STAND-ALONE PROJECT

FINAL REPORT

Project number	**P23296-N13**
Project title[1]	**Void Evolution due to Electromigration**
	Lunkerwanderung aufgrund von Elektromigration
Project leader	**SELBERHERR Siegfried**

---

[1] Short title in English and German language

I. Summary for public relations work

1. Zusammenfassung für die Öffentlichkeitsarbeit

Ein allgemeines Elektromigrationsmodell für das Verhalten von Lunkerstrukturen wurde theoretisch entwickelt, in einem Simulationswerkzeug implementiert und numerisch untersucht. Die kontinuierliche Skalierung der Verbindungsstrukturen in integrierten Schaltungen verursacht erhöhte Betriebs-Stromdichten und Temperaturen. Diese Entwicklung erhöht nach und nach den Druck auf das Verbindungstruktur-Design und die Herstellung, da Zuverlässigkeits-Probleme, wie die Elektromigration, zunehmend an Bedeutung in modernen, integrierten Schaltungen gewinnen, welche den kontinuierlichen Fortschritt im Bereich der Mikroelektronik behindern.

Im heutigen modernen Kupfer-Dual-Damascene-Verfahren tragen verschiedene physikalische Mechanismen zur Lunkerwanderung durch Elektromigrations-induzierten Stress bei. Im Besonderen, sind die Oberflächenenergie, Elektromigration und elastische Deformations-Energie die primär verantwortlichen Kräfte, welche Materialtransport entlang der Lunkerstruktur-Oberfläche auslösen. Zusätzlich beeinflusst die Wechselwirkung der Lunkerstruktur mit den lokalen geometrischen Eigenschaften (zum Beispiel Materialgrenzflächen und Mikrostrukturen) die Lunkerstruktur-Migration, Wachstum und Form-Stabilität. Insbesondere ist die hohe Diffusivität an der Kupfer/Deck-Schicht eines der Hauptprobleme, welches die Lunkerstruktur-Migration und das Wachstum entlang einer Verbindungsstruktur bestimmt.

Die Mängel früher Ansätze, welche auf Oberflächen-Verfolgungs-Methoden basierten, wurden durch ein sogenanntes Diffusions-Grenzflächen-Modell bewältigt. Ein internes, dreidimensionales Simulationswerkzeug (FEDOS) wurde mit diesem Modell erweitert, welches Simulationen von Elektromigrations-induzierten Lunkerwanderungen, basierend auf unserer allgemeinen Elektromigrations-Lunkerstrukturentwicklung, ermöglicht.

Die Ergebnisse, die durch unser Simulationswerkzeug generiert wurden, welches unsere entwickelten Modelle verwendet, haben gezeigt, dass die Fähigkeit der Vorhersage der Lunkerstrukturentwicklung im Vergleich zu früheren Ansätzen signifikant verbessert wurde. Der Stand der Technik wurde somit signifikant vorangebracht.

2. Summary for public relations work

A general electromigration void evolution model has been theoretically developed, implemented in a simulation tool, and numerically investigated. The continuous scaling of interconnects in integrated circuits causes increased operating current densities and temperatures. This development increasingly puts pressure on the interconnect design and fabrication, as reliability issues, such as electromigration, are more and more a concern for modern integrated circuits, impeding continuous advancement in the area of microelectronics.

In state-of-the-art copper dual-damascene technology different physical mechanisms contribute to void evolution under electromigration-induced stress. In particular, surface energy, electromigration, and elastic strain energy are the primary forces at play, triggering material transport along the void surface. Additionally, the interaction of the void with local geometric features (e.g. material interfaces and microstructures) further impacts void migration, growth, and shape stability. In particular, the high diffusivity at the copper/capping layer interface is one major issue which controls void migration and growth along an interconnect structure.

The shortcomings of early approaches based on surface-tracking methods have been tackled with a so-called diffusive interface model. An in-house, three-dimensional simulation tool (FEDOS) has been augmented with this model, enabling simulations of electromigration-induced void evolutions based on our general electromigration void evolution model.

The results obtained from our simulation tool, utilizing our developed models, have demonstrated, that the ability of predicting the void evolution has been significantly improved as compared to previous approaches. The state-of-the-art has thereby been significantly advanced.

II. Brief project report

1. Report on research work

1.1 Information on the development of the research project

During the boot-up phase of the project, we investigated moving boundary methods, in particular the level set method (LSM) and the diffuse interface model (DIM). Our initial investigations were based on an in-house level set tool, providing the core procedures for the solution of the Hamilton-Jacobi equation as well as the level set handling based on the sparse field level set method (SFLSM). By using this tool, void migration in interconnects, preserving the void's shape, was simulated. Although those initial results were interesting, the extraction of the velocity via numerical methods applied to the void surface introduced a complication: The numerical surface velocity extraction step required the solution of several partial differential equations, in turn requiring surface extraction. As a consequence, important features of the beneficial SFLSM are lost, in particular the implicit description of the surface, efficient storage, and computation for mesh points near the surface only.

Due to these disadvantages, the research focus moved from the LSM to the DIM. Besides the implicit description of the void surface by a phase field parameter, the main advantage of this method is that it can be efficiently combined with the finite element method (FEM). In this way, the velocity field can be readily calculated, since the solution of the corresponding PDEs requires only a simple modification of their coefficients. Based on the DIM, an in-house three-dimensional finite element tool (FEDOS) has been enhanced, which was used throughout the project as the primary platform for numerical investigations. Although the chosen approach based on the DIM proved promising, some issues remained. In particular sufficiently locally adapted meshes are required to properly resolve the phase field parameter. This, however, introduces more mesh elements, in turn increasing the memory and computing demands, ultimately leading to longer simulation times.

The successful implementation of our models in the simulation platform (FEDOS) followed an in-depth investigation of the mathematical and physical modelling of the void evolution due to electromigration (EM). Initially, the numerical solution of the Cahn-Hilliard equation was investigated. The numerical discretization of the time-dependent equation for the phase field parameter in connection with the surface chemical potential equation was studied and implemented. In order to verify the implementation correctness, numerous simulations were carried out, which focused on analyzing the void shape change due to gradients of the surface chemical potential, in particular, due to gradients of the void surface curvature. First, two-dimensional test cases were run. For that purpose elliptical voids were initially set and the Cahn-Hilliard equation was solved. The curvature gradients generate atomic transport from regions of larger curvatures to smaller ones. Under such conditions an elliptical void relaxes to a circular shape. Tests were also carried out in fully three-dimensional structures, so that an ellipsoidal void relaxes to a spherical one. Although the correct physical behavior was obtained, the solution of this system of equations proved to be very challenging numerically, since significant instability and convergence problems were observed. This is mainly critical when the time steps for the discretization are large, so larger fluxes and shape variations occur. A second test case studied was the migration of the void due to the EM driving force. Atomic transport along the void surface in the direction of the electron flow causes void movement in the opposite direction, towards the cathode end of the line. Again, despite the correct physical behavior, the same instability and convergence issues were observed.

To further improve the accuracy of our model, we incorporated additional physical effects into FEDOS. In particular, the equations governing the vacancy transport through an interconnect line due to the various driving forces for vacancy migration (EM itself, diffusion, stressmigration) have been implemented. The combination of these equations together with the already previously implemented Cahn-Hilliard equation forms the main part of the by EM induced void evolution model. Various simulation tests were designed to check the implementation and model behavior, in particular:

- Transport only through the void surface region;
- Transport only through the bulk;
- Transport through the surface and bulk without transfer fluxes between these regions;
- Full transport including transfer fluxes.

In the first three tests the correctness of the implementation was verified. The expected transport behavior was clearly observed at sites of vacancy accumulation and depletion. The simulations were also rather stable and no critical problems, like convergence issues, were observed. However, the fourth test, in particular the transfer fluxes, posed several problems for the simulation. During this test a rather poor convergence behavior for the solution of the Cahn-Hilliard equation was observed.

The narrow band approach we had previously developed has been improved, in such a way that the exchange fluxes of vacancies between the bulk and the diffuse interface region are properly placed. Another important issue we have dealt with is the control of the time stepping scheme: We have observed that our standard approach is too aggressive for the solution of the model equations. Therefore, we have tested numerous published schemes and we finally decided to use a polynomial time step prediction scheme, which significantly improved the simulation flow.

Finally, we applied our simulation capabilities to investigate a novel interconnect structure, being open through-silicon via (TSV), where the conducting materials are aluminum and tungsten. For the diffuse interface approach conservation law was used where - beside the EM of the surface - the vacancies from the inside of the metal moving to the interface are taken into account. For modeling of the thermal mechanical problem the Navier-Cauchy and the heat equation were employed. These were linked to the EM-induced vacancy dynamics model used inside metal which in turn is based on a drift-diffusion model, using the so called Rosenberg-Ohring creation/annihilation term.

The conducted work described above has led to some minor changes of the work plan described in the proposal, triggered by our research findings; however, the overall plan was followed as foreseen in the proposal.

1.2 Most important results and brief description of their significance

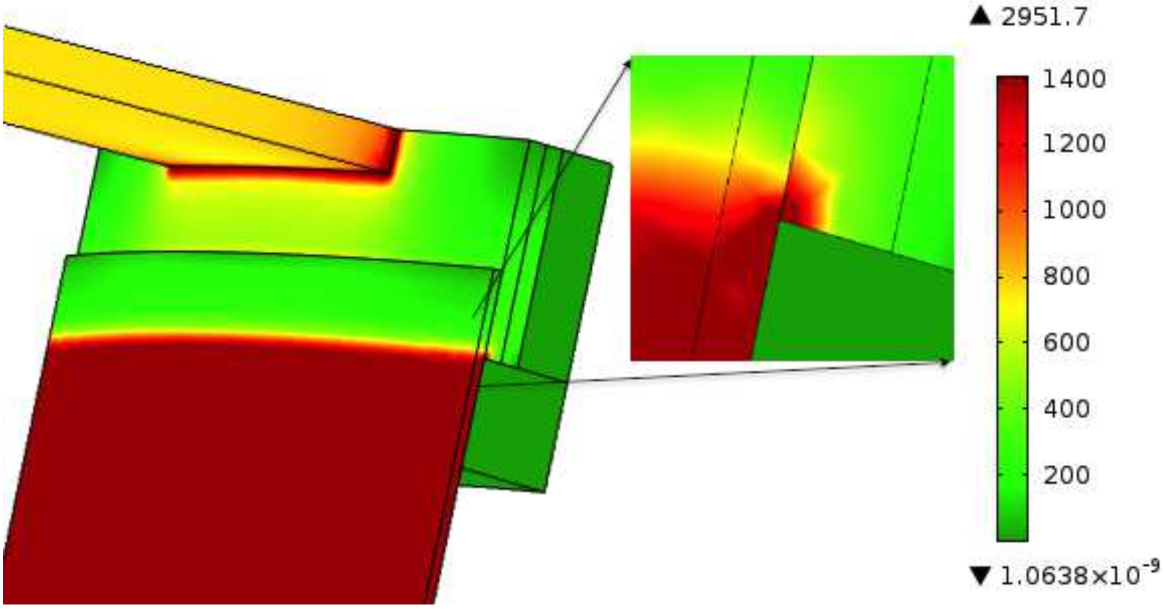
Our research yielded a general EM void evolution model as well as numerical techniques for an implementation in simulation tools, as was carried out for our simulation tool FEDOS. Our model incorporates void growth, migration, shape change, the impact of material interfaces, and microstructures, as well as the interactions with grain boundaries. We have specifically focused on three-dimensional problems, due to the importance to cutting-edge applications, such as open TSVs. Due to the complicated shapes and the ever-increasing demand for improved accuracy, three-dimensional simulations, as tackled in our research, are indeed essential to obtain an appropriate accuracy of the results. Additionally, we can treat multiple void scenarios, to investigate void agglomeration or break-up.

In particular, it was shown that the DIM is more suitable to EM-based void evolution research than the LSM; contrary to the latter, the first allows for a direct interface with the FEM, enabling the coupled solution of numerical models in concert with the boundary tracking step.

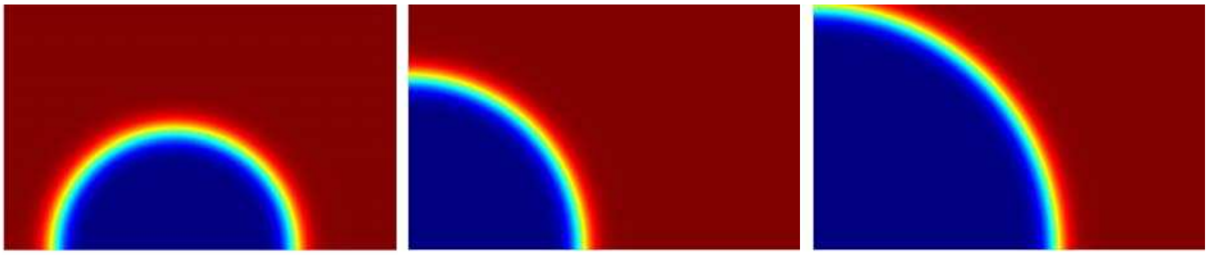
In order to improve the implementation and speed-up of the computation time a method applying a narrow band approach to the solution of Cahn-Hilliard equation was developed. In this method the phase field parameter solution is obtained for the mesh points located only within the diffuse interface region. Thus, the size of the linear system of equations to be solved is significantly reduced. This approach also led to an improvement in the stability by removing non-smooth solutions of the surface chemical potential at the diffuse interface boundaries.

Our investigations of open TSVs showed that a void is moved in the direction of the current. Due to the much larger resistance against EM of tungsten compared to aluminum the interface represents a barrier for vacancies and, therefore, the EM-induced transported material leads to the shrinking of the aluminum, resulting in the development of stress and the growth of the void. To investigate this peculiar effect, we specifically covered cases where the current, and thus the void, moves to the tungsten/aluminum interface. After reaching the interface, the surface (and therefore the surface energy) of the void is minimized as the void reshapes itself into a half-circle. Also, we have analyzed the resistance growth and qualitatively verified our findings relative to measurements in other structures.

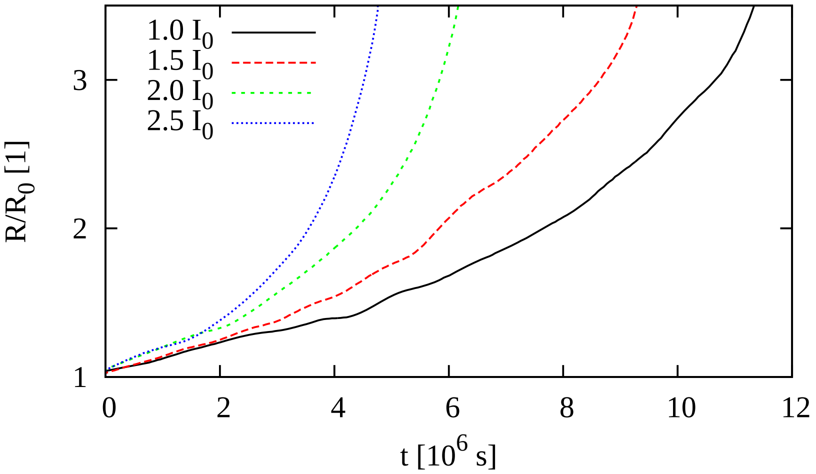
The following figure shows the current distribution in an open TSV segment. The current densities in the two metals differ strongly due to the different thicknesses of the metal layers. In the regions where the aluminium is overlapped by the tungsten the current is mainly flowing in the aluminium due to its lower resistance.



The movement of a void due to EM can be accurately tracked by our modelling approach, as can be seen in the following figure sequence. A void is migrating over timer from left to right.



Based on our model, the relative resistance of a TSV over time for different current densities can be computed, as shown in the following. With the growth of the void, the current density at the void surface also increases as the conducting cross-section is decreasing and leads to a higher EM flux, resulting in a nonlinear resistance increase.



1.3 Information on the execution of the project, use of available funds and any changes to the original project plan

The complete duration of the project was 48 months, 36 months were planned and an extension of 12 months without change of funding was granted. In the first years, the project team consisted solely of Dr. Roberto Lacerda De Orio; due to a shortage of suitable and interested PhD candidates in this highly challenging field. In the last phase of the project, a talented and interested PhD student, Mr. Wolfhard H. Zisser, and a postdoctoral researcher, Dr. Josef Weinbub, joined the team; the latter took over the postdoctoral position of Dr. Roberto Lacerda De Orio, who accepted a professoral position at a university in Brazil in spring 2014. In general, Dr. Roberto Lacerda De Orio laid the foundation of the research work, which was carried on by the PhD student Mr. Wolfhard H. Zisser. Dr. Josef Weinbub complemented the team's skills with respect to mesh generation and advanced computational science-related issues.

During the project all members regularly published and presented their results at international conferences and in scientific journals. The available funding was entirely spent as planned in the proposal. No significant changes to the original project plan were necessary.

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

The knowledge and experience gained during this FWF project serves as an excellent basis for further scientific work and personal development for all project members, including the project leader who supervised and guided the project member.

Dr. Roberto Lacerda de Orio had the opportunity to obtain valuable experience in organizing research work on the complex problem of EM-induced void migration, requiring time and personal management. All members benefited from the great opportunity to develop and improve their strategies for publishing obtained results and from the communication with the scientific community.

Mr. Wolfhard H. Zisser, the PhD student, had the opportunity to gain deeper understanding in the physical phenomena involved in the EM-processes as well as in the appropriate ways to mathematically model them. He will formally finish his doctoral studies in the coming autumn.

Dr. Josef Weinbub could extend his expertise in computational science with a new field, further extending his understanding and experience.

3. Effects of the project beyond the scientific field

Augmented by the knowledge gained during the project, Dr. Josef Weinbub helped organizing science summer internship programs for (under)graduate students at the TU Wien. These programs enable to foster young academics which is especially valuable as the highly specific field of simulation-based micro- and nanoelectronics lacks a broad visibility among the students regarding potential future careers in research. This puts further pressure on the availability of suitable candidates for future positions in research, which was also felt by during the beginning of this project by the lack of suitable PhD candidates.

4. Other important aspects

III. Attachments

1. Scholarly / scientific publications

1.1 Peer-reviewed publications / already published

Journals:

1. H. Ceric, R. Lacerda de Orio, W. H. Zisser, S. Selberherr:"Microstructural Impact on Electromigration: A TCAD Study", Facta Universitatis - series: Electronics and Energetics, 27 (2014), 1 – 11. doi: 10.2298/FUEE1401001C (Other OA)
2. **W. H. Zisser, H. Ceric, J. Weinbub, S. Selberherr:"Electromigration Reliability of Open TSV Structures", Microelectronics Reliability, 54 (2014), 2133 – 2137. doi:10.1016/j.microrel. 2014.07.099 (Other OA)**
3. **R. Orio, H. Ceric, S. Selberherr:"*Electromigration Failure in a Copper Dual-Damascene Structure with a Through Silicon Via",* Microelectronics Reliability, 52 (2012), 1981 – 1986. doi:10.1016/j.microrel.2012.07.021 (Other OA)**
4. **R. Orio, H. Ceric, S. Selberherr:"A Compact Model for Early Electromigration Failures of Copper Dual-Damascene Interconnects", Microelectronics Reliability, 51 (2011), 1573 – 1577. doi:10.1016/j.microrel.2011.07.049 (Other OA)**

Conference Proceedings:

1. W. H. Zisser, H. Ceric, J. Weinbub, S. Selberherr: "*Electromigration Induced Resistance Increase in Open TSVs*"; Poster: International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Yokohama, Japan; 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, 249 – 252. doi:10.1109/SISPAD.2014.6931610 (Other OA)
2. W. H. Zisser, H. Ceric, J. Weinbub, S. Selberherr: "*Electromigration Reliability of Open TSV Structures*"; 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: 978-1-4799-3931-2, 317 – 320. doi:10.1109/IPFA.2014.6898179 (Other OA)
3. R. Orio, H. Ceric, S. Selberherr: "*Influence of Temperature on the Standard Deviation of Electromigration Lifetimes*"; Poster: International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Glasgow, Scotland, United Kingdom; 2013-09-03 - 2013-09-05; in "*Proceedings of the 18th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*", (2013), 232 – 235. doi:10.1109/SISPAD.2013.6650617 (Other OA)
4. R. Orio, S. Selberherr: "*Physically Based Models of Electromigration*"; Talk: Conference on Electron Devices and Solid-State Circuits (EDSSC), Hong Kong; (invited) 2013-06-03 - 2013-06-05; in "*Proceedings of the International Conference on Electron Devices and Solid-State Circuits (EDSSC)*", (2013), 1 – 2. doi:10.1109/EDSSC.2013.6628175 (Other OA)
5. R. Orio, S. Selberherr: "*Formation and Movement of Voids in Copper Interconnect Structures*"; Talk: International Conference on Solid State and Integrated Circuit Technology (ICSICT), Xi'an, China; (invited) 2012-10-29 - 2012-11-01; in "*Proceedings of the International Conference on Solid-State and Integrated Circuit Technology (ICSICT)*", (2012), 378 – 381, doi:10.1109/ICSICT.2012.6467675. (Other OA)

6. R. Orio, H. Ceric, S. Selberherr: "*Electromigration Failure in a Copper Dual-Damascene Structure with a Through Silicon Via*"; Poster: 23rd European Symposium on the Reliability of Electron Devices, Failure Physics and Analysis, Cagliari, Italy; 2012-10-01 - 2012-10-05; in "*Proceedings of the 23rd European Symposium on the Reliability of Electron Devices, Failure Physics and Analysis*", (2012), 1981 – 1986. (Other OA)
7. R. Orio, H. Ceric, S. Selberherr: "*Modeling of Electromigration Induced Resistance Change in Three-Dimensional Interconnects with Through Silicon Vias*"; Talk: International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Denver, USA; 2012-09-05 - 2012-09-07; in "*Proceedings of the 17th International Conference on Simulation of Semiconductor Processes and Devices*", (2012), 268 – 271. (Other OA)
8. R. Orio, H. Ceric, S. Selberherr: "*Analysis of Resistance Change Development due to Voiding in Copper Interconnects ended by a Through Silicon Via*"; Talk: International Symposium on Microelectronics Technology and Devices (SBMicro), Brasilia, Brazil; 2012-08-30 - 2012-09-02; in "*ECS Transactions*", (2012), 273 – 280, doi:10.1149/04901.0273ecst. (Other OA)
9. R. Orio, H. Ceric, S. Selberherr: "*A Compact Model for Early Electromigration Lifetime Estimation*"; Talk: International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Osaka, Japan; 2011-09-08 - 2011-09-10; in "*Proceedings of the 16th International Conference on Simulation of Semiconductor Processes and Devices*", (2011), 23 – 26. doi: 10.1109/SISPAD.2011.6035068 (Other OA)
10. R. Orio, H. Ceric, S. Selberherr: "*Modeling Electromigration Lifetimes of Copper Interconnects*"; Talk: Intl. Symposium on Microelectronics Technology and Devices (SBMicro), Joao Pessoa, Brazil; 2011-08-30 - 2011-09-02; in "*ECS Transactions*", (2011), 163 – 169, doi:10.1149/1.3615190. (Other OA)

1.2 Non peer-reviewed publications / already published

1.3 Planned publications

2. Most important academic awards

3. Information on results relevant to commercial applications

4. Publications for the general public and other publications

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

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		1		1
Venia thesis (*Habilitation*) / Equivalent senior scientist qualification				
Postdoc		2		2
Ph.D. theses	1			1
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: Wählen Sie ein Element aus.		
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: Wählen Sie ein Element aus.		
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	**+2**
	Clarity	**+2**
	Intelligibility	**+2**

Procedures (submission, review, decision)

	Advising	**+2**
	Duration of procedure	**-1**
	Transparency	**0**

Project support

Advising	Availability	**+2**
	Level of detail	**+2**
	Intelligibility	**+2**

Financial transactions (credit transfers, equipment purchases, personnel management)	**+2**

Reporting / review / exploitation

	Effort	**+2**
	Transparency	**X**
	Support in PR work / exploitation	**X**

Comments on cooperation/interaction with the FWF: