END OF PROJECT REPORT

Project title	**Simulation of Si-Ge Heterojunction Bipolar Transistors**
Project leader	**Univ.Prof.Dipl.-Ing.Dr. Siegfried SELBERHERR**
Project number	**P14483-N05**

1 Summary for public relations work

Nowadays Heterojunction Bipolar Transistors (HBTs) attract much industrial interest. In particular, Silicon-Germanium (SiGe) HBTs exhibit promising properties stretching the intrinsic advantages of the established CMOS technology into high-frequency electronics. SiGe HBTs increasingly challenge the III-V (GaAs, InP, etc.) devices in the highest frequency ranges. The devices employ strained SiGe layers to achieve better performance. SiGe devices have seen a major development to industrial maturity in the recent five years, further extending the applicability of the Silicon technology towards higher frequencies. Major contributions come from Hitachi (Japan), IBM (USA), Infineon (Germany). The Austrian company Austriamicrosystems AG has also attained a good position with these devices,

In this project new models for the material properties of SiGe have been developed. This includes models for effective carrier masses, density of states, carrier mobility, and bandgap energies for strained and relaxed SiGe, and their application to the simulation of SiGe HBTs. The thermal material properties have been modeled to allow for electro-thermal simulation. Attention has been paid to the high-field/high-energy transport especially at the heterointerfaces.

The developed models for SiGe were implemented in the two-dimensional device simulator MINIMOS-NT. The emphasis has been put on the simulation application of SiGe HBTs to industrial requirements. Physics-based DC- and AC- simulations were carried out for SiGe HBT structures provided by Austriamicrosystems AG.

Model verification through a comparison between simulated and measured forward and reverse Gummel plots of several SiGe HBTs with different Ge content at several ambient temperatures was performed. Simulation of the output characteristics including self-heating effects and impact ionization is cross-checked against measured data. The successful match between measured and simulated S-parameters gives the possibility to go for large-signal modeling. Optimization of the doping for specific requirements (high speed or high breakdown voltage) was performed. In frame of the project a complete set of models which is needed to investigate industrial technologies by means of Technology Computer-Aided Design (TCAD), was developed.

Heterostruktur-Bipolar-Transistoren (HBTs) sind zur Zeit für die Industrie von großem Interesse. Im Besonderen besitzen Silizium-Germanium (SiGe) HBTs sehr attraktive Eigenschaften, welche es erlauben die der etablierten CMOS Technologie inhärenten Vorteile für die Hochfrequenzelektronik zu nutzen. Mehr und mehr werden SiGe HBTs in den höchsten Frequenzbereichen zu einer echten Herausforderung für Bauelemente, die auf III-V (GaAs, InP, etc.) Halbleitermaterialien basieren. SiGe Bauelemente benutzen verspannte SiGe Schichten, um bessere Eigenschaften zu erreichen. Diese Bauelemente haben in den letzen fünf Jahren große Schritte in Richtung Industriereife gemacht und die Leistungsfähigkeit der Siliziumtechnologie für immer höhere Frequenzen erweitert. Wichtige Beiträge für diese Technologie kommen von Hitachi (Japan), IBM (USA), und Infineon (Deutschland). Auch die österreichische Firma Austriamicrosystems AG hat eine gute Position mit diesen Baulementen erreicht.

Im Rahmen des vorliegenden Projektes wurden neue Modelle für die Materialeigenschaften von SiGe entwickelt. Darunter sind Modelle für die effektiven Massen, die effektive Zustandsdichten, die Beweglichkeiten, die Bandkantenenergien für verspanntes und unverspanntes Silizium-Germanium (SiGe), und die Anwendung dieser Modelle für die numerische Simulation von SiGe HBTs. Um eine elektro-thermische Simulation zu ermöglichen, wurden Modelle der thermischen Werkstoffeigenschaften entwickelt. Besondere Sorgfalt wurde für den Energietransport unter Hochfeldbedingungen an den Heteroübergängen aufgewandt.

Die entwickelten Modelle wurden in den zweidimensionalen Bauelement-Simulator MINIMOS-NT implementiert. Der Schwerpunkt lag auf der Anwendung der numerischen Simulation zur Erfüllung industrieller Bedürfnisse. Physikalisch basierte DC und AC Simulationen wurden für SiGe HBTs von Austriamicrosystems durchgeführt.

Die Modelle wurden mittels Vergleich von bei verschiedenen Temperaturen simulierten und gemessenen Eingangskennlinien für verschiedene SiGe HBTs mit unterschiedlichem Germaniumgehalt verifiziert. Die Simulation der Ausgangskennlinien wurde unter Berücksichtigung der Selbsterwärmung und der Impaktionisierung anhand von Messergebnissen überprüft. Die bestehende Übereinstimmung zwischen gemessenen und simulierten S-Parametern gibt weiters die Möglichkeit zur Großsignalanalyse. Optimierungen der Verteilung der Dopanten im Bauelement wurden in Hinblick auf unterschiedliche Erfordernisse (Hochgeschwindigkeit oder Durchbruchfestigkeit) durchgeführt. Insgesamt wurde im Rahmen dieses Projektes ein vollständiger Satz von Modellen entwickelt, der die Anforderungen, welche die Erforschung industrieller Bauelemente mit einer computerunterstützten Entwicklungsumgebung stellt, erfüllt.

2 Brief project report

2.1 Report on the scientific work

2.1.1 Development of the research work

The original project was scheduled for 24 months in total. The main scientific concept and goals of the original project include:

- theoretical work on derivation of models for strained and relaxed SiGe validated by Monte Carlo simulations
- implementation of the developed models and algorithms in the device simulator MINIMOS-NT including extension of the source code, testing, and documentation
- application of the implemented models and algorithms to realistic device structures under various DC operating conditions including verification against experimental data
- industrial application of the simulation of SiGe HBTs, e.g. mixed-mode device/circuit simulation and S-parameter simulation, verification against experimental data, analysis of device reliability issues

The time schedule was followed but not strictly as some interesting industrial applications occurred at earlier stages. On the other hand, some of the theoretical work was delayed due to incomplete Monte Carlo simulation data available in the literature. Thus, own Monte Carlo simulations needed to be performed. A proposal for 12 months project prolongation includes:

- derivation of models for SiGe:C and implementation
- investigation of quantization effects
- small-signal analysis will be performed both for SiGe HBTs and Si/SiGe MOSFETs.

The approved prolongation period of 6 months allowed small-signal analysis of SiGe HBTs and investigation of quantization effects using simple approximations. The project results are systematically summarized and discussed in detail in a monograph book [B1]. The international scientific community acknowledged our work with several invitations for conference presentations.

2.1.2 Important results

All theoretical work was accomplished including the derivation of models for strained and relaxed SiGe in accordance with the research plan.

Development of Models for Strained and Relaxed SiGe Layers
New models for physical properties of SiGe with respect to material composition and strain conditions due to lattice mismatch were developed. These models are valid for the whole composition range and in the temperature range between 70 K and 500 K. The material properties of $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ are treated as a function of the material composition x for all mole fractions based on the properties of both Si and Ge (strained Ge grown on Si). The new models were verified against experimental data and/or Monte Carlo calculations.

Models for effective carrier masses, density of states, bandgap energies, and carrier mobility for strained and relaxed SiGe were developed to allow simulation of SiGe HBTs.

For the effective carrier masses of Si and Ge a linear and a quadratic temperature dependence are used in the case of electrons and holes, respectively. For SiGe a quadratic interpolation of these masses was chosen as a function of the material composition. The model for the density of states is based on a theoretical expression which takes into account the number of equivalent energy minima. In case of a transition between a direct and an indirect bandgap, the valley degeneracy factor is treated accordingly. The anisotropic properties of SiGe are modeled based on several theoretical investigations.

The temperature dependent bandgaps of Si and Ge are calculated first. Then, the SiGe bandgap and the energy offset are calculated as a function of the material composition and considering the strain condition. Finally, the energies of the conduction and valence band edges are computed. The bandgap narrowing model accounts for the semiconductor material, the dopant species, and the lattice temperature. Special attention was paid to the band offsets at the hetero-interfaces and the thermionic-field emission model which must be used in the case of abrupt heterojunctions.

The mobility model for SiGe employs the low-field mobilities of Si and Ge and combines them by a harmonic mean. The respective interpolations between Si and Ge are also used in the models for the saturation velocities and, in the case of hydrodynamic simulation, of the energy relaxation times. The temperature dependence of the lattice mobility preserves the expression from the mobility model of MINIMOS 6. A mobility model which distinguishes between majority and minority carriers is now available for Si and SiGe.

The Monte Carlo simulation data available in the literature for the carrier mobility in SiGe turned out to be incomplete. The data do not contain sufficient information for all Ge contents (most often less than 30%), temperatures, doping levels, and applied electrical fields.

Thus, we performed Monte Carlo simulations with our own simulator. The band structure parameters serve as input for Monte Carlo transport calculations. Bulk simulations for n-type semiconductors were carried out. The fundamental properties of electron transport are captured by an analytical, multi-valley band structure model. Dependence of mobility on strain, material composition, lattice temperature, and doping concentration is considered.

The Monte Carlo simulations give the in-plane and out-of plane components of carrier mobility and are hence equally suited to deal with transport in lateral devices such as SiGe MOSFET and vertical devices such as SiGe HBT. In case of HBTs, the minority mobility was investigated. Parameters for both the drift-diffusion and hydrodynamic transport models were considered. Complete sets of simulation data for in-plane/out-of-plane, majority/minority electron mobility at various temperatures was obtained. Analytical expressions based on these data were derived, implemented in MINIMOS-NT, thoroughly tested, and documented.

To allow for electro-thermal simulation, proper models for mass density, specific heat, and thermal conductivity of SiGe were created. A linear interpolation between the values of the mass density of Si and Ge is used to model the mass density of SiGe. The temperature dependence of the thermal conductivity of Si and Ge is modeled by a power law. A harmonic mean is taken to model the material composition dependence of the thermal conductivity of SiGe. The lattice temperature dependence of the specific heat capacity is computed by a new model. The models are based on experimental data. The permittivity in SiGe is modeled by a linear interpolation between the values of the ones of Si and Ge. The existing generation/recombination models for Si appear to be suitable for SiGe.

Implementation in MINIMOS-NT, Simulation Verification, and Application

The developed models for SiGe were implemented in the two-dimensional device simulator MINIMOS-NT. This phase of the project included extension of the source code, testing, and documentation.

The convergence behavior was improved and the complexity of the models was cross-checked with the computational effort in order to ensure the efficiency of the new models.

Physics-based DC- and AC- simulations were carried out for realistic SiGe HBT structures [1], provided by Austriamicrosystems AG.

Model verification through a comparison between simulated and measured forward and reverse Gummel plots of several SiGe HBTs with different Ge content at several ambient temperatures was performed. Simulation of the output HBT characteristics including self-heating (SH) effects and impact ionization (II) generation is cross-checked against measured data. Two different methods were used to extract the current gain cutoff frequency. The first one employs transient simulation and the second employs a small-signal AC-analysis. We found that the results from both methods are in very good agreement. The successful match between measured and simulated S-parameters at several bias points gives the possibility to go for large-signal modeling.

Optimization of the doping for specific requirements (high speed or high breakdown voltage) was performed. In frame of the project, a complete set of models which is needed to investigate industrial technologies by means of TCAD, was developed.

2.1.3 Running of the project, funding, and changes to the original project

The project was run in accordance with the research plan. The research was conducted by one PostDoc person funded by FWF. Two PhD students were partially involved in the project without being funded by FWF.

Due to the excellent infrastructure of the research institute no additional equipment was required to be purchased for this project. The original project duration of 24 months was extended by 6 additional months.

2.2 Personnel development

The project was performed by one PostDoc scientist: Dr.techn. Vassil Palankovski. For him the project gave the opportunity to complement results from his dissertation on modeling and simulation of GaAs HBTs with results on SiGe HBTs. This allowed him and Dr. Rüdiger Quay to write a book on 'Analysis and Simulation of Heterostructure Devices', which is currently in print at Springer Verlag in the series on 'Computational Microelectronics'.

Dr. Palankovski will use the results of the project for further activities at the Technische Universität Wien and for submitting a habilitation work.

Some PhD students, who were not funded by the project, also got partially involved in the project activities. The project brought them significant motivation and scientific results for their dissertations.

The project had an excellent response from the international scientific community, resulting in several invited presentations. The project brought higher national and international reputation for the project leader, the project co-workers, and their institution.

The project intensified several international collaborations with University research partners and industry.

2.3 Effects of the project outside the scientific field

The project gives perspectives for research of other novel materials and novel devices. The methodology applied in this project can be used for research on other Group IV semiconductor materials, as well as ternary and quarternary III-V materials, such as phosphides, arsenides, antimonides, and nitrides. Next to SiGe devices, several III-V heterostructure devices, such as GaAs and InP HBTs, and GaAs, InP, and GaN HEMTs can be analyzed based on the project experience.

The research results from the project are relevant for teaching activities and will be incorporated in a course of lectures on ‘RF Semiconductor Devices’.

One of the project results is a software product, which has been given free of charge for download via Internet since September 2002. Today, there are 55 registered users from all over the world.

The results of the project are of interest for companies from the semiconductor industry. In the course of the project, a close co-operation on the topic was developed between the Institut für Mikroelektronik and Austriamicrosystems AG. Some particular tasks were supplied from Infineon AG, Germany, and Sony, Japan.

3 Project participants

co-workers	number	man-months	
PhD Students	2	6	not funded by FWF
PostDocs	1	30	funded by FWF

4 Attachments

4.1 Scientific publications

Books

[B1] V. Palankovski and R. Quay, *Analysis and Simulation of Heterostructure Devices*, Springer, Wien–New York, 2003, (in press).

Contributions in peer-reviewed scientific journals

[J1] S. Wagner, V. Palankovski, T. Grasser, G. Röhrer, and S. Selberherr, "A Direct Extraction Feature for Scattering Parameters of SiGe-HBTs,", *J.Appl.Surf.Science*, 2003, (in press).

[J2] V. Palankovski, G. Röhrer, T. Grasser, S. Smirnov, H. Kosina, and S. Selberherr, "Rigorous Modeling Approach to Numerical Simulation of SiGe-HBTs," *J.Appl.Surf.Science*, 2003, (in press).

[J3] V. Palankovski and S. Selberherr, "The State-of-the-Art in Simulation for Optimization of SiGe-HBTs," *J.Appl.Surf.Science*, 2003, (in press).

4.2 Project-related participation in international scientific conferences

Invited lectures

[1] V. Palankovski, "Simulation von SiGe Baulementen," in *GMM Workshop "Integrierte-Silizium-Hetero-Bauelemente"*, Munich, Germany, 24-25 Apr. 2002.

[2] V. Palankovski and S. Selberherr, "Optimization of SiGe HBTs for Industrial Applications," in *Intl. SiGe Technology and Device Meeting ISTDM*, (Nagoya, Japan), pp. 267–268, 15-17 Jan. 2003.

[3] V. Palankovski and S. Selberherr, "Critical Modeling Issues of SiGe Semiconductor Devices," in *Symposium on Diagnostics & Yield*, (Warszawa, Poland), pp. (7-2)1–11, 22-25 June 2003.

[4] V. Palankovski, S. Wagner, and S. Selberherr, "Numerical Analysis of Compound Semiconductor RF Devices," in *Tech.Dig. GaAs IC Symposium*, (San Diego, California, USA), 9-12 Nov. 2003, (in press).

[5] V. Palankovski and S. Selberherr, “Rigorous Modeling of High-Speed Semiconductor Devices,” in *IEEE Conference on Electron Devices and Solid-State Circuits EDSSC*, (Hong Kong), 16-18 Dec. 2003, (in press).

[6] V. Palankovski and S. Selberherr, “Challenges in Modeling of High-Speed Electron Devices,” in *Proc. Intl. Workshop on the Physics of Semiconductor Devices IWPSD*, (Madras, India), 16-20 Dec. 2003, (in press).

Lectures

[1] V. Palankovski, G. Röhrer, E. Wachmann, J. Kraft, B. Löffler, J. Cervenka, R. Quay, T. Grasser, and S. Selberherr, “Optimization of High-Speed SiGe HBTs,” in *Proc. Intl. Symposium on Electron Devices for Microwave and Optoelectronic Applications EDMO*, (Vienna, Austria), pp. 187–191, 15-16 Nov. 2001.

[2] S. Wagner, V. Palankovski, T. Grasser, G. Röhrer, and S. Selberherr, “A Direct Extraction Feature for Scattering Parameters of SiGe-HBTs,” in *Intl. SiGe Technology and Device Meeting ISTDM*, (Nagoya, Japan), pp. 83–84, 15-17 Jan. 2003.

[3] V. Palankovski and S. Selberherr, “Modeling High Speed Semiconductor Devices of Modern Communication Systems,” in *Proc. World Multi Conf. on Systemics, Cybernetics and Informatics SCI*, (Orlando, Florida, USA), pp. 97–102, 27-30 July 2003.

Posters

[1] V. Gopinath, V. Palankovski, S. Selberherr, and S. Aronowitz, “Effects of Stress-Induced Bandgap Narrowing on Reverse-Biased Junction Behavior,” in *Proc. 32nd European Solid-State Device Research Conference ESSDERC*, (G. Baccarani, E. Gnani, and M. Rudan, editors), (Firenze, Italy), pp. 631–634, 24-26 Sept. 2002.

[2] V. Palankovski, G. Röhrer, T. Grasser, S. Smirnov, H. Kosina, and S. Selberherr, “Rigorous Modeling Approach to Numerical Simulation of SiGe-HBTs,” in *Intl. SiGe Technology and Device Meeting ISTDM*, (Nagoya, Japan), pp. 97–98, 15-17 Jan. 2003.

4.3 Development of collaborations

1. National (N), extensive (E3), in the discipline (D):
   Austriamicrosystems AG, Simulation of SiGe HBTs
2. European (E), medium (E2), transdisciplinary (T):
   Infineon AG, Münich, Simulation of HBTs
3. European (E), low (E1), in the discipline (D):
   Universitaät, Stuttgart, Simulation of SiGe HBTs
4. Other (I), low (E1), in the discipline (D):
   Sony, Japan, Simulation of SiGe HBTs
5. Other (I), low (E1), transdisciplinary (T):
   LSI Logic, USA, Simulation of strained layers

4.4 Habilitations and PhD theses

The project was important for the habilitation of Dr.techn. Vassil Palankovski (in progress) and for the PhD theses of Dipl.-Ing. Stephan Wagner (in progress) and Sergey Smirnov (in progress).

4.5 Effects outside the scientific field

An application for a follow-up project (START) was submitted in Nov. 2002 to FWF, but to our regret was refused.