STAND-ALONE PROJECT - FINAL REPORT

Project number	P-17927-N13
Project title	**Ionenimplantation für die SiGe Halbleitertechnologie**
Project leader	Dipl. Ing. Dr. Andreas HÖSSINGER

1 Summary for public relations work

In order to manufacture integrated circuits a lot of processing steps have to be performed to transfer a circuit physically into silicon. One of these process steps is ion implantation, which is used to selectively put dopant atoms into the device structures which are established in the substrate material. The process of ion implantation ensures a very high spatial selectivity, which is a must due to the very small dimensions of the devices in state of the art and future integrated circuits. In order to estimate and predict the spatial distributions of the dopant atoms in the final device structures, simulations of the ion implantation process can be performed. The ion implantation simulation tool which has been extended and improved within the scope of the project is capable of predicting the full three-dimensional dopant distribution in a full three-dimensional device geometry. This simulation tool uses the physically based Monte-Carlo method (in contrast to empirical analytical methods) to predict the dopant distribution, by calculation the trajectories after entering the substrate, of a large number of ions. Anyhow this method still uses some empirical models to describe the interaction of the implanted ions with the substrate material.

In former technologies semiconductor devices were made up mainly of crystalline silicon in combination with several other amorphous and poly-crystalline materials. In state of the art technologies adding epitaxial crystalline regions made of silicon-germanium is getting more prominent to introduce stress into the devices. For simulation this means that the simulation tool has to be capable of handling multiple regions with different crystalline topology in a single device. This single device is usually the spatial domain for simulation analysis. Within the scope of the project the Monte-Carlo simulation tool MCIMPL-II has been extended to make this capability available. Actually the object oriented design of the simulator was used to implement completely independent models for the various crystalline regions of the device. Nevertheless adding the capability to simulate new types of materials namely silicon-germanium, also means adjusting the empirical models selectively for these new types of materials. Therefore also a well selected set of experiments has been performed within the scope of the project to evaluate the empirical models and to calibrate the empirical parameters within these models. The experiments have covered various dopant species typically used in semiconductor technology. A large set of substrates (different germanium content and different wafer orientation) have been implanted with various types of doping species and implantation conditions. The implantation conditions were chosen such that various empirical parameters in the simulation models could be investigated independently. Secondary ion mass spectroscopy (SIMS) techniques have been used to measure the doping distributions in the implanted samples. Analysing the experimental results and comparing with simulations has verified the fact that the models for silicon germanium, which has been derived from the models for silicon are well applicable also for silicon germanium alloys. But it has also shown that some empirical model parameters have to be adjusted for alloys with various silicon germanium content. Nevertheless the experience gained has allowed to come up with predictive simulation capabilities since the adjustments are a smooth function of the germanium content.

2 Brief project report

2.1 Report on the scientific work

2.1.1 Scientific concepts and goals

The goal of the project was to develop and improve an extendible simulation tool for the simulation of ion implantation and the calibration of this simulation tool for a new field of applications. The main target was the accurate and predictive simulation of the implantation of doping atoms into silicon-germanium substrates and silicon-germanium layers in advanced semiconductor devices. In order to obtain the required accuracy, a simulation tool based on the Monte-Carlo method had to be extended to be flexible enough to handle simultaneously multiple crystalline materials with distinct material properties. The main motivation was that such a simulation tool could be applied to ion implantation simulation into state of the art semiconductor devices which are composed of several types of semiconductor (active) materials (e.g. silicon in various strain states and silicon-germanium to introduce strain). Thereby the main challenge was to handle multiple crystalline materials within one simulation structure, so that the ion implantation characteristics in devices made of silicon and silicon-germanium alloys can be reasonable analysed by the simulation tool.

Even so the Monte-Carlo method for the simulation of ion implantation is based on principle physical concepts and behaviour of atoms, some modelling parameters have to be calibrated to correctly reproduce experimentally obtained doping profiles. For the purpose of calibration a series of experiments had to be carried out within the scope of the project to derive these calibrations parameters. Carefully selected experiments for the various calibration parameters were set-up. The goal was to distinguish energy loss calibration parameters from crystal damage related parameters. As a consequence experimental conditions have been defined which were extremely challenging for the experimental analysis. Moreover the experimental conditions were chosen such that the calibration parameters could be investigated under various process conditions (different energies, doses and ion beam angles) and for varying material properties (different germanium content in the alloys). Thereby the simulation tool could not only be calibrated, also the applicability of the applied models for a wide variety of process conditions should be evaluated.

The analysis was focused on typical n-type and p-type doping species applied in advanced semiconductor technology. There arsenic is the most prominent n-type dopant and boron the most prominent p-type dopant. In order to implant boron not only single atomic boron ions, but also BF_2 ions are frequently used to obtain shallow doping profiles. All three doping species were considered in the experimental investigations.

Finally some experiments were carried out to investigate whether stress has an influence on the doping profiles, because it was speculated that stress could change the activation energy for damage generation.

2.1.2 Activities and Results

Within the scope of the project two major tasks had to be carried out. On the one hand the simulation tool MCIMPL-II had to extended and adapted in a way that it is capable of handling multiple crystalline materials simultaneously. On the other hand a serious of experiments had to be carried out to provide an experimental data basis for calibration and verification of the simulation tool.

2.1.2.1 Extension of the Monte-Carlo simulator MCIMPL-II

When applying the Monte-Carlo method for the simulation of ion-implantation the trajectories of a large number of ions when passing though the target material are calculated. The doping profile is obtained by counting the final positions of the ions in a cellular mesh covering the simulation domain. The interaction with the target material is described on an atomistic basis. In order to be able to correctly simulate and model the implantation into a structure which is composed of multiple materials, especially of multiple crystalline materials and of materials with special atomistic arrangements like surfaces it is necessary to represent the target somehow on an atomistic level. Since this is not feasible due to the size of the simulated structures, special techniques are used to obtain proper collision partners along the trajectory of the ion. The standard techniques rely on targets being composed only of single crystalline materials. Usually these materials can only be simulated in combinations with amorphous materials. Doing so the atoms of the crystal have well defined positions in the three-dimensional space. In this approach multiple materials are handled by selecting collision partners either from this infinite crystal (single crystalline material) or randomly (amorphous material). This approach cannot be used for simulating ion implantation into several crystalline materials with locally varying crystal structure (e.g due to lattice mismatch).

In order to make the implantation into multiple crystalline materials feasible an object oriented modelling system has been implemented in MCIMPL-II. This means that the target structure is represented on two scale levels. The structure with

- all its material regions,
- all properties within these material regions,
- all interfaces of these material regions and
- all properties assigned to these interfaces

is represented on the basis of an unstructured grid. For means of ion implantation simulation the structure is split into regions, whereby one region is characterised by homogenous atomistic properties. A separate model set is assigned to each of these regions. When the ion enters a region while it moves through the target the model set related to this regions is activated. Thereby different model sets with different calibration parameters can be applied to various parts of the simulation domain. This allows to distinguish crystalline bulk regions form crystalline epitaxial regions, or from strained epitaxial layers, or from amorphous regions, or from poly-crystalline regions or from material interface regions. A model set contains models which determine,

- how the atomistic neighbourhood of the ion looks like and how the next collision partner can be found (atomistic material model),
- how the scattering is calculated in the neighbourhood of the ion (nuclear stopping model),
- how the electronic stopping is calculated in the neighbourhood of the ion (electronic stopping model),
- how the damage generation is calculated in the neighbourhood of the ion (damage generation model).

Within the course of the simulation and on the basis of these models also additional information is generated which is stored on a simulation grid (e.g. amount of crystal damage). This information can be used by all models later throughout the simulation. The models of the model-sets have been implemented in an object oriented manner. This object oriented structure is especially relevant for the atomistic material model, which most significantly differs for the various types of regions. This model mainly transforms the information stored on the unstructured grid and the simulation grid into an atomistic representation of the material around the current ion position. It is quite obvious that the models used for the various material types significantly differ in calculation speed. While the fast standard

algorithms can be used in the model for crystalline bulk materials or amorphous materials slower and more explicit algorithms have to be used for the other types of materials to translate the continuum information into an atomistic material representation.

2.1.2.2 Experimental work

Beside the enhancement of the simulation tool MCIMPL-II a major task within the scope of the project was to obtain experimental data which could be used as a data basis for calibration of the model parameters applied within silicon-germanium bulk, silicon-germanium epitaxial region and strained silicon regions. A series of implantation experiments for the implantation of the typical n-type dopant arsenic and of the most frequently used p-type dopants boron and BF_2 have been carried out. Performing the experiments has raised a series of issues and problem which were not anticipated when starting the project.

Initially the goal was to cover wide range of substrate types with the experimental analysis. The plan was to use silicon-germanium substrates with a germanium content of up to 75%. During the wafer acquisition process it turned out that the wafer suppliers contacted could deliver a the requested substrates with appropriate specifications. Since it was not intended to start a research task on substrate manufacturing, it was decided to narrow the range down to 30% germanium content. This was still a reasonable range to investigate the variations of the model parameters. Even so the wafer supplier had promised to provide also <110> substrates within the requested specification, analysis of the samples had turned out that the <110> wafers with the higher germanium content were not mono-crystalline but poly-crystalline or even amorphous. Nevertheless some influence of the germanium content could be investigated also on the basis of the <110> substrates.

Moreover the SIMS analysis of the samples has raised some issues. In order to be able to neglect the influence of implantation induced damage quite low implantation doses have been chosen for the implantation experiments with arsenic and with BF_2 ions. It turned out that none of the applied SIMS analysis techniques was able to resolve the arsenic doping profiles with sufficient accuracy to provide suitable profiles for calibration purposes from the experiments with the <100> wafer substrates. Nevertheless high quality boron profiles have been obtained from the implantation experiments with boron and with BF_2 ions. In further experimental runs arsenic implantations with significantly higher doses have been performed into the <110> wafers. Unfortunately damage parameters cannot be distinguished from stopping parameters under these conditions, which leaves some uncertainty in the calibration.

The comparisons between the experimental data and the simulation results based on calibration parameters for silicon have shown that especially the electronic stopping behaviour was highly optimised for the simulation of ion implantation into crystalline silicon. Even so the electronic stopping model applied for silicon theoretically already considers the influence of various atom species in the target, the comparisons have shown that the model was highly optimised only for pure silicon targets, while the influence of the presence of germanium atoms was overestimated. On the basis of the experimental data it was found that different empirical calibration parameters have to be derived for different silicon germanium composition. Since these empirical parameters are a smooth function of the germanium content, at least within the investigated range of germanium content, still a good predictability of simulation results also for substrates with higher germanium content (beyond the range of experimental investigation) can be expected.

As far as the damage generation is concerned no significant impact of the germanium content could be observed. Using the same damage generation parameters as previously used for the

simulation of ion implantation into silicon did properly reproduce the dose dependency observed in the experimental analysis. This means that as far as the empirical model parameters are concerned, strained silicon regions can be treated as bulk silicon regions. Nevertheless the deformed crystal structure in the strained silicon regions has to be taken into account.

2.1.3 Project administration

2.1.3.1 Project duration and organization

Initially it was planned to carry out the project within a one year period. While all software implementation aspects could be finished as planned, several unforeseen problems in performing the experiments and the experimental analysis have caused a delay of the experimental tasks and also a delay of the software calibration activities. The substrate material for the implantation experiments was delivered quite late and part of the requested substrate material (<110> silicon germanium wafers) could not be delivered with the specifications requested. Moreover the SIMS analysis of arsenic profiles in silicon germanium substrates has turned out to be a very challenging issue, especially if the doping concentrations are quite low, because the presence of germanium significantly deteriorates the resolution of the SIMS technique. For these reasons the project was extended by one year to be able to complete the experimental analysis and to perform the simulator calibration. The difficulties observed while performing the experiments were also the reason why the initially planned experimental analysis of silicon germanium carbide materials could not be carried out within the scope of the project. As initially planned the simulator implementation activities and the software calibration tasks have been carried out by A. Hössinger and by R. Wittmann from the Institute for Microelectronics, TU-Wien, the ion implantation experiments have been carried out by Prof. Palmetshofer from the Institute of Experimental Physics, Johannes Kepler University Linz, together with his students and the SIMS analysis have been carried out by Prof. Hutter, from the Institute of Chemical Technologies and Analytics, TU-Wien, together with his students. The project has been coordinated by A. Hössinger from the Institute for Microelectronics, TU-Wien.

2.1.3.2 Project equipment

In order to carry out the ion implantation experiments mainly consumables like substrate material and ion sources had to be purchased for the purpose of the project. Apart from these consumables some equipment had to be purchased to handle also toxic gas sources. A gas system for the implant engine was required as well as some security equipment to allow handling of toxic gases. Finally a PC for software development activities has been acquired. Other than that no special large equipment has been has been purchased. All large equipment has already been available at the institutes participating in the project and was made accessible to the project.

2.2 Personal

Within the coarse of the project P. Haas from the Institute of Chemical Technologies and Analytics, who has carried out the challenging attempts to measure the arsenic doing profiles in silicon-germanium via the SIMS analysis technique could complete his diploma thesis on the basis of the performed measurements and on reporting and analysing the difficulties observed while measure arsenic doping within silicon germanium substrates. Moreover R. Wittmann from the Institute for Microelectronics was able to complete his PhD thesis partially on the basis of the simulation calibration activities and on the application of the developed ion implantation simulation tool for silicon germanium substrates and devices using epitaxial silicon germanium and strained silicon layers. By carrying out this project A.

Hössinger has extended his expertise from simulation tool development and process modelling also to process characterization.

3 Information on project participants

Not funded by the FWF			Funded by the FWF (project)		
Co-worker	Number	Person-month	Co-worker	Number	Person-month
			Diploma students	1	6
PhD students	1	10	PhD students	1	7
			Post-doctoral Co-workers	1	6,7
Professors	2	5			

4 Attachments

List 1

1.a Scientific publications

1 .a.1 Peer-reviewed publications

R. Wittmann, A. Hössinger and S. Selberherr,
Monte Carlo Simulation of Ion Implantation for Doping of Strained Silicon MOSFETs,
In Proc. International Conference on the Simulation of Semiconductor Processes and Devices (SISPAD) 2005, pp. 191 -- 194, Tokyo, Japan, 2005.

R. Wittmann, S. Uppal, A. Hössinger, J. Cervenka and S. Selberherr,
A Study of Boron Implantation into High Ge Content SiGe Alloys,
In SiGe and Ge: Materials, Processing, and Devices , Vol. 3, Nr. 7, The Electrochemical Society; ECS Transactions, pp. 667 -- 676, 2006.

R. Wittmann, S. Uppal, A. Hössinger, J. Cervenka and S. Selberherr,
A Study of Boron Implantation into High Ge Content SiGe Alloys,
In Proc. Meeting of the Electrochemical Society (ECS) 2006, Cancun, Mexico, 2006.

List 2 Conference participations

2.a Conference participations – lectures

1) Meeting of the Electrochemical Society (ECS) 2006, Cancun, Mexico

2.b Conference participations – posters

1) International Conference on the Simulation of Semiconductor Processes and Devices (SISPAD) 2005, Tokyo, Japan

List 3 Development of collaborations

N	**E**	**D**	Collaboration partner / Content of collaboration
N	E2	D	Name : Prof. Palmetshofer Institution: Institute of Experimental Physics, Johannes Kepler University Linz Content: Perform the ion implantation experiments required for the project
N	E2	D	Name : Prof. Hutter Institution: Institute of Chemical Technologies and Analytics, TU-Wien Content: Perform the SIMS analysis required for the project

List 4 PhD these and Diploma theses

4.a PhD Theses

R. Wittmann,
Miniaturization Problems in CMOS Technology: Investigation of Doping and Reliability,
Institute for Microelectronics, TU-Wien, 2007.

4.b Diploma Theses

P. Haas,
Investigation of Implantation in Silizium-Germanium with TOF-SIMS,
Institut für Chemische Technologien und Analytik, TU-Wien, 2007.