STAND-ALONE PROJECT - FINAL REPORT

Project number P18825-N14

Project title Electromigration Simulation

Project leader O.Univ.Prof.Dipl.-Ing.Dr. Siegfried SELBERHERR

1. Summary for public relations work

English version:

Electromigration is the biggest reliability problem for interconnect structures in modern integrated circuits. Electromigration is the transport of material caused by electric current. It is kind of a ‘time bomb’, which can cause total failure of a circuit at an unspecified time. Electromigration is often accompanied by stress migration, a diffusion controlled process in which the driving force for the transport of material is the gradient of mechanical stress. Highly integrated microelectronic circuits (eg. microprocessors) require dense wiring structures. With the resulting increase in current density, electromigration induced failure becomes a more and more challenging issue. Significant advance has been made by choosing copper instead of aluminum as interconnect metal, because copper has an improved electromigration bulk resistance. On the other hand the low copper affinity introduces high diffusivity paths along copper/barrier interfaces and thereby promotes nucleation of intrinsic voids in the interconnect metal. The design of an electromigration compatible interconnect layout is a complex task which can not be handled by using simple design rules.

There exists a lot of theoretical work available for explaining and modeling of the manifold physical phenomena behind electromigration, but only a very small part of it was actually implemented in software tools and tested on real world applications. In the scope of this project the state of the art of the physical models was evaluated and weak points were identified and eliminated. With the best models a widely applicable interconnect reliability characterization tool was then developed and verified on real world applications.

The achieved findings will enable the fabrication of more reliable integrated circuits.

German version:

Die Elektromigration stellt das größte Zuverlässigkeitsproblem für Verdrahtungsstrukturen in modernen integrierten Schaltungen dar. Unter Elektromigration versteht man einen Materialtransport, der durch elektrischen Strom verursacht wird. Es ist eine Art ‚Zeitbombe', welche einen totalen Ausfall des Schaltkreises zu einem unbestimmten Zeitpunkt auslösen kann. Die Elektromigration wird oft von Stressmigration begleitet, einem diffusionsgesteuerten Prozess, bei dem die treibende Kraft für den Materialtransport im Gradienten der mechanischen Spannung begründet ist. Hoch integrierte mikroelektronische Schaltungen (z.B. Mikroprozessoren) verlangen dichte Verdrahtungsstrukturen. Mit der daraus resultierenden Zunahme an Stromdichte, werden Ausfälle durch Elektromigration ein immer kritischeres Problem. Bedeutender Fortschritt wurde durch die Verwendung von Kupfer statt Aluminium als Verbindungsmetall erreicht, weil Kupfer eine höhere Elektromigrationsfestigkeit hat. Andererseits führt die niedrige chemische Affinität des Kupfers zu schnellen Diffusionspfaden entlang der Kupfer/Barriere-Übergänge und fördert dadurch die Keimbildung von Lunkern innerhalb des Verbindungsmetalls.

Der Entwurf einer elektromigrationsgerechten Verdrahtungsstruktur ist eine komplizierte Aufgabe, die nicht durch die Anwendung von simplen Regeln gelöst werden kann. Viel theoretische Arbeit wurde mit Bemühungen geleistet, die vielfältigen Phänomene hinter der Elektromigration zu erklären, aber nur ein kleiner Teil davon wurde wirklich in Computerprogramme, die der Entwurf von Verdrahtungsstrukturen unterstützen, umgesetzt und an realen Anwendungen getestet. Im Rahmen dieses Projektes wurden die neuesten physikalischen Modelle evaluiert und mögliche Schwachpunkte erkannt und beseitigt. Die besten Modele wurden dann in ein allgemeines Simulationsprogramm für die Beschreibung der Zuverlässigkeit moderner Verdrahtungsstrukturen implementiert und an realen Anwendungen verifiziert.

Die gewonnenen Erkenntnisse werden die Fertigung von zuverlässigeren integrierten Schaltungen ermöglichen.

2. Brief project report

2.1. Report on the scientific work

2.1.1. Information on the development of the research work

The microstructure of interconnects, e.g. network of grain boundaries, crystal orientation inside the grains, and stress dependence of grain bulk diffusivity, now plays a crucial role in determining interconnect behavior under the impact of electromigration.

Current electromigration models, used for simulation and analysis of interconnect reliability, lack an appropriate description of the metal microstructure and consequently have a very limited predictive capability. The goal of this project was an adaptation and further development of models describing electromigration in connection with the metal microstructure and the integration of these models in an overall electromigration material transport model.

There were three key aspects of microstructure modeling located around a central problem, namely, the role of grain boundaries in the development of electromigration failure. The first aspect is point defect dynamics, including the grain boundary as a fast diffusion path, while the second is the role of grain boundaries as a medium capable of producing and annihilating point defects. Finally, the third aspect is the interaction between a grain boundary and the metal interfaces, which has a crucial significance in the void nucleation process.

The project began with an evaluation of available theoretical work and an adjustment of the most adequate models which describe the microstructure impact on electromigration-induced material transport in interconnects. The models describing the metal microstructure have been implemented in a simulation tool, following a careful study of the corresponding numerical algorithms. A final decision about optimal models for simulation has been made after a comparison of simulation results with relevant experiments. Parallel to this work, a general electromigration model has been implemented, including an electro-thermal model, a point defect (vacancy) transport model, and a model connecting electromigration and stress migration.

Beyond the initial plan of developing grain boundary models, the work has been successfully extended to the study of stress-dependent diffusivity and statistical aspects of electromigration failure. This extension was a necessary step in order to fully exploit the developed grain boundary models. Most notably, statistical studies involving the artificial generation of microstructures similar to the copper microstructure in state-of-the-art interconnects have enabled new and significant insight into the nature of electromigration failure.

2.1.2. Most important results and their significance

The project has made contributions in three distinct areas. The first and central contribution is the physical modeling of microstructural characteristics, such as grain boundaries and stress dependence of material transport. The second contribution is the numerical optimization of the spatial discretization for an accurate simulation of microstructural features. The third and final contribution is the development of an application methodology for the newly developed models and numerical methods.

The previous grain boundary models are all based on a Rosenberg-Ohring recombination term and are highly phenomenological. Detailed insight into the vacancy dynamics and the role of stress was lacking. Based on recent experimental observations and our theoretical analysis, a new grain boundary model was developed. The model includes the detailed balance relationship at the grain boundary and in the vicinity of the grain boundary. The grain boundary is considered to be a medium capable of capturing and releasing vacancies. Captured vacancies induce tensile stress, while at the same time, the capacity of a grain boundary to absorb vacancies depends on stress.

A general electromigration tool, also implemented during the project period, has been extended by an implementation of this new grain boundary model. Additionally, after initial testing, some optimization regarding efficiency and numerical accuracy has been performed.

Residual process stress, thermo-mechanical stress, and stress induced by vacancy migration sums up to a complex stress picture, which causes the anisotropy of material transport to be consequently modeled with tensorial diffusivity. The first step involved the careful study of all available models and the analysis of their applicability to modern copper interconnect technologies. Furthermore, a numerically efficient integration in the previously implemented macroscopic electromigration environment had to be considered.

For the purpose of obtaining an accurate simulation, grain boundaries and, more generally, every interface of the problem geometry had to be supplied with an appropriately fine finite element mesh. This is necessary in order to provide sufficient resolution for the local dynamics described with the grain boundary model. In the scope of the project, a novel numerical method has been developed for setting slices of fine mesh around grain boundary planes that depend on the physical parameters of the model.

The complexity of the mathematical model has made it necessary to invent and test novel concepts for the handling of sub-models. The goal was to attain sufficient accuracy and stability of numerical algorithms without significantly increasing the computational costs. The solution was found in a hierarchical handling of sub-modules, according to a unique priority list. The electro-thermal model has the highest priority, followed by material transport equations and the mechanical problem.

For a given interconnect layout and monocrystalline material, simulation will provide a unique time-to-failure. All impact factors, e.g. geometry of the layout, bulk diffusivity, interface diffusivity, and mechanical properties are deterministic, resulting in a deterministic time-to-failure. However, the situation changes, when the interconnect possesses a microstructure. The microstructure has a significant impact on electromigration, since it introduces a diversity of possible electromigration paths and local mechanical properties.

The purpose of the simulation is the extrapolation of extended-time interconnect behavior on the basis of the results of accelerated electromigration tests. The methodology developed and used in this project is clearly capable of going beyond an extrapolation by standard statistical methods, which rely on Black’s equation and extrapolate a time-to-failure for a single interconnect structure. The usage of TCAD tools enables a prediction of the behavior for structures obtained by varying the geometrical properties and operating conditions of a previously investigated initial test structure. The applied scenario for the application of an electromigration reliability TCAD tool is:

- Model Calibration. For this purpose we use one layout and many test units. At the end of the calibration, all parameters of the model are fixed. During this process, different microstructures are considered and simulation parameters are varied in order to reproduce experimental failure time statistics.
- Model Application. The calibrated model is used for simulation. The simulation extrapolates the behavior of an interconnect under real life conditions.

The experimental electromigration data is regularly described by lognormal distributions. Although the origin of the lognormal distribution for electromigration lifetimes is not entirely clear, it has been argued that the diffusion process, in connection with the effect of the microstructure on electromigration, provides the basis for the lognormal distribution. Understanding of the electromigration lifetime distribution is crucial for the extrapolation of the times to failure obtained empirically, from accelerated tests, to the real operating conditions, as performed by a modified form of the Black equation. Also, it has been shown that the microstructure plays a key role regarding the failure mechanisms in dual-damascene copper interconnects.

Since the copper grain sizes seem to follow lognormal distributions in typical dual-damascene process technologies and, due to the influence of the microstructure on the electromigration process, the lognormal distribution has been used as the underlying statistics for electromigration lifetimes. The models and methods developed in the project have enabled a thorough study of the relationship between the grain size distribution and the distribution lifetime.

In order to include the grain distribution in the numerical simulations, a microstructure generation tool has been developed. Given a specific interconnect structure and providing the tool with a median grain size and corresponding standard deviation, it generates a lognormal distribution of grain sizes.

Careful and extensive simulations have shown a direct connection between the lognormal distribution of grain boundaries and the lognormal distribution of electromigration lifetimes. Moreover, simulations have revealed an interesting relationship between the statistical properties of grain size distribution, such as the mean value and variance, to the corresponding properties of lifetime distribution. These new insights will enable significant improvements for the extrapolation capabilities of electromigration models.

During the final reporting period, investigations were carried out for both failure development prior to void nucleation as well as during the void evolution phase. Theoretical studies of the void nucleation condition were also carried out. The significance of the nucleation condition lies in the fact that it is a connection between void nucleation and void evolution models. Subsequently, in order for these models to be applied properly, the nucleation condition must be understood and modeled sufficiently well. In the final reporting period, a Level-Set based model of the evolving void surface was developed and implemented. The model describes void evolution under the influence of surface electromigration and self-diffusion.

The three-dimensional void evolution modeling and simulation was not initially intended to be part of the project, but it was included due to the successful overall progress and concurrent research interests. With a simple void evolution model, it was possible to make an additional plausibility study of novel grain boundary models by observing how encounters with grain boundaries influence the evolving void surface. Even without including stress effects on the void surface (which would have been numerically very demanding) the obtained simulation results reproduced the experimental results very well. The simulated shape of the void after consecutive encounters with grain boundaries has matched well with experimental scanning electron microscope pictures. Simulation has also accurately predicted the run of the time-resistance curve during void evolution. Nevertheless, modeling void evolution still requires considerable research.

With the implementation of a three-dimensional grain boundary model and void evolution model, all necessary models for a comprehensive electromigration simulation were completed and prepared for verification. The verification procedure has been performed by separately applying the model developed for the void nucleation and the void evolution phase, in combination with the corresponding experimental results. The new grain boundary model, embedded in a comprehensive electromigration model already implemented in FEDOS (Finite Element Diffusion and Oxidation Simulator), was fully verified by comparing its prediction for the distribution of failure times during an accelerated electromigration test with experimental results. The interaction of evolving voids with grain boundaries, predicted by the developed model, appeared to be in excellent agreement with experimental observations. Finally, we conclude that, with the implementation of the electro-thermal model, the vacancy-dynamics model, the stress-electromigration interaction model, and the grain boundary model, along with their complete verifications, the overall goals of the project have been completely reached.

The further development of the applied methodology of using statistical simulations, combined with the results of accelerated electromigration tests, will surely prove fruitful in reliability engineering.

2.1.3. Information on the running of the project

The complete duration of the project was 36 months. The project team consisted of Dr. Hajdin Ceric and M.Sc. Roberto Lacerda de Orio. The literature study was carried out by both project members, with Dr. Ceric having his focus on theoretical models and M.Sc. Lacerda de Orio predominantly studying experimental publications. The development of new models was mostly performed by Dr. Ceric, but in discussion with M.Sc. Lacerda de Orio. Both members of the project were active in developing numerical algorithms, where their practical implementation in a software tool was carried out by M.Sc. Lacerda de Orio.

The software tool was gradually developed and each step was concluded by carrying out extensive tests to assess physical plausibility of the models. The simulation tests were carried out by M.Sc. Lacerda de Orio. Both project participants took part in discussing and evaluating the results.
During the project, Dr. Ceric and M.Sc. Lacerda de Orio periodically published and presented their results at international conferences and in scientific journals.

2.2. Personnel development

The knowledge and experience acquired during the FWF project has founded an excellent basis for further scientific work and personal development of both project members.
Problems and limitation of physical modeling for reliability related phenomena on macroscopic level recognized during the project have motivated Dr. Ceric to apply for a Christian Doppler Laboratory which was approved in December 2009. During the project Dr. Ceric has also gained a valuable experience in organizing research work around a complex problem, which demands careful time and personal management. For both project members, the project has also been a unique opportunity to develop and improve strategies for publishing the achieved results and for communicating with scientific community.
M.Sc. Lacerda de Orio, as doctoral student during the project, has attained the ability to deal with problems within three different areas. First, he significantly improved his programming skills in C++, second he developed his own methodological approach in designing numerical algorithms, and third he gained the capability to recognize the weaknesses and limitations of studied physical models and make improvements.
Both Dr. Ceric and M.Sc. Lacerda de Orio have made a valuable and useful experience in dealing with experimental data obtained either from published materials or obtained from industrial partners.

2.3. Effects of the project outside the scientific field

In September 2007, the project members with support of the Institute for Microelectronics organized an ‘International Workshop on Electromigration Reliability’, where practically all international electromigration experts participated. In front of this eminent audience Dr. Ceric also gladly presented work performed in the scope of the project.

http://www.sispad.org/sispad/sispad-events/sispad-2007/companion-workshops/workshop-on-electromigration-reliability.html

Following the workshop a Special Issue of IEEE Transaction on Device and Materials Reliability was published in March 2009, where speakers from the workshop and the FWF project members have published their newest achievements.

3. Information on project participants

not funded by the FWF			**funded by the FWF (project)**		
co-workers	**number**	**Person-months**	**co-workers**	**number**	**Person - months**
non-scientific co-workers			non-scientific co-workers		
diploma students	1	6	diploma students		
PhD students	1	36	PhD students		
post-doctoral co-workers			post-doctoral co-workers	1	36
co-workers with “Habilitation” (professorial qualifications)			co-workers with “Habilitation” (professorial qualifications)		
professors	1	6	professors		

4. Attachments

List 1

1.a. scientific publications

1.a.1. Peer-reviewed publications (journals, contribution to anthologies, working papers, proceedings etc.)

1) R. L. de Orio, H. Ceric, S. Selberherr, "Effect of Strains on Anisotropic Material Transport in Copper Interconnect Structures under Electromigration Stress," in: *Journal of Computational Electronics*, vol.7, no.3, pp.128 -131, (2008).
2) H. Ceric, R. L. de Orio, J. Cervenka, S. Selberherr, “A Comprehensive TCAD Approach for Assessing Electromigration Reliability of Modern Interconnects,” in: *IEEE Transactions on Device and Materials Reliability*, vol.9, no.1, pp.9-19, (2009).
3) R. L. de Orio, H. Ceric, S. Selberherr, “Analysis of Electromigration in Dual-Damascene Interconnect Structures,” in: *Journal of Integrated Circuits and Systems*, vol.9, no.2, pp.67-72, (2009).

1.a.2. Non peer-reviewed publications (journals, contribution to anthologies research reports, working papers, proceedings, etc.)

1.a.3. Stand-alone publications (monographies, anthologies)

1.b. publications for the general public and other publications

List 2 project-related participation in international scientific conferences

2.1. Conference participations - invited lectures

1) H. Ceric, S. Selberherr: "Electromigration in Interconnect Structures of Microelectronic Circuits," in: *Proc. Microelectronics, Electronics, and Electronic Technologies,* pp. 23 – 28, (2007).
2) H. Ceric, S. Selberherr, "Electromigration Modeling for Interconnect Structures in Microelectronics," in: *Proc. Intl. Symp. on Microelectronics Technology and Devices*, pp. 295-304, (2007).
3) H. Ceric, R. L. de Orio, S. Selberherr. "Comprehensive Modeling of Electromigration Induced Interconnect Degradation Mechanisms," in: *Proc. Intl. Conf. on Microelectronics,* pp. 69-76, (2008).

2.2. Conference participations - lectures

1) R. L. de Orio, H. Ceric, S. Selberherr, "Strain-Induced Anisotropy of Electromigration in Copper Interconnect," in: *Proc. Intl. Semiconductor Device Research Symp.*, pp.TA4-01.1-2, (2007).
2) H. Ceric H., R. L. de Orio, J. Cervenka, S. Selberherr, "TCAD Solutions for Submicron Copper Interconnect"; in: *Proc. Intl. Symp.on the Physical and Failure Analysis of Integrated Circuits*, pp.78-81, (2008).
3) R. L. de Orio, Carniello S., H. Ceric, S. Selberherr, "Analysis of Electromigration in Dual-Damascene Interconnect Structures," in: *Proc. Intl. Symp. on Microelectronics Technology and Devices*, pp. 337-348, (2008).
4) R. L. de Orio, H. Ceric, J. Cervenka, S. Selberherr, "The Effect of Microstructure on the Electromigration-Induced Failure Development," in: *Proc. Intl. Symposium on Microelectronics Technology and Devices*, pp.345-352, (2009).
5) H. Ceric, R. L. de Orio, J. Cervenka, S. Selberherr, "The Effect of Microstructure on Electromigration Induced Voids," in: *Proc. Intl. Symp. on the Physical and Failure Analysis of Integrated Circuits*, pp. 694-697, (2009).
6) R. L. de Orio, H. Ceric, J. Cervenka, S. Selberherr, "The Effect of Copper Grain Size Statistics on the Electromigration Lifetime Distribution," in: *Proc. Intl. Symp. on Microelectronics Technology and Devices*, pp. 182-185, (2009).
7) H. Ceric, R. L. de Orio, J. Cervenka, S. Selberherr, "Copper Microstructure Impact on Evolution of Electromigration Induced Voids," in: *Proc. Intl. Symp. on Microelectronics Technology and Devices*, pp. 178-181, (2009).
8) R. L. de Orio, H. Ceric, J. Cervenka, S. Selberherr, "Electromigration Failure Development in Modern Dual-Damascene Interconnects," in: *Proc. Intl. Conference on Very Large Scale Integration*, pp.15.1-15.5 (2009).
9) R. L. de Orio, H. Ceric, J. Cervenka, S. Selberherr, "The Effect of Microstructure on the Electromigration Lifetime Distribution," in: *Proc. Intl. Symp. on the Physical and Failure Analysis of Integrated Circuits*, pp. 731-734, (2009).

2.3. Conference participations - posters

1) R. L. de Orio, H. Ceric, S. Selberherr, "Effect of Strains on Anisotropic Material Transport in Copper Interconnect Structures under Electromigration Stress," in: *Proc. Intl. Workshop on Computational Electronics*, pp. 62 – 63, (2007).
2) R. L. de Orio, H. Ceric, S. Carniello, S. Selberherr. "Analysis of Electromigration in Redundant Vias," in: *Proc. Intl. Conf. on Simulation of Semiconductor Processes and Devices*, pp. 237-240, (2008).
3) H. Ceric H., R. L. de Orio, J. Cervenka, S. Selberherr. "Analysis of Microstructure Impact on Electromigration," in: *Proc. Intl. Conf. on Simulation of Semiconductor Processes and Devices*, pp. 241-244, (2008).

2.4. Conference participations - other

List 3 Development of collaborations

Indication of the most important collaborations (maximum 5), that took place (initiated or continued) in collaboration please give the name of the collaboration partner (name, title, institution) and a few words about the scientific content. Please also assign one of the following **categories** to each collaboration:

N			Nature	**N** **E** **I**	(national); (European); (other international cooperation)
	E		Extent	**E1** **E2** **E3**	**low** (e.g. no joint publications but mention in acknowledgements or similar); **medium** (collaboration e.g. with occasional joint publications, exchange of materials or similar but no longer-term exchange of personnel); **high** (extensive collaboration with mutual hosting of group members for research stays, regular joint publications etc.)
		D	Discipline	**D** **T**	within the discipline transdisciplinary

N	E	D	Collaboration partner / content of the collaboration
			1) Name: Title: Institution: Content:
			2) Name: Title: Institution: Content:
			3) Name: Title: Institution: Content:
			4) Name: Title: Institution: Content:
			5) Name: Title: Institution: Content:

Note: general scientific contacts and occasional meetings should not be considered as collaborations in the above sense.

List 4 “Habilitations” (professorial qualifications) / PhD theses / diploma theses

with an indication of the status (in progress / completed)

4.1. Professorial Qualifications

The work performed in this project is the basis for a Habilitation thesis of Dr. Ceric.

4.2. PhD Theses

During the project period M.Sc. Lacerda de Orio completed his doctoral thesis: ‘Electromigration modeling and simulation’.

4.3. Diploma Theses

During the project period Karl Rupp completed his master thesis ‘Multiphysics Modelling in the Context of Generative Programming’.

List 5 Effects of the project outside the scientific field (where appropriate)

Sections of the list:

5.1. Organization of scientific events

In September 2007, in the scope of “The International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)” the “International Workshop on Electromigration Reliability” was organized.
http://www.sispad.org/sispad/sispad-events/sispad-2007/companion-workshops/workshop-on-electromigration-reliability.html

5.2. Particular honours, prizes etc.

5.3. Information on results relevant to commercial applications

5.4. Other effects beyond the scientific field

5.5. Relevance of the project in the organization of the relevant scientific discipline

List 6. Applications for follow-up projects

6.1 Applications for follow-up projects (FWF projects)
In April 2009 Prof. Selberherr inspired by the findings in this research applied for the project ‘Void Evolution due to Electromigration’.

6.2 Applications for follow-up projects (Other national projects)
In Mai 2009 Dr. Ceric applied for the ‘Christian Doppler Laboratory for Reliability issues in Microelectronics’. The laboratory was approved in December 2009.

6.3 Applications for follow-up projects (International projects)