STAND-ALONE PROJECT

FINAL REPORT

P23390-N24

Project number

Project title[1]	**Mikroskopische Modellierung von NBTI** **Microscopic Modeling of NBTI**
Project leader	**Tibor Grasser**

1 Short title in English and German language

I. Summary for public relations work

The project's most significant results (scientific advances) from the project leader's point of view should be presented on a single page (DIN A4, 11 pt font, line spacing 1.5) in a way that is comprehensible to the general public. In this text, it is important to use as few technical terms as possible in order to ensure that the text is interesting and understandable to people not familiar with the field. The main point should be mentioned at the very start of the summary. Please keep descriptions of the issues addressed and results obtained short and succinct. Possible applications to or implications for social, cultural, ecological, medical, economic or technological areas should also be mentioned briefly.

The summary should be submitted both in **German** and in **English** (without special characters). The summaries will be made available via the FWF's project database. The FWF will not edit the summaries, meaning that the authors bear full responsibility for the content of these texts.

1. Zusammenfassung für die Öffentlichkeitsarbeit

Transistoren begegnen uns alltäglich in zahlreichen elektronischen Geräten und nehmen daher eine wesentliche Rolle in unserer technologiegeprägten Gesellschaft ein. Die stetige Weiterentwicklung dieser elektronischen Bauteile geht mit ihrer Minaturisierung einher. Die Dimensionen dieser elektronischen Bauteile dringen bereits in Größenordnungen vor, in denen einzelne im Dielektrikum eingefangene Ladungen die Bauteilkennlinien stark beeinflussen. Dies stellt ein schwerwiegendes Zuverlässigkeitsproblem dar, das unter dem Namen Bias-Temperature-Instability (BTI) bekannt ist. Eine Erklärung für dieses Phänomen wurde durch eine kürzlich entwickelten Methode names Time-Dependent-Defect-Spectroscopy geliefert, die die Untersuchung einzelner Defekte erlaubt und zur Entwicklung des Four-State-NMP-Modell führte. Wie der Name schon verrät, basiert dieses mikroskopische Modell auf vier Defektzuständen, welche sich in ihrer Atomkonfiguration, ihrer Stabilität und ihrem Ladungszustand unterscheiden. Auch wenn diese Defekteigenschaften durch die Kalibrierung des Modells auf experimentelle Daten extrahiert werden können, gehen sie als rein empirische Werte in das Modell ein und beschreiben daher einen hypothetischen Defekt. Im Zuge der Suche nach dem tatsächlichen BTI-Defekt wurde eine Reihe von möglichen Kandidaten mittels atomistischer First-Principles-Simulationen untersucht.

Unsere Studien gingen von Defektstrukturen aus, welche in Siliziumdioxid (SiO_2) vorkommen aber auch in anderen, z.B. geschichteten, Dielektria vermutet werden. Da die meisten bekannten Defekte mit dem Four-State Modell inkomptibel sind, beschränkte sich die Anzahl der im Detail untersuchten Defektkandidaten auf eine kleine Auswahl, einschließlich der Sauerstoffvakanz, der Wasserstoffbrücke und dem Hydroxyl-E'-Center. Es wurde gezeigt, dass nur die letzteren beiden bistabile Konfigurationen besitzen, welche laut unserer TDDS-Analysen ein besonderes Merkmal eines BTI-Defekts sind und deren Existenz daher als ein strenges Kriterium für die Defektvalidierung herangezogen wurden. Ein anderes stark einschränkendes Kriterium war die Position des Traplevel, welches aber nicht von der Sauerstoffvakanz erfüllt wurde. Dieses Kriterium wurde von der Sauerstoffvakanz auch unter Berücksichtigung der amorphen Beschaffenheit von SiO_2, welche Variationen in lokalen Bindungsstrukturen zulässt und daher zu einer Streuung der Trapleveln führt, nicht erfüllt. Derartige statistische Untersuchungen wurden nicht nur für die Sauerstoffvakanz sondern auch für die Wasserstoffbrücke und das Hydroxyl-E'-Center durchgeführt und haben beide Defekte als vielversprechende Kandidaten bestätigt.

Jüngste Langzeit-TDDS-Studien haben auch Defekte zum Vorschein gebracht, die zeitweise in ihrem neutralen oder positiven Ladungszustand verschwinden und wieder auftrauchen. Dieses als Defektvolatilität bezeichnete Phänomen spielt sich üblicherweise auf längeren Zeitskalen ab und ist daher mit der Lebensdauer von Transistoren, einem wesentlich Aspekt der Bauteilzuverlässigkeit, verbunden. Die Erkenntnisse aus diesen TDDS-Studien haben eine Erweiterung des Four-State-NMP-Modells mit zusätzlichen Zuständen erfordert. Unter Zuhilfenahme von First-Principles-Simulationen konnten diese neuen Zustände nur für das Hydroxyl-E'-Center identifiziert werden. Damit erfüllt das Hydroxyl-E'-Center alle aus TDDS-Studien stammenden Kriterien und wird daher als der wahrscheinlichste für BTI verantwortliche Defektkandidat betrachtet.

2. Summary for public relations work

Microelectronic devices have become the foundation to many aspects of our modern lives and take an important role in our technology-driven society. The ongoing advancement of those devices is strongly related to their continuous miniaturization. Due to this, device dimensions have entered scales where even a single charge trapped in the dielectric can severely alter the transistor characteristics. This poses a serious reliability issue, referred to as the bias temperature instability (BTI). Unfortunately, its behavior for different gate biases and temperatures as well as its physical origins have eluded our understanding so far. However, the recently developed time dependent defect spectroscopy (TDDS) allows for the investigation of single defects, leading to a new microscopic model called four-state NMP model. As its name suggests, this model is based on several different defect states, which differ in their configuration, their stability, and the trapped charge. These defect properties can be extracted from a calibration of this model to experimental data but solely enter as empirical values for a hypothetical defect. As such, the actual defect responsible for BTI remains unknown. Hence, we set out on the search for the atomistic structure of the responsible defect, by employing density functional theory (DFT) simulations.

Our studies started from defects located in amorphous silicon dioxide (SiO_2) as this is the material in which BTI was discovered initially. The number of defects that had to be investigated in detail could be narrowed down to a few candidates, including the oxygen vacancy, the hydrogen bridge, and the hydroxyl E' center, as only they have a metastable in addition to a stable configuration according to our DFT studies. This was a special feature, which has been deduced from our TDDS studies and used as a stringent criterion for defect identification throughout this work. Another restrictive criterion was that the trap level of the defect must lie close to the valence band edge of the silicon substrate, which is not met by the oxygen vacancy. This was found to hold even if the amorphous nature of SiO_2 was considered, which gives rise to large variations in the local atomic bonding structure and thus in the trap level of the defects at different sites. Such statistical studies have also been performed for the hydrogen bridge and the hydroxyl E' center, demonstrating that both of them are still good candidates for a BTI defect.

Recent long-time TDDS studies have revealed that defects involved in BTI occasionally disappear and reappear in the neutral or positive charge state. This phenomenon termed “defect volatility” usually occurs on large time scales and is thus related to the device lifetime of transistors, an important aspect for device reliability. These TDDS findings required an extension of the four-state NMP model with additional states. Using DFT simulations, these new states could only be indentified for the hydroxyl E' center. As such, the hydroxyl E' center was the only one meeting the TDDS criteria and is therefore regarded as the sought as the most likely defect responsible for the BTI phenomenon, the identification of which being the primary goal of this project.

II. Brief project report

1. Report on research work

1.1 Information on the development of the research project

The proposal was initially developed around our two-stage model (TSM), which appeared to be the most promising model for defects involved in bias temperature instability (BTI) at the time of the project application. It was based on two stages, where the first described the recoverable component of BTI via de-/trapping of charge carriers. The second stage fixes the captured charge within the defect via a defect transformation and thereby models defects which contribute to the permanent component of BTI. Even though this model could already describe a variety of experimental features, it could not give an explanation for the observations made by a subsequently developed measurement technique, termed time-dependent defect spectroscopy (TDDS). This new technique has allowed us to monitor single charge capture and emission events into and out of individual defects, thereby providing unprecedented insight into the physical mechanisms underlying charge capture and emission. One of the most interesting findings of TDDS has been that a considerable portion of the detected BTI defects show a pronounced gate bias dependence of their emission times while the other defects remain insensitive to the gate bias. The new experimental findings were taken into account by our newly developed four-state nonradiative multi-phonon (NMP) model. It was build upon the concept of bistable defects, which feature two neutral (1, 1') and two positive (2, 2') states. Each of these charge states has a metastable counterpart (1', 2'), which is only passed temporarily during a complete charge capture or emission process. The possible transitions within the four-state NMP model are either defect deformations between same charge states (1↔1' or 2↔2') or actual charge capture and emission processes (1↔1' or 2↔2'), described by NMP theory. The availability of this new single-defect data together with the development of the new model at the beginning of this project required substantial changes in our first-principles investigations, primarily the identification of bistable defects together with their numerous states.

As the goal of this project was to identify the particular defect responsible for BTI at the atomistic level, we had to develop an advanced theoretical description of the BTI defect, which can be directly linked to our DFT calculations. This description relies on the shape of the potential energy surfaces (PES) extractable from DFT calculations. In particular, it allows calculating trap levels that can be determined by experiments. To reduce the computational costs, an efficient method was devised to calculate the NMP transition rate assuming a single-mode approximation. This method is particularly suitable for the evaluation of the NMP rates using the experimentally relevant classical high-temperature limit as well as the quantum mechanical formulation for low temperatures and weak electron-phonon coupling. Furthermore, the description had to be refined to account for the charge exchange with the excited conduction and valence band states and not only with their band edges as assumed previously. All the above improvements have proven to be necessary for an accurate description of the NMP processes, especially with regard to stress-induced leakage currents (SILC), as discussed later.

In parallel, we implement a code for simulated annealing - a Metropolis Monte Carlo scheme combined with a bond switching algorithm - for generating amorphous host structures for the DFT simulations of BTI defects. This code was tested for silicon dioxide (SiO_2) material based on pair-correlations functions and bond angle distributions and was extended for Si/SiO_2 interface structures with different stoichiometries. Furthermore, it has also been parallelized for a faster generation of defect host structures.

The actual search for possible defects started from the SiO_2 host material. This decision was motivated by the fact that the BTI phenomenon shows a quite similar behavior in all transistor technologies, including those with a silicon oxynitride and high-k materials as dielectric. This suggests that the sought BTI defect is the same or at least similar in all technologies, especially given the fact that high-k dielectrics are attached to a defective SiO_2 interlayer and silicon oxynitrides exhibit a quite small nitrogen content. The frequently suspected oxygen vacancy in its dimer configuration was found to have a trap level which is energetically far too low for a significant contribution to hole trapping to BTI. Therefore, the E' center model, which was at the heart of the initial two-stage model, had to be ruled out. Experimental investigations from our industrial partners focused on wafer splits with different hydrogen contents and suggested that the sought defect is likely to involve hydrogen. Following this hint, the hydrogen bridge was selected as our next defect candidate and investigated in crystalline and amorphous SiO_2. This work included the generation of amorphous SiO_2 structures and numerous DFT calculations at various sites within these structures. Our DFT simulations demonstrated that the hydrogen bridge shows the essential features of a BTI defect, including a bistable configuration and a trap level in the region close to the substrate bandgap.

In addition to defects in SiO_2, we have also investigated nitrogen-related defects, first of all the nitrogen bridge. Based on our DFT simulations, the nitrogen bridge was found to be an electron trap rather than a hole trap. As BTI is primarily ascribed to hole trapping, this nitrogen-related defect had to be ruled out as well.

As the DFT investigations are quite labor-intensive, we started a close collaboration with another internationally recognized research group, namely Prof Alex Shluger’s group at UC London. In a joint research activity, we studied a new defect candidate termed hydroxyl E' center in amorphous SiO_2. The DFT investigations for both the hydrogen bridge and the hydrogen E' center were again carried out in amorphous SiO_2 based on large statistics. The obtained results for both defects were compared to the experimental results, showing that both candidates meet the criteria established by our earlier TDDS studies.

During the course of this project, later long-time TDDS studies revealed that defects involved in BTI occasionally disappear and reappear in the neutral as well as the positive charge state. This phenomenon was termed “defect volatility” and usually occurs at large time scales. This volatility, at least, may affect the long-term and „more permanent“ degradation of BTI. It is thus related to the device lifetime of transistors, one of the most important aspects of reliability. The above TDDS findings required an extension of the four-state NMP model. While the bistable defect is still at the heart of this new model, additional states had to be introduced into our four-state NMP model to account for the defect volatility. These new states could be indentified for the hydroxyl E' center by testing their stability and formation barriers using DFT simulations. With this, we have been able to establish a more detailed picture of BTI that does not only account for the recoverable but also for the permanent component of BTI.

In our DFT investigations, the PESs were sampled at special configurations, i.e. equilibrium configurations and the saddle points of energy barriers. Using this information, we reconstructed the PES of the investigated defects within the relevant range of the four-state NMP model. For evaluating the simulated defects, their DFT results were compared with the calibrations of the four-state NMP model to the experimental data of mostly SiON- but also HfO_2-based transistors. These calibrations included electrical measurements of ensembles of defects on large-area devices as well as TDDS studies for single defects on small-area devices, whereby large statistics of the relevant PES parameters have been obtained for the experimental verification of the simulated BTI defects.

In summary, two promising defect candidates, namely the hydrogen bridge and the hydroxyl E' center, have been found as a possible BTI defect within the four-state NMP model using DFT simulations. In the course of the project, the initial version of this model had to be extended due to new experimental findings, which have narrowed down the selection of possible defect candidates to the hydroxyl E' center alone.

1.2 Most important results and brief description of their significance (main points) with regard to the following:

During this project, the hydroxyl E' center was identified as the most likely defect which can explain a variety of features obtained from short- and long-time TDDS. The result constitutes a genuine progress in the long-standing research topic BTI. This progress was based on our atomistic modeling approach, which has been pursued with unprecedented thoroughness. This concerns our rigorous theoretical description of the mechanisms behind BTI, our efforts to consider the newest findings from TDDS studies, and especially our attempts to support the four-state NMP model with an atomistic picture based on a particular defect. The atomistic picture has been derived from our in-depth DFT calculations, which account for the statistical variations of the defect properties due to the amorphous nature of the dielectric material.

This approach has also been extended to random telegraph noise (RTN) in the drain currents and SILC, both of which could be related to the four-state NMP model (details mentioned in 3.). Furthermore, this model was shown to also explain the electron traps observed in nMOSFETs. As such, all the above investigations can be understood as an additional benchmark of our model, which therefore can be regarded as a comprehensive description of oxide defects in reliability issues.

1.3 Information on the execution of the project, use of available funds and (where appropriate) any changes to the original project plan relating to the following:

The permitted funding allowed for the financing of both a PostDoc and a Ph.D. over the course of three years. In the initial stage of the project, the available funding was mostly used to support the dissertation of Dr. Wolfgang Goes, who successfully defended his Ph.D. thesis in December 2011 and could continue his scientific work as a PostDoc until the end of the project. During his time as a PostDoc, the possibility opened up to work as a visiting researcher at IMEC, thereby deepening the collaboration with the experimental reliability group of Guido Groesenecken/Ben Kaczer. In addition, DI Paul-Jürgen Wagner worked on the project as a Ph.D. for 12 months in 2012. In 2012/2013, DI Michael Waltl contributed for 24 months. In total, 29 PhD months and 33 PostDoc months were spent during the duration of the project.

2. Personnel development – Importance of the project for the research careers of those involved (including the project leader)

As the largest portion of permitted funding was invested for the research of Dr. Wolfgang Goes, the project was primarily to the benefit of his research career. During the project, he has broadened his expertise with the required knowledge and skills regarding first-principles investigations. In addition, a scientific network has been developed which is a prerequisite for future interdisciplinary research. In particular, the collaboration with IMEC resulted in a series of well received publications, one of which was honoured with a best paper award at IPFA 2013. Furthermore, this publication allowed the Dr. Goes to enter a new scientific topic (SILC) in addition to the BTI phenomenon. All these achievements have provided the group of Prof. Grasser with a solid theoretical foundation for their reliability efforts, thereby further strengthening the international standing of the group.

3. Effects of the project beyond the scientific field

The research activities within the project were primarily focussed on BTI, which is attributed to charge trapping. Besides that, also RTN in the drain current has become a severe reliability issue since already a single trapped charge may affect the device functionality. In the course of this project, it could be demonstrated that RTN and BTI have the same physical origin and are caused by the same defects. We have also given an explanation for other noise phenomena, such as temporary and anomalous RTN.

Further progress has been achieved regarding SILC. The phenomenon of correlated drain and gate current fluctuations could be explained within the four-state NMP model by a mechanism called trap-assisted tunneling, which is triggered by a charge capture from the substrate. Similar to SILC, our explanation relies on the generation of defects opening a leakage current paths and, therefore, our work has also provided a valuable contribution to the research field of SILC. (Both works were only mentioned in passing in 1.2.)

4. Other important aspects

The results of our research activities could be disseminated at several acknowledged international conferences, which include the IRPS and the IEDM among others. The number of given talks amount to seven conference contributions (listed below), where a high fraction resulted from collaborations with other research groups, most notably at Infineon and IMEC. A couple of these talks were invited or have even received a best-paper award.

1. P.-J. Wagner, B. Kaczer, A. Scholten, H. Reisinger, S. Bychikhin, D. Pogany, L.K.J. Vandamme, T. Grasser: "*On the Correlation Between NBTI, SILC, and Flicker Noise*"; IEEE International Integrated Reliability Workshop, California; 2012-10-14 – 2012-10-18.
2. M. Waltl, P.-J. Wagner, H. Reisinger, K. Rott, T. Grasser: "*Advanced Data Analysis Algorithms for the Time-Dependent Defect Spectroscopy of NBTI*"; IEEE International Integrated Reliability Workshop, California; 2012-10-14 - 2012-10-18.
3. T. Grasser, W. Gös, Y. Wimmer, F. Schanovsky, G. Rzepa, M. Waltl, K. Rott, H. Reisinger, V. Afanas'ev, A. Stesmans, A. El-Sayed, A. Shluger: "*On the Microscopic Structure of Hole Traps in pMOSFETs*"; International Electron Devices Meeting (IEDM), San Francisco, CA, USA; 2014-12-15 – 2014-12-17.
4. W. Gös, M. Waltl, Y. Wimmer, G. Rzepa, T. Grasser: "*Advanced Modeling of Charge Trapping: RTN, 1/f noise, SILC, and BTI*"; International Conference on Simulation of

Semiconductor Processes and Devices (SISPAD), Yokohama, Japan; (**invited**) 2014-09-09 – 2014-09-11.

5. W. Gös, M. Toledano-Luque, F. Schanovsky, M. Bina, O. Baumgartner, B. Kaczer, T. Grasser: "*Multi-Phonon Processes as the Origin of Reliability Issues*"; Meeting of the Electrochemical Society (ECS), San Francisco, USA; (**invited**) 2013-10-27 – 2013-11-01.

6. W. Gös, M. Toledano-Luque, O. Baumgartner, M. Bina, F. Schanovsky, B. Kaczer, T. Grasser: "*Understanding Correlated Drain and Gate Current Fluctuations*"; International Symposium on the Physical and Failure Analysis of Integrated Circuits (IPFA), Suzhou, China; (**best paper**) 2013-07-15 – 2013-07-19.

7. T. Grasser, K. Rott, H. Reisinger, M. Waltl, J. Franco, B. Kaczer: "*A unified perspective of RTN and BTI*"; International Reliability Physics Symposium (IRPS), Waikoloa, Hawaii, USA; (**best paper**) 2014-06-01 – 2014-06-05.

III. Attachments

(lists may be as long as required)

1. Scholarly / scientific publications

Publications may only be listed if they relate directly to the project. **Up to three of the most important publications** should be highlighted as such (e.g. printed in bold letters).
Please note that funding for publication costs can be requested (under the original project number) for up to three years following completion of a project.

Please make sure that all publications are freely available on the Internet. For details, see the Open Access Policy of the FWF. (In the Life Sciences category, all refereed publications are to be made available through Europe PubMedCentral)

Please indicate at the end of every peer-review publication (in brackets) the Open Access (OA) type as following:

- Gold OA = published in Open Access Journal, with or without an author fee (see register of all Open Access Journals http://www.doaj.org/)
- Hybrid OA = published in a subscription journal but Open Access by an author fee (see http://en.wikipedia.org/wiki/Hybrid_open_access_journal)
- Green OA = self-archived electronic copy of the final "accepted manuscript" which might include an embargo period (see: http://www.fwf.ac.at/en/research-funding/open-access-policy/)
- Other OA = any other type of Open Access
- No OA = not published Open Access

1.1 Peer-reviewed publications / already published (journals, monographs, anthologies, contributions to anthologies, proceedings, research data, etc.)

Citations should be provided in a **commonly used format.** For each work, the publication list **must mention the following**:

- Author(s)
- Title
- Journal
- Issue
- Year
- Pages
- DOI or ISBN (for books)
- If Open Access: URL
- Open Access (OA) Type

T. Grasser, P.-J. Wagner, H. Reisinger, T. Aichinger, G. Pobegen, M. Nelhiebel, B. Kaczer: "*Analytic Modeling of the Bias Temperature Instability Using Capture/Emission Time Maps*"; Talk: International Electron Devices Meeting (IEDM), Washington DC, USA; 2011-12-05 - 2011-12-07; in "*2011 International Electron Devices Meeting (IEDM) Technical Digest*", (2011), ISBN: 978-1-4577-0505-2, 4 page(s) doi:10.1109/IEDM.2011.6131624. (No OA)

P.-J. Wagner, B. Kaczer, A. Scholten, H. Reisinger, S. Bychikhin, D. Pogany, L.K.J. Vandamme, T. Grasser:
"*On the Correlation Between NBTI, SILC, and Flicker Noise*";
Talk: IEEE International Integrated Reliability Workshop, California; 2012-10-14 - 2012-10-18; in "*IEEE International Integrated Reliability Workshop Final Report*", (2012), 60 - 64. (No OA)

T. Grasser, B. Kaczer, H. Reisinger, P.-J. Wagner, M. Toledano-Luque:
"*On the Frequency Dependence of the Bias Temperature Instability*";
Poster: International Reliability Physics Symposium (IRPS), California, USA; 2012-04-17 - 2012-04-19; in "*Conference Proceedings of International Reliability Physics Symposium (IRPS 2012)*", (2012), ISBN: 978-1-4577-1680-5, 6 page(s). (No OA)

T. Grasser, H. Reisinger, K. Rott, M. Toledano-Luque, B. Kaczer:
"*On the Microscopic Origin of the Frequency Dependence of Hole Trapping in pMOSFETs*";
Talk: International Electron Devices Meeting (IEDM), San Francisco, CA, USA; 2012-12-10 - 2012-12-12; in "*2012 International Electron Devices Meeting (IEDM) Technical Digest*", (2012), 470 - 473 doi:10.1109/IEDM.2012.6479076. (No OA)

T. Grasser, K. Rott, H. Reisinger, P.-J. Wagner, W. Gös, F. Schanovsky, M. Waltl, M. Toledano-Luque, B. Kaczer:
"*Advanced Characterization of Oxide Traps: The Dynamic Time-Dependent Defect Spectroscopy*";
Talk: International Reliability Physics Symposium (IRPS), Monterey, CA, USA; 2013-04-14 - 2013-04-18; in "*Conference Proceedings of International Reliability Physics Symposium (IRPS 2013)*", (2013), 1 - 6. (No OA)

M. Waltl, P.-J. Wagner, H. Reisinger, K. Rott, T. Grasser:
"*Advanced Data Analysis Algorithms for the Time-Dependent Defect Spectroscopy of NBTI*";
Talk: IEEE International Integrated Reliability Workshop, California; 2012-10-14 - 2012-10-18; in "*IEEE International Integrated Reliability Workshop Final Report*", (2012), 74 - 79. (No OA)

T. Grasser, K. Rott, H. Reisinger, P.-J. Wagner, W. Gös, F. Schanovsky, M. Waltl, M. Toledano-Luque, B. Kaczer:
"*Advanced Characterization of Oxide Traps: The Dynamic Time-Dependent Defect Spectroscopy*";
Talk: International Reliability Physics Symposium (IRPS), Monterey, CA, USA; 2013-04-14 - 2013-04-18; in "*Conference Proceedings of International Reliability Physics Symposium (IRPS 2013)*", (2013), 1 - 6. (No OA)

T. Grasser, K. Rott, H. Reisinger, M. Waltl, P.-J. Wagner, F. Schanovsky, W. Gös, G. Pobegen, B. Kaczer:
"*Hydrogen-Related Volatile Defects as the Possible Cause for the Recoverable Component of NBTI*";
Talk: International Electron Devices Meeting (IEDM), Washington, DC, USA; 2013-12-09 - 2013-12-11; in "*2013 International Electron Devices Meeting (IEDM) Technical Digest*", (2013), 409 - 412 doi:10.1109/IEDM.2013.6724637. (No OA)

W. Gös, M. Toledano-Luque, O. Baumgartner, F. Schanovsky, B. Kaczer, T. Grasser:
"*A Comprehensive Model for Correlated Drain and Gate Current Fluctuations*";
Talk: International Workshop on Computational Electronics (IWCE), Nara, Japan; 2013-06-04 - 2013-06-07; in "*Book of Abstracts of the 16th International Workshop on Computational Electronics (IWCE)*", (2013), ISBN: 978-3-901578-26-7, 46 - 47. (No OA)

W. Gös, M. Toledano-Luque, O. Baumgartner, M. Bina, F. Schanovsky, B. Kaczer, T. Grasser:
"*Understanding Correlated Drain and Gate Current Fluctuations*";
Talk: European Symposium on Reliability of Electron Devices, Failure Physics and Analysis (ESREF), Arcachon, France; (invited) 2013-09-30 - 2013-10-04; in "*20th IEEE International Symposium on the Physical and Failure Analysis of Integrated Circuits (IPFA)*", (2013), 51 - 56. (No OA)

W. Gös, M. Toledano-Luque, F. Schanovsky, M. Bina, O. Baumgartner, B. Kaczer, T. Grasser:
"*Multi-Phonon Processes as the Origin of Reliability Issues*";
Talk: Meeting of the Electrochemical Society (ECS), San Francisco, USA; (invited) 2013-10-27 - 2013-11-01; in "*ECS Transactions 2013 - "Semiconductors, Dielectrics, and Materials for Nanoelectronics 11"*", (2013), Vol.58/7/, 31 - 47 doi:10.1149/05807.0031ecst. (No OA)

T. Grasser, W. Gös, Y. Wimmer, F. Schanovsky, G. Rzepa, M. Waltl, K. Rott, H. Reisinger, V. Afanas´Ev, A. Stesmans, A. El-Sayed, A. Shluger:
"*On the Microscopic Structure of Hole Traps in pMOSFETs*";
Talk: International Electron Devices Meeting (IEDM), San Francisco, CA, USA; 2014-12-15 - 2014-12-17; in "*2014 International Electron Devices Meeting (IEDM) Technical Digest*", (2014), ISBN: 978-1-4799-8001-7, 530 - 533 doi:10.1109/IEDM.2014.7047093. (No OA)

W. Gös, M. Waltl, Y. Wimmer, G. Rzepa, T. Grasser:
"*Advanced Modeling of Charge Trapping: RTN, 1/f noise, SILC, and BTI*";
Talk: International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Yokohama, Japan; (invited) 2014-09-09 - 2014-09-11; in "*Proceedings of the 19th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*", (2014), ISBN: 978-1-4799-5285-4, 77 - 80 doi:10.1109/SISPAD.2014.6931567. (No OA)

T. Grasser, K. Rott, H. Reisinger, M. Waltl, F. Schanovsky, B. Kaczer:
"*NBTI in Nanoscale MOSFETs-The Ultimate Modeling Benchmark*";
IEEE Transactions on Electron Devices, **61** (2014), 3586 - 3593
doi:10.1109/TED.2014.2353578. (No OA)

T. Grasser, K. Rott, H. Reisinger, M. Waltl, W. Gös:
"*Evidence for Defect Pairs in SiON pMOSFETs*";
Talk: International Symposium on the Physical and Failure Analysis of Integrated Circuits (IPFA), Singapore, Singapore; 2014-06-30 - 2014-07-04; in "*Proceedings of the 21st International Symposium on the Physical and Failure Analysis of Integrated Circuits*", (2014), ISBN: 978-1-4799-3929-9, 262 - 267. (No OA)

T. Grasser, G. Rzepa, M. Waltl, W. Gös, K. Rott, G. Rott, H. Reisinger, J. Franco, B. Kaczer:
"*Characterization and Modeling of Charge Trapping: From Single Defects to Devices*";
Talk: IEEE International Conference on IC Design and Technology (ICICDT), Austin, TX, USA; (invited) 2014-05-28 - 2014-05-30; in "*Proceedings of IEEE International Conference on IC Design and Technology*", (2014), ISBN: 978-1-4799-2153-9, 1 - 4
doi:10.1109/ICICDT.2014.6838620. (No OA)

1.2 **Non peer-reviewed publications / already published** (journals, monographs, anthologies, contributions to anthologies, research reports, working papers / preprints, proceedings, research data, etc.)

Citations should be provided in a **commonly used format.** For each work, the publication list **must mention the following**:

- Author(s)
- Title
- Journal
- Issue
- Year
- Pages
- DOI or ISBN or URL / if applicable
- Open Access / if applicable
- Open Access (OA) Type

W. Gös, F. Schanovsky, T. Grasser:
"*Advanced Modeling of Oxide Defects*";
in "*Bias Temperature Instability for Devices and Circuits*", T. Grasser (ed); Springer New York, 2013, ISBN: 978-1-4614-7909-3, 409 - 446 doi:10.1007/978-1-4614-7909-3_16. (No OA)

1.3 Planned publications

(journals, monographs, anthologies, contributions to anthologies, proceedings, research data, etc.)

Author(s)	Y. Wimmer, W. Goes, A.-M. El-Sayed, A.L. Shluger, and T. Grasser		
Title	On the Validity of the Harmonic Potential Energy Surface Approximation for Nonradiative Multiphonon Charge Transitions in Oxide Defects		
Sources	Proceedings of the 18th International Workshop on Computational Electronics		
URL (if applicable)	https://nanohub.org/groups/iwce2015/		
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☒	submitted ☐	in preparation ☐

Author(s)	Y. Wimmer, W. Goes, A.-M. El-Sayed, A.L. Shluger, and T. Grasser		
Title	A Density-Functional Study of Defect Volatility in Amorphous Silicon Dioxide		
Sources	Proceedings of the 20th International Conference on Simulation of Semiconductor Processes and Devices		
URL (if applicable)	https://www.ece.umd.edu/sispad2015/		
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☒	submitted ☐	in preparation ☐

Author(s)	W. Gös, Y. Wimmer, A.-M. El-Sayed, M. Jech, A. Shluger, T. Grasser		
Title	Linking Charge Transfer Theory with First-Principles Calculations		
Sources	Physical Review B		
URL (if applicable)			
Peer Review	yes ☒	no ☐	
Status	in press/accepted ☐	submitted ☐	in preparation ☒

2. Most important academic awards

(Specific academic awards, honours, prizes, medals or other merits)

Name of award	n=national / i=international
“Best Paper Reliability”, IPFA2013	I
“Outstanding Paper Award”, IRPS 2014	I

3. Information on results relevant to commercial applications

- Type of commercial application:
    1. Patent
    2. Licensing
    3. Copyrights (e.g. for software; no publications)
    4. Others

Type of commercial application		
Subject / title of the invention / discovery		
Short description of the invention / discovery		
Year		
Status	granted ☐	pending ☐
Application reference (or patent number)		

4. Publications for the general public and other publications

(Absolute figures, separate reporting of national / international publications)

- Type of dissemination activities:

  Self-authored publications on the World Wide Web
  Editorial contributions in the media (print, radio, TV, www, etc.)
  (Participatory) contributions within science communication
  Popular science contributions (books, lectures, exhibitions, films, etc.)

	national	International
Self-authored publications on the www		
Editorial contributions in the media		
(Participatory) contributions within science communication		
Popular science contributions		

5. Development of collaborations

Indication of the most important collaborations (no more than 5) that took place (i.e. were initiated or continued) in the course of the project. Please provide the name of the collaboration partner (name, title, institution) and a few words about the scientific content. Please **categorise** each collaboration arrangement as follows:

N				Nationality of collaboration partner (please use the ISO-3-letter country code)
	G			Gender **F (**female) **M** (male)
		E		Extent **E1** **low** (e.g. no joint publications, but mention in acknowledgements or similar); **E2** **medium** (collaboration e.g. with occasional joint publications, exchange of materials or similar, but no longer-term exchange of personnel); **E3** **high** (extensive collaboration with mutual hosting of group members for research stays, regular joint publications, etc.)
			D	Discipline **W** **within the discipline** (within the same scientific field) **I** **interdisciplinary** (involving two or more disciplines) **T** **transdisciplinary** (collaborations outside the sciences)

N	G	E	D	Name	Institution
GB	M	E2	I	Prof. Alex Shluger	University College London
GB	M	E2	I	PhD Al-Moatasem El-Sayed	University College London
BE	M	E3	W	Dr. Ben Kaczer	IMEC
BE	F	E3	W	Dr. Maria Toledano-Luque	IMEC

Note: General scientific contact and occasional meetings should not be considered collaborations for the purposes of this report.

6. Development of human resources in the course of the project

(Absolute figures with an indication of status (in progress / completed)

Note: It is not possible to assign a *venia* thesis / work (*Habilitation*) to a single project; here it is necessary to mention those *venia* theses for which the project was important. A similar caveat applies to Ph.D. and diploma theses: The FWF does not support thesis work, but instead funds the scientific work that forms the basis for such theses.

	In progress	**Completed**	**Gender**	
			f	**m**
Full professorship				
Venia thesis (*Habilitation*) / Equivalent senior scientist qualification				
Postdoc				
Ph.D. theses	2	1		3
Master’s theses				
Diploma theses				
Bachelor‘s theses				

7. Applications for follow-up projects

(Please indicate the status of each project and the funding organisation)

7.1 Applications for follow-up projects (FWF projects)

Please indicate the project type (e.g. stand-alone project, SFB, DK, etc.)

Project number (if applicable)			
Project type			
Title / subject			
Status	granted ☐	pending ☐	in preparation ☐
Application reference (if a patent is applied)			

7.2 Applications for follow-up projects (Other national projects)

(e.g. FFG, CD Laboratory, K-plus centres, funding from the Austrian central bank [OeNB], Austrian federal government, provincial agencies, provincial government or similar sources)

Funding agency	Please choose an item:		
Other national funding agencies			
Project number (if applicable)			
Project type			
Title / subject			
Status	granted ☐	pending ☐	in preparation ☐
Total costs (granted)			

7.3 Applications for follow-up projects (international projects) (e.g. EU, ERC or other international funding agencies)

Country			
Funding agency	Please choose an item:		
Project number (if applicable)			
Project type			
Title / subject			
Status	granted ☐	pending ☐	in preparation ☐
Total costs (granted)			

IV. Cooperation with the FWF

Please rate the following aspects with regard to your interaction with the FWF. Please provide any **additional comments (explanations)** on the supplementary sheet with a reference to the corresponding question/aspect.

Scale:
-2 highly unsatisfactory
-1 unsatisfactory
0 appropriate
+1 satisfactory
+2 highly satisfactory
X not used

Rules
(i.e. guidelines for: funding programme, application, use of resources, reports)

		Rating
Application guidelines	Length	**+1**
	Clarity	**+1**
	Intelligibility	**+1**

Procedures (submission, review, decision)

	Advising	**+1**
	Duration of procedure	**0**
	Transparency	**0**

Project support

Advising	Availability	**+1**
	Level of detail	**+1**
	Intelligibility	**+1**

Financial transactions (credit transfers, equipment purchases, personnel management)	**+1**

Reporting / review / exploitation

	Effort	**+1**

Transparency	**+1**
Support in PR work / exploitation	**0**

Comments on cooperation/interaction with the FWF:

The FWF is the ***only*** funding source which allows us to focus on science rather than on writing reports and being entangled in lengthy book-keeping activities.

THANK YOU FOR THAT, PLEASE KEEP THINGS THE WAY THEY ARE AND DO NOT LET THE FWF BE TAKEN OVER BY CONTROLLERS AND OTHER MANAGEMENT-LIKE PEOPLE WHO SIMPLY FAIL TO SEE HOW SCIENCE WORKS!!!