vocabulary of an LM with these terms and fine-tune it on domain-specific texts.

## 2.2 Transformer

The transformer in the field of NLP is a new architecture which is able to solve sequence-to-sequence tasks while handling dependencies in the text. Transformers basically consist of an encoder and a decoder. The encoder reads the input text and the decoder produces a prediction. Transformers work in small increments. In each step, an attention mechanism is applied to understand the relationships between the words in a sentence, regardless of their positions.

## 2.3 Evolution of Language Models

### 2.3.1 BERT

BERT stands for Bidirectional Encoder Representations from Transformers. It makes use of a transformer and an attention mechanism that learns contextual relations between words or sub-words in a text. The BERT model was developed by Google and is already pre-trained using a combination of masked language modeling objective and next sentence prediction on a large corpus comprising the Toronto Book Corpus and Wikipedia. In contrast to previous language models which looked at a text sequence either from left to right or combined left-to-right and right-to-left training, BERT is using the bidirectional approach. The paper's results show that a language model which is bidirectionally trained can have a deeper sense of language context and flow than single-direction language models. To do this, the authors introduced a new technique which is called Masked Language Modelling (MLM).

A Transformer usually includes two separate mechanisms, an encoder that reads the text input and a decoder that produces a prediction for the task. For producing a language model, only the encoder mechanism is necessary. Previous models have read the text input sequentially either left-to-right or right-to-left. BERT's transformer encoder reads the entire sequence of words at once. This allows the model to learn the context of a word based on all of its surroundings [?].

The input to BERT's encoder is a sequence of tokens previously converted into vectors. Later, these tokens can be processed in the neural network. In order to be able to do this, however, a few steps must first be carried out:

1. CLS and SEP tokens at the beginning and end of each sentence
2. Segment embeddings for each token to distinguish between sentences.

3. Position embeddings for each token to identify the position in a sentence.

### 2.3.2 Difference from BERT and word2Vec

Word2Vec is context-independent, so it only has a numeric vector to represent a word. If a word has several meanings, these are combined into a vector.

BERT, on the other hand, is context-dependent and thus allows multiple numeric vectors as a representation for a word, depending on the context in which the word occurs.

An example of the difference is the word bank, which can appear in a financial context as well as in a beach or park context. Word2Vec will always generate the same vector for this word and can therefore lead to an inaccurate representation. BERT can distinguish the two different semantic meanings and thus also generate two different vectors.

1. The next difference is that Word2Vec doesn't care about the position of words in a sentence. BERT, on the other hand, uses the position (index) of a word as input for calculating the vector.
2. Word2Vec only needs one word as input and delivers a vector as output. BERT, on the other hand, needs an entire sentence as input because it needs the context of the sentence to calculate the vector.
3. Word2Vec can have problems if a word is not stored in the vocabulary and no vector can be generated. BERT can also create a vector for subwords that are not stored in the vocabulary and is therefore not limited by the vocabulary.

### 2.3.3 From BERT to SciBERT

The development of BERT was a milestone in Natural language processing. Since the vocabulary of BERT is restricted, the application of the model in some domains does not lead to a satisfactory performance. To achieve this goal in different scientific fields, the model of BERT got adapted to SciBERT. The SciBERT model follows the same architecture as BERT but is instead pre-trained on scientific text. The corpus consists of 1,14M papers derived from *Google Scholar*, 18% papers from the computer science domain and 82% from the broad biomedical domain. The authors used the full text of the papers instead of only the abstracts. The average paper length is 154 sentences which results in 2.769 tokens. The final corpus size has 3.17B tokens, similar to the 3.3B tokens on which BERT was trained [?].

The S2ORC-SciBERT is a SciBERT model which was further trained on the S2ORC dataset presented above. It got published simultaneously with the dataset itself from the same developers. Compared to SciBERT it has a wider corpus including 20 different domains like Computer Science, Mathematical Science and Engineering which could be beneficial for the FA domain. However it was also trained on Medical and Biology data which again could be a drawback for the model as with SciBERT.

## 2.4 Masked Language Modelling

## 2.5 Named Entity Recognition





## 3 Analysis

This chapter will cover the first two research questions about existing BERT models and how well they fit to the semiconductor domain. In this way we were able to find a suitable entrypoint for training our FA-BERT model.

### 3.1 BERT based Language Models

### 3.2 Finding the Model Entrypoint

Since BERT models studied in this paper were trained on different text corpora, their tokenizers might provide different coverage of important terms used in the FA domain, such as the ones stored in FA ontology. To determine the coverage, we first analyze the tokenization of the ontology keywords with the three language models: traditional BERT, SciBERT and S2ORC-SciBERT. With this analysis it was possible to gain a first impression about the vocabulary of the models and how well they fit to the electrical domain.

The models got downloaded from the website [Huggingface](#) and can be load into the notebook as follows:

```
model = BertModel.from_pretrained("/path/to/model/")
tokenizer = BertTokenizer(vocab_file = '../path/to/tokeizer/vocab.txt')
```

To receive the keywords, we executed an existing function provided from our supervisor Christian Burner. It executes a script with a request to the SparQL Database receiving the ontology keywords in a list. This keywords also occur in the reports as indicators for the content.

After receiving the keywords from the ontology and having a deeper look at them, we found some misspellings like in the word *flasover*, which misses a h to become *flashover*. These typos could confuse the models and lead to some mistokenization. To prevent this, we will first run some spell checking and correction methods on the keywords before further processing it. Therefore we tried different packages like the *Pyspellchecker* or *SymSpellPy* which are based on the Peter Novig's method. As both of the two packages did not work, we skimmed the keywords manually and corrected misspellings.

With the correct spelled keywords we started the experiment of tokenizing them with the three different BERT models. The code for tokenization was the same for every model:

```
# Run tokenizer.
tokenized_word = s2orc_scibert_tokenizer.tokenize(word)

#differentiate good and badly tokenized words
if len(tokenized_word) == 2:
```

```

        good_tokenized_words_s2orc += 1
        good_words.extend(tokenized_word)
    elif len(tokenized_word_c) > 2:
        badly_tokenized_words_s2orc += 1
        bad_words.extend(tokenized_word)

```

We created a loop which hands every word over to the tokenizers and also analyzes if the resulting word is included in the models vocabulary or not. A word which is already in the vocabulary will not be divided into subtokens and so consists of only one token. If it is not included in the vocabulary, we determined if the word was good or badly tokenized. A word got considered as badly tokenized if it was split in more than two tokens. Otherwise the tokenization got considered as good. At the end of the execution, we created a dataframe depicting how the individual words got splitted into tokens. An example of the dataframe is depicted in Figure 3.1. Here the keyword "lifted clip" would get considered as badly tokenized word and the keyword "requestor" as good.

lifted clip				
	0	1	2	3
0	SciBERT:	lift	##ed	clip

requestor			
	0	1	2
0	SciBERT:	request	##or

Fig. 3.1: Example of tokenization with SciBERT

Next we analyzed the word stems of the failure analysis reports and again examined the tokenization of the words with the language models. We did not analyze the word stems of the whole reports, but only the word stems of the most frequently used words. To obtain the frequency distribution and the word stems of the reports, we used the NLTK (Natural Language Toolkit) library. It includes the so called *SnowballStemmer*, because according to the documentation, this stemmer works better for English text. Stemmers remove morphological affixes from words, leaving only the word stem. To run the tokenization experiment, we also had to lower case the word stems and transform plural words into singles. The code can be seen in the code below. For the tokenization itself, the same code has been used as already explained above.

```

#create a new stemmer
stemmer = SnowballStemmer("english")

#test the stammer on pluralized words
most_common_stems = nltk.word_tokenize(str(most_common))
singles = [stemmer.stem(plural) for plural in most_common_stems]

```

```
word_stems = set(singles)
print(' '.join(singles))
```

As a result of the tokenization of the keywords it can be seen that SciBERT and S2ORC-SciBERT both perform better on the keywords as the traditional BERT model. Both models contain a few more keywords in their vocabulary than the BERT model. The resulting statistic can be seen in Figure 3.2. We expected this result because the training data of these two models fits better to our electrical domain than the data BERT was trained with which is more widespread.

```
#Keywords: 362
#Words in BERT vocabulary: 166
#Words in SciBERT vocabulary: 169
#Words in S2ORC SciBERT vocabulary: 178
```

Fig. 3.2: Comparison of the performance of the three models on the keywords

For the tokenization of the FA reports and their word stems we assumed to see at least a slight difference between SciBERT and S2ORC-SciBERT but without fine-tuning the models it is not possible to determine a better model which can be seen on the results of the tokenization analysis in Figure 3.3.

```
SciBERT:
In vocabulary: 39
Good tokenized words: 7
Badly tokenized words: 1
S2ORC-SciBERT:
In vocabulary: 39
Good tokenized words: 7
Badly tokenized words: 1
```

Fig. 3.3: Comparison of the performance on the word stems

In order to finally decide between SciBERT and S2ORC-SciBERT, a further analysis was performed in which the keywords were assigned a weighting based on their occurrence frequency. This makes it possible to assign an importance to the keywords. The more often they appear in the reports, the more important it is that the model tokenizes the keywords well. Therefore, using the frequency and the number of subtokens, a weight is calculated as follows:

$$n = |t_1, t_2, \dots, t_n| \quad (3.1)$$

$$\rightarrow w = n \cdot sx_m \quad (3.2)$$

The resulting weights looked like the following:

```
[('thin', 0.002654), ('backside', 0.062375), ('metallization', 0.12209), ...]
```

After this weighting we again performed a tokenization and examined the good and badly tokenized keywords, but both models performed again very similar. SciBERT tokenized 129 keywords good, S2ORC-SciBERT 120. Because the FA reports contain out of more than only keywords, we decided to choose the S2ORC-SciBERT as an entrypoint for our further exper-

iments. It has more electrical and physical papers in its training corpus than the original SciBERT and therefore might work better for us.

## 4 Data Collection

In order to train a language model, a sufficiently large amount of data is needed. Since the model presented in this paper will be used for textual classification, the data must be available in written form. Most of the data used for the report classification come from the FA laboratory. The laboratory has two sources to save information: an ontology which is the formalization of FA knowledge in a computer-friendly format, and the FA reports which comprise information that describes all diagnostic steps, results, and observations for a job analysis. These two resources would have a large enough amount of data to train the model. However, experiments with previous models indicated that these documents are too specific to serve as the sole data source for a model in the semiconductor domain. The content of the documents in the ontology and the FA reports contains too specific vocabulary and too little general vocabulary about electronics and semiconductors. Models which were trained only with this data did not have sufficient performance. For this reason, additional sources were sought to train the model more extensively. This chapter starts by introducing the individual datasets and how they got collected before covering the data cleaning process to prepare it as an input for the PikaBERT model.

### 4.1 Data Sources

The remaining dataset was created out of different data sources which got categorized in four datasets for an easier use in later experiments. The four datasets are: the *FA ontology and reports*, the *S2ORC Dataset*, the *Infineon Dataset* and the *Additional Dataset*. The following chapters introduce every dataset with its content, size and characteristics.

#### 4.1.1 Failure Analysis Ontology and Reports

The FA laboratory stores most of its knowledge as free texts, thus they might be ambiguous and cannot be processed by the software automatically. To avoid these issues, standard definitions of FA concepts used in the domain are required. Moreover, these definitions must be stored in a way that they can be used by both engineers and software tools alike. One possible solution to this challenge is to formalize the knowledge about the FA domain as an ontology, a knowledge base specifically designed to store terminological definitions. This is the case for the FA laboratory, where an ontology is being developed, currently storing hundreds of failures, tasks, tools, etc. The structure of an ontology includes classes, instances of these classes and properties. Individuals are descriptions of real-world entities, like sample integrated circuits of a job or tools available in a lab. Classes are defining parts of the world by summarizing properties of a collection of individuals.

For training the classification models, we have considered the historical data of the FA laboratory. These reports contain a series of fields, including the job identification number, customer comment regarding the issues found in devices, an analysis report describing applied methods, found physical defects, their locations, electrical characterization, and other details. Some of this data is structured and can be retrieved from corresponding databases. However, the essential parts relevant to the fault identification process are described only in textual form and, therefore, cannot be processed automatically. Consider three samples taken from fault analysis reports of an FA Laboratory presented in Error! Reference source not found.. The examples show selected sentences describing the findings of an engineer and the labels indicating the physical faults and their electrical signatures. Both types of labels are organized in an ontology, which is a hierarchical structure representing a taxonomy of faults. This ontology allows for the development of software tools helping to label reports manually and working with the classification results. Along with the job summary, the reports contain a series of fields including, an identification number of the device, lists of tasks performed on the device, the images obtained by certain tools such as X-Ray, the description of such images attached, etc. A subset of the reports also includes fault labels, both of the electrical signature of the faulty device and of the final physical failure. For the classification phase, these two faults are considered the target output while the job summary and image descriptions will constitute the input.

#### 4.1.2 S2ORC Dataset

The S2ORC Dataset was collected by the Allen Institute of Artificial Intelligence and it has a corpus of 81.1M English-language academic papers from different domains. Around 40% of the papers belong to the biomedical field, as in Figure 4.1. The texts got extracted from PDFs including abstracts and inline mentions of citations. The S2ORC-SciBERT is a SciBERT model which was further trained on the S2ORC dataset presented above. It got published simultaneously with the dataset itself from the same developers. Compared to SciBERT it has a wider corpus including 20 different domains like Computer Science, Mathematical Science and Engineering which could be beneficial for the FA domain. However, it was also trained in Medical and Biology data which again could be a drawback for the model as with SciBERT.

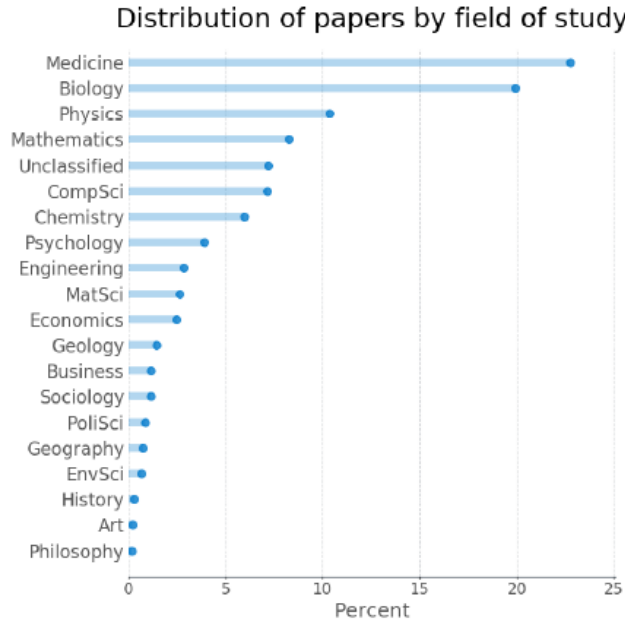


Fig. 4.1: Different Domains in the S2ORC Dataset.

#### 4.1.3 Infineon Dataset

In addition, we created an Infineon Dataset comprising relevant textual data available on the company's intranet. This dataset comprises 1,687 papers covering research topics and best-practices methods in the semiconductor domain. It was collected by employees and engineers of Infineon. Because these papers got collected from engineers in different countries, we had to filter out non-English language papers. After filtering and extracting the raw text, we used approximately 31.5MB of text data to create a dataset.

#### 4.1.4 Additional Data

To increase the specificity of the training data for the FA domain, we also searched the Web for FA and electrical engineering papers. In this work we were using open search engines, like FreeFullPDF and GoogleScholar, as well as specific sources, like IEEE, to collect the data. The text was extracted from the papers and converted into a text representation. The resulting dataset comprises 12.31MB of raw text, where 2.33MB got collected from FreeFullPDF and Google-Scholar and the other 9.98MB from IEEE.

## 4.2 Data Preprocessing

For later usage during training, we combined the Infineon and the Additional Datasets in one. Moreover, since the biggest part of the S2ORC Dataset was medical and biomedical data, we filtered this dataset by using the FA ontology keywords, retaining only documents that comprise at least one keyword. The resulting filtered dataset contains approximately 542MB of raw text. For later discussions, we introduce the following abbreviations for the datasets:

- **inf**: Infineon Dataset + Additional Dataset;

- **s2:** a part of the documents from S2ORC dataset filtered on keywords extracted from the ontology.

After finishing collecting the papers for the dataset, it was necessary to extract the raw text out of the documents. Therefore we got access to a text extractor API developed by Infineon colleagues in Bangalore. The raw texts got extracted and UTF8 converted to be saved as excel sheets.

Not all of the extracted text is important or useful for the dataset. To remove unuseful data, a notebook was created where the text got prepared before being cleaned. Authors, metadata about the images, tables and other not contiguous text was removed. The resulting text got again saved as excel sheets.

### 4.2.1 Data Cleaning

To use the FA reports for AI purposes, their content must be pre-processed and cleaned to erase all data that can disrupt the training process. One of the biggest issues regarding the FA reports is the wide variety of styles in which they are written, as they come from several laboratories around the globe, some of them dealing with specific purposes, while others deal with a broader range of failures. It is also essential to consider that although all they are written in English, this is not a standard language as engineers are only rarely native speakers.

The data cleaning process was the same for all datasets. A notebook was created where the excel sheets got loaded into dataframes. The methods used for cleaning the text are imported from the **Natural Language Toolkit (nltk)** package which implements functions for normalization, stemming and lemmatization. The following steps describe the procedure of text cleaning:

1. **Remove Punctuations and Special Characters:** Punctuations and special characters got removed inbetween and at the end of every sentence by using regular expressions because a language model is not able to interpret those characters.
2. **Remove Numbers:** The input got checked if it is a number or not. Also all words which are not strictly all letters got removed to avoid confusing the model.
3. **Normalization:** After removing undesired words and characters, the entire text got normalized. This means that the resulting text contains only out of lowercased letters.
4. **Remove Stop-Words:** The nltk package contains a collection of english stop-words like "and", "or", "but", "for" etc. Due to their low entropy they are useless for the training and therefore removed from the text.
5. **Lemmatization:** Lemmatization considers the context of a word and converts it to its meaningful base form, which is called Lemma. For instance, lemmatizing the word "Caring" would return "Care". This has been done for the entire dataframe by iterating over the words.
6. **Remove Empty Lines:** Due to the previous cleaning some cells or lines of the dataframe may be empty now and represented as NaN values in the dataframe. These NaN values have to be replaced with spaces, otherwise they will cause errors during further processing.



### 4.2.2 Dataset Formatting

In comparison to traditional neural networks, BERT-based models are like a black box for the engineer. For training the model we used the so-called “transformer” class from [Huggingface](#). The `train` method of the `transformer` class needs a model, a tokenizer and the training dataset as input. This input dataset needs to have a specific format and datatype otherwise the function would rise an error. To do so the previous created dataframes got converted into dataframes of two cells, an index and a text cell. An example is shown in Table 4.1.

	text
0	The following parameters are most often considered...
1	Nitrogen fertilization stands out as an important...

Tab. 4.1: Example of transformed dataframe shape

The base class *Dataset* from Huggingface implements a Dataset backed by an Apache Arrow table. This type of object can be created out of the dataframe just created with the following code:

```
train_dataset = Dataset.from_dict(df)
datasets = datasets.DatasetDict({"train:" train_dataset})
```

The dataset object allows to specify a training and a test dataset. Since training the language model is an unsupervised learning method, only the training dataset is needed. The resulting dataset objects were saved and could be loaded later for training.

[Tokenizing dataset split into blocks](#)



## 5 Experiments

In this section we will cover the process of preparing the collected dataset, described in section 4 and training different types of tokenizers and language models until we found the best performing one.

### 5.1 Tokenization of the dataset

In order to use the dataset created earlier in the chapter 4 for the BERT based model as training input, it must be transformed into a suitable format. Since we are using the Huggingface trainer, we also need to follow the Huggingface training data format.

In the first step, the entire text from the CSV file is converted into a dataset dictionary. This is possible with one line of code after importing the datasets package.

Listing 1: Creating the Dataset Dictionary

```
from datasets import Dataset
training_data = Dataset.from_dict(df)
datasets = datasets.DatasetDict({"train": train_data})
```

When using this method, training and test data can be stored together in one object and accessed via the `datasets["train"]` or `datasets["test"]` index. The resulting `datasets["train"]` dictionary has the feature "text" to access the data and 1.052.587 rows as visible in the output depicted in Figure 5.1.

```
Dataset({
  features: ['text'],
  num_rows: 1052587
})
```

Fig. 5.1: Format of Dataset Dictionary

The next step is to apply the tokenizer to the entire text. For this we use the map method from the datasets library. First we define a method shown in Listing 2 which calls the tokenizer on the text.

Listing 2: Tokenize Function to call on the text

```
def tokenize_function(examples):
    return tokenizer(examples["text"])
```

The map function, shown in Listing 3, can be used to apply the tokenizer function from Listing 2 to the entire dataset. To speed up the process, we pass the `number_poc=4` attribute, which enables multithreading and splits the process into four threads.

Listing 3: Applying the tokenize function on the Text

```
tokenized_datasets = datasets.map(tokenize_function, batched=True, num_proc=4,
                                remove_columns=["text"])
```

The "text" column from the dictionary has now been replaced by the `input_ids` which is needed by the model as an input for training.

```
DatasetDict({
  train: Dataset({
    features: ['input_ids', 'token_type_ids', 'attention_mask']
    num_rows: 1052587
  })
})
```

Fig. 5.2: Text column has been replaced by calling tokenizer on the dataset.

After the dataset has been tokenized, the next step is to split it into individual chunks. The size of these chunks depends on the available resources and the maximum context size of the model. The context size can be determined with the method `model_max_length`. For BERT based models, like ours, it is 512 tokens. We need to concatenate all of our texts together and then split the result in small chunks of a certain `chunk_size`. To do this, we will use the `map` method again, with the option `batched=True`. This option actually lets us change the number of examples in the datasets by returning a different number of examples than we got. This way, we can create our new samples from a batch of examples.

First, we grab the maximum length our model was pretrained with. This might be a bit too big to fit in our GPU RAM. In the first try we chose a chunk size of 64, which turned out not to be suitable because longer sentences were truncated, while shorter sentences were populated with [PAD] tokens (id: 0) until they reach the desired length. Using a small chunk size can be detrimental in real-world scenarios, so it is recommended to use a size that corresponds to the use case the model will be applied to. Because of that we chose a chunk size of 128.

Listing 4: Definition of the method `group_text`

```
chunk_size = 128
```

```
def group_texts(examples):
    # Concatenate all texts
    concatenated_examples = {k: sum(examples[k], []) for k in examples.keys()}
    # Compute length of concatenated texts
    total_length = len(concatenated_examples[list(examples.keys())[0]])
    # We drop the last chunk if it's smaller than chunk_size
    total_length = (total_length // chunk_size) * chunk_size
    # Split by chunks of max_len
    result = {
        k: [t[i : i + chunk_size] for i in range(0, total_length, chunk_size)]
```

```

        for k, t in concatenated_examples.items()
    }
    # Create a new labels column
    result["labels"] = result["input_ids"].copy()
    return result

```

## 5.2 Training of the Tokenizer

Also the tokenizer itself can be improved before using it in the training method together with the model. Training a tokenizer can be done in two ways:

1. Extending the vocabulary manually
2. Pre-training the tokenizer

Tokenizers of BERT-derived models usually have empty positions allowing us to add required tokens directly. Extending the vocabulary of a tokenizer means that it won't get trained explicitly but important words like our ontology keywords can be added to the vocabulary of the tokenizer and therefore recognized as one single token by the model later. Pre-training the tokenizer means that the tokenizer will get trained on a prepared dataset without using the model. Again the engineer has no impact on the behavior of the tokenizer during the training loops. We created four types of trained tokenizers. For later discussions we introduce the following abbreviations:

- **ext**: A tokenizer with the ontology keywords added to its vocabulary manually
- **small**: A tokenizer trained on inf dataset
- **large**: A tokenizer trained on inf+s2 dataset;
- **fit**: A tokenizer trained on the s2 dataset

### 5.2.1 Extending the tokenizers vocabulary

For the first experiment we tried to enhance the language models performance by extending the tokenizers vocabulary. The tokens which we added to the vocabulary were the ontology keywords. As already discussed in the [section before](#), some of the keywords included misspellings. We again removed or corrected these keywords to avoid to sabotage our model.

Before extending the tokenizer, it's vocabulary had a size of 31944. To add the keywords to the tokenizers vocabulary, we had to execute the following code:

Listing 5: Extending the Tokenizer Vocabulary

```

for keyword in keywords:
    tokenizer.add_tokens(keyword)

```

The keywords got added to the vocabulary and increased the vocabulary size to 32131. After saving the tokenizer it can be used in the training process like any other pretrained tokenizer.

### 5.2.2 Pre-Training the tokenizer

Training a tokenizer is very simple with the [huggingface](#) methods. To train a tokenizer we first need to create a training dataset again. This dataset should have the same format as already

described in chapter 4. For our experiments, we assembled four different datasets to train four tokenizers. These were then to be trained together with the language model in different tests. The different data sets were used for testing purposes to find the best possible model.

### creating of the training corpus

After creating the training corpus, the tokenizer can be trained with one single line of code. The `train_new_from_iterator` method needs the training corpus and the new vocabulary size as an input. We chose the highest possible vocabulary size, which is 52.000.

Listing 6: Training the Tokenizer and resize Vocabulary

```
tokenizer = old_tokenizer.train_new_from_iterator(training_corpus, 52000)
```

After training the tokenizer with the smaller training corpus, it tokenized the ontology keywords into 542 tokens instead of 661, which means an improvement in performance.

## 5.3 Training Process

The training process for all of the following experiments is the same and will be described below. After creating the training data as described in section ??, it is necessary to prepare some requirements for the training process. The whole training is executed on the HPC Cluster, described in section ??, to ensure the training can be executed as fast as possible. Most of the training code got copied from the huggingface notebook. The relevant code is described in the section Masked Language Modeling. It also includes the process of how to chunk the training dataset into a specific block size which is needed by the model as an input. We adapted the code regarding to our needs.

The training itself contains out of the five steps:

1. Defining the model and tokenizer checkpoints
2. Chunking the dataset into blocks
3. Defining the training arguments
4. Defining the Huggingface Trainer
5. Call the train method

Defining the model and tokenizer checkpoints can be done in the same way as shown in the code ?. The chunking of the dataset is described in section ?. The training arguments are variables which are needed by the trainer object. Here different values like the learning rate, the name of the model and how to report the logging can be set.

Listing 7: Creating the Training Arguments

```
training_args = TrainingArguments(
    "checkpoint_LM_s2_s2orc",
    evaluation_strategy = "epoch",
    learning_rate=2e-5,
    weight_decay=0.01,
    report_to="tensorboard",
    logging_strategy="steps"
)
```

Listing 8: Creating the Trainer Object

```

trainer = Trainer(
model=model,
args=training_args,
train_dataset=lm_datasets["train"],
data_collator=data_collator,
)

```

The training can be started by calling the method `train()` from the `transformers trainer object`.

Listing 9: Starting the training

```

trainer.train()

```

### 5.3.1 Moving the bias towards FA domain

In the first training experiments it was our goal to move the bias of the pretrained S2ORC-SciBERT further towards the semiconductor and failure analysis domain. Therefore we use different datasets.

[describe datasets here](#)

For later discussions and easier use we introduce the following abbreviations:

- inf: Infineon Dataset (FA-reports, FA-papers, IEEE papers, FreeFullPDF papers)
- s2: S2ORC dataset filtered on keywords

For the first few experiments we used the inf dataset together with the different trained and extended tokenizers explained in section 5.2. The inf dataset should be a good complement to the BERT based model which has already been pre-trained with the S2ORC dataset. With the help of the trained tokenizers, this training material should prepare for the classification of FA reports. We trained the models for 10 epochs and a learning rate of  $2e-5$  as described in Listing 8.

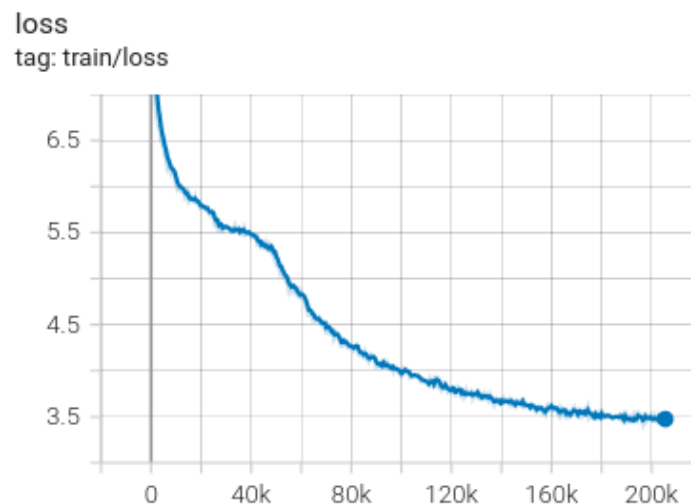


Fig. 5.3: Loss Function during Training with Infineon Dataset and small trained tokenizer.

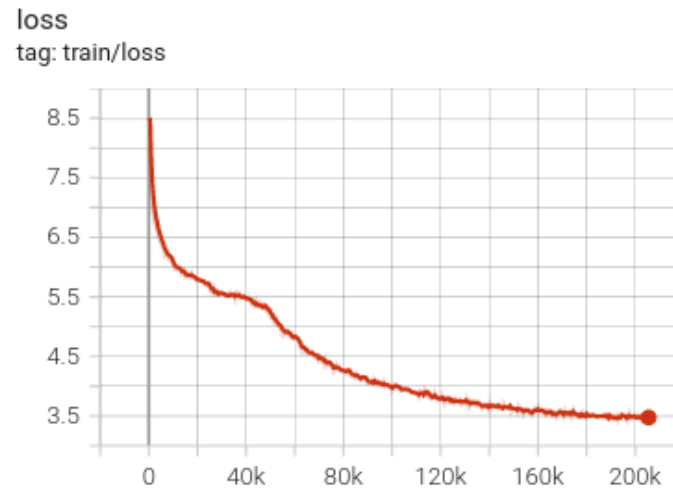


Fig. 5.4: Loss Function during Training with Infineon Dataset and large trained tokenizer.

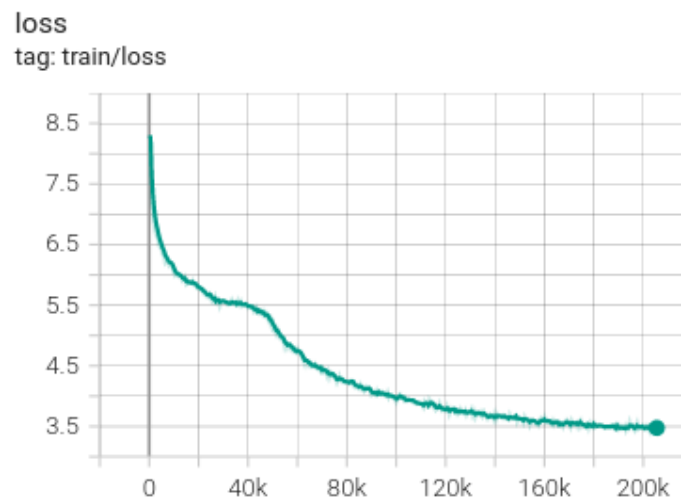


Fig. 5.5: Loss Function during Training with Infineon Dataset and extended tokenizer.



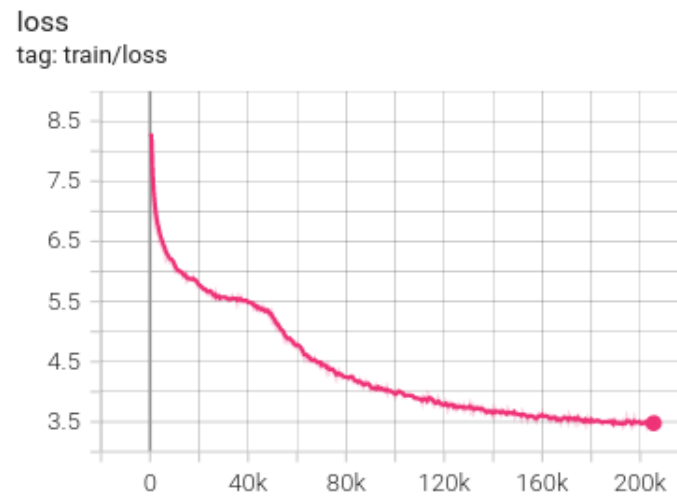


Fig. 5.6: Loss Function during Training with tokenizer trained on s2.

Bild später ersetzen

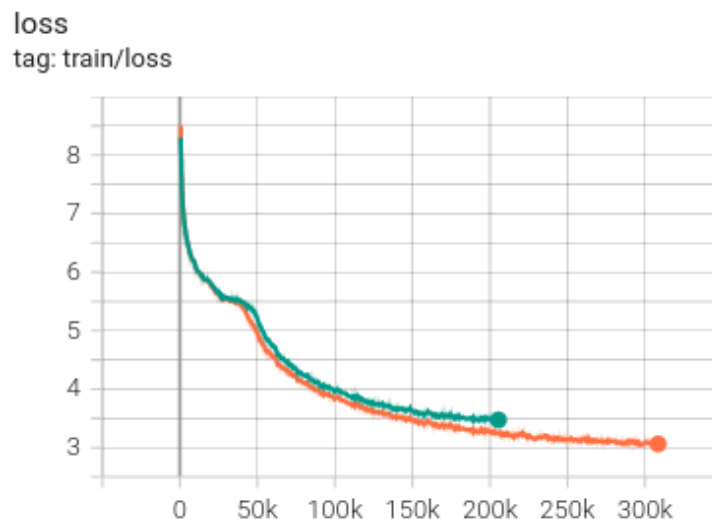


Fig. 5.7: Loss Function during Training with largest dataset and tokenizer trained on large.

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The various loss functions hardly differ from each other. On the basis of the last curve, which was trained for 15 epochs, it can be seen that the longer training could certainly lead to a better performance. Nevertheless, the loss function already flattens out too much in this area. For this reason, further **measures** regarding the improvement of the training were researched.

### 5.3.2 Trying different types of losses

Another attempt to improve the performance of the model is to implement a different loss function. Cross entropy loss seemed to be particularly suitable. In the case of masked language modeling, this metric compares the token predicted by the model with the ground truth and

assigns a value between 0 and 1 to the prediction. 0 stands for a perfect prediction. During training, the values are aggregated to represent the loss function.

The loss function used by the `Trainer` object from `Huggingface Transformers` is shown in Listing 10.

Listing 10: Trainer compute loss function

```
def compute_loss(self, model, inputs, return_outputs=False):
    if self.label_smoother is not None and "labels" in inputs:
        labels = inputs.pop("labels")
    else:
        labels = None
    outputs = model(**inputs)
    # Save past state if it exists
    if self.args.past_index >= 0:
        self._past = outputs[self.args.past_index]

    if labels is not None:
        loss = self.label_smoother(outputs, labels)
    else:
        # We don't use .loss here since the model may return tuples
        # instead of ModelOutput.
        loss = outputs["loss"] if isinstance(outputs, dict) else outputs[0]

    return (loss, outputs) if return_outputs else loss
```

quelle: <https://github.com/huggingface/transformers/blob/v4.17.0/src/transformers/trainer.py#L2006>

which means that, by default, the model itself is responsible for computing some sort of loss and returning it to outputs. To implement an own loss function, we had to overwrite the `Trainer` class and the loss function and defining a cross entropy loss function to return it to outputs. The code is shown in listing 11. We use the cross entropy loss function from `torch.nn` here. In most cases the `CrossEntropyLoss()` function gets some weights as inputs, but because in our case pretraining a BERT model is an unsupervised learning task, we have no weights to assign and leave it empty.

Listing 11: Cross Entropy Loss

```
class MyTrainer(Trainer):
    def compute_loss(self, model, inputs, return_outputs = False):
        labels = inputs.pop("labels")
        outputs = model(**inputs)
        logits = outputs.get("logits")

        loss_fct = nn.CrossEntropyLoss()
        loss = loss_fct(logits.view(-1, tokenizer.vocab_size),
                        labels.view(-1))
        return (loss, outputs) if return_outputs else loss
```

### 5.3.3 Changing the Masking Method

The original masking method which is used by all BERT based models is that every token in an input blocked gets masked by the probability of 15%. **hier fehlt noch was**

Based on the latest experiments, it can be seen that our models are not sufficiently well trained in the semiconductor area. Another attempt to improve the performance is to adjust the masking strategy during the training. After some research we came across the Whole Word Masking strategy. With this method, not only some tokens are randomly masked, but it is also checked whether the token to be masked is a standalone token or a subtoken. If a subtoken, which is part of a word, should get masked, the algorithm also masks all the surrounding tokens that belong to the word. In addition we increased the masking probability from 15% to 20%. The code is visible in Listing 12. Therefore we created a new data collator class **which has the whole word masking method implemented** and handed this data collator to the trainer shown in Listing 13. **nicht vergessen tokenizer map funktion geändert damit word ids im dataset**

```
DatasetDict({
  train: Dataset({
    features: ['input_ids', 'token_type_ids', 'attention_mask', 'word_ids'],
    num_rows: 1052587
  })
})
```

Fig. 5.8: Loss Function during Training with Infineon Dataset and large trained tokenizer.

Listing 12: Data Collator implementing Whole Word Masking

`wmm_probability = 0.2`

```
def whole_word_masking_data_collator(features):
    for feature in features:
        word_ids = feature.pop("word_ids")

        # Create a map between words and corresponding token indices
        mapping = collections.defaultdict(list)
        current_word_index = -1
        current_word = None
        for idx, word_id in enumerate(word_ids):
            if word_id is not None:
                if word_id != current_word:
                    current_word = word_id
                    current_word_index += 1
                mapping[current_word_index].append(idx)

        # Randomly mask words
        mask = np.random.binomial(1, wmm_probability, (len(mapping),))
        input_ids = feature["input_ids"]
        labels = feature["labels"]
        new_labels = [-100] * len(labels)
        for word_id in np.where(mask)[0]:
```

```

word_id = word_id.item()
for idx in mapping[word_id]:
    new_labels[idx] = labels[idx]
    input_ids[idx] = tokenizer.mask_token_id
    feature["labels"] = new_labels

return torch_default_data_collator(features)

```

Figure 5.9 shows an example of how the whole word masking method works. The green examples shows how the algorithm is masking all surrounding subtokens which belong to a word were the blue example show some random picked tokens to mask which do not belong to any other word.

```

'>>> [['[CLS]', 'content', 'downloaded', 'i', '##ops', '##ci', '##ence', 'scr', '##oll', 'text', '[SEP]', '[CLS]',
'download', '[MASK]', 'ip', 'address', '137', '222', '24', '##9', '19', 'content', '[MASK]', '26', '02', '2015',
'19', '34', 'note', 'terms', '[MASK]', 'apply', '[SEP]', '[CLS]', 'high', 'performance', 'microm', '##achi', '##n
ed', 'ga', '##n', 'si', 'high', 'electron', 'mobility', 'transistor', 'back', '##side', 'diamond', '##like', 'car
bon', 'titanium', 'heat', 'dissipation', 'layer', 'view', 'table', 'contents', 'issue', 'journal', 'home', '##pa
', '##ge', '[MASK]', 'appl', 'phys', '[MASK]', '8', '011', '##00', '##1', '[MASK]', 'i', '##ops', '##ci', '##ence
', 'i', '##op', 'org', '188', '##2', '07', '##86', '8', '1', '011', '##00', '##1', 'home', '[MASK]', '[MASK]',
'[MASK]', 'contact', 'i', '##ops', '##ci', '##ence', '[SEP]', '[CLS]', '[MASK]', 'performance', 'microm', '##achi
', '##ned', 'ga', '##n', 'si', 'high', 'electron', 'mobility', 'transistor', 'back', '##side', 'diamond', '##like
', 'carbon', 'titanium', 'heat', 'dissipation', '[MASK]', '[MASK]', '[MASK]', '[MASK]', 'chi', '##u', '##1', '*',
'chi']]

```

Fig. 5.9: Example of Whole Word Masking Method.

Listing 13: Trainer

```

trainer = MyTrainer(
model=model.to(device),
args=training_args,
train_dataset=lm_datasets['train'],
data_collator=whole_word_masking_data_collator,
tokenizer=tokenizer
)

```

We trained the model with the new masking method again for 20 epochs and the same learning rate and weight decay as in the other experiments. The results show a final loss of 2.51, which is the lowest loss in all experiments so far. The loss curve is depicted in Figure 5.10. This model could allow a good performance for the FA classifier after further training epochs.

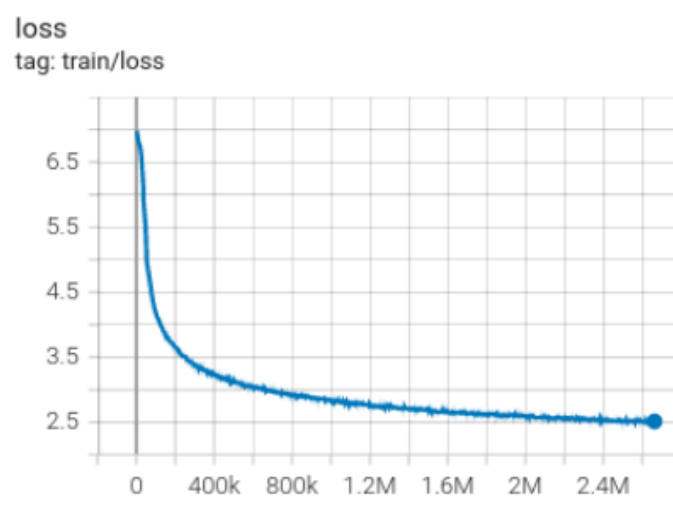


Fig. 5.10: Loss Function during Training with Whole Word Masking.



## **6 Results**

### **6.1 Performance Measures**

### **6.2 Discussion of Results**

Inhalt...





## **7 Conclusion**

From the previous experiments, we can conclude that a BERT-based model was a good choice for the FA model due to the broadly pre-trained training corpus and ease of use. It is also easy to apply and incorporate for the following classification. Since no suitable models exist in the semiconductor domain yet and most of the BERT models were trained with mainly medical and biomedical papers, it was cumbersome to find a suitable model entry point since the medical vocabulary can lead to a degradation of performance on semiconductor texts.

### **7.1 Future Work**



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