

INTERNATIONAL CO-OPERATION PROJECT FINAL REPORT

Title of programme or call ESF EUROCORES, FoNE
(e.g. in the frame of ESF EUROCORES, CERC3, ERA-Net Calls, Bi- multilateral Memoranda of Understanding)

Title of collaborative research project title Device Electronics Using Nanowires and Nanotubes (DEWINT)
(if applicable)

Title of national (sub)project FONE-Bauelemente-Elektronik mit Nanowires und Nanotubes (DEWINT)

Project leader KOSINA Hans

Role of applicant Project Coordinator) Principal Investigator of (sub)project
 Associated Partner

Project duration Months 39

Project number

1. Summary for public relations work (English)

One dimensional nanostructures are currently subject of intensive research as they often show exceptional mechanical, electrical, and also optical properties. In this project one dimensional nanostructures made from carbon and silicon have been studied using a computer model. Carbon can form nanotubes with diameters in the nanometer range. These carbon nanotubes show excellent electrical transport properties and, therefore, are promising starting materials for electronic devices such as novel transistors. A simulation program for field effect transistors with carbon nanotubes forming the current-conducting channel has been developed. Because of the small dimensions of the structures considered a computer model including all relevant quantum mechanical effects has been utilized. By means of this program the electrical characteristics of carbon nanotube transistors and a variety of effects occurring in these devices can be better understood and described quantitatively. Thus this program is a tool aiding the design and optimization of such devices. Various transistor structures have been investigated in the course of this project. It has been demonstrated, how the static characteristics of a carbon nanotube field effect transistor can be optimized by suitably tuning some of the geometrical parameters. Scattering of charge carriers in the thermally excited crystal lattice has been taken into account. A significant effect of scattering processes due to phonons in particular on the dynamic switching behavior of the transistors has been shown. In addition to the conventional transistor designs a tunnel transistor has been studied in detail. Because of their specific electronic structure carbon nanotubes can also be used as the active elements of optoelectronic devices. The computer model has been extended to account for the electron-light interaction and then applied to study carbon nanotube-based infrared photodiodes. A method to reduce the dark current has been proposed. Furthermore, it has been shown that the local approximation of the selfenergy for electron-photon interaction is not valid. Instead, the full non-locality of this term has to be considered to obtain realistic results. The calculated quantum yield of carbon nanotubes showed good agreement with published experimental data. Silicon, the second semiconductor material considered here, can form nanowires. In this project the thermoelectric properties of silicon nanowires have been investigated. The thermoelectric effect allows one to directly convert temperature differences into usable electrical energy. Specifically designed nanowires achieve considerably higher conversion efficiency than the comparable bulk material. The effect of nanowire cross section, doping, and crystal orientation on the efficiency has been studied and optimum parameter ranges been identified.

Summary for public relations work (German)

Wegen ihrer außergewöhnlichen mechanischen, elektrischen und auch optischen Eigenschaften sind eindimensionale Nanostrukturen derzeit Gegenstand intensiver Forschungen. In diesem Projekt wurden derartige Nanostrukturen bestehend aus Kohlenstoff beziehungsweise Silizium mit Hilfe von Computermodellen untersucht. Kohlenstoff kann Nanoröhren mit Durchmessern im Nanometerbereich, so genannte Carbon Nanotubes, bilden. Diese weisen exzellente Stromleitungseigenschaften auf, wodurch sie als Ausgangsmaterial für elektronische Bauelemente wie neuartige Transistoren interessant werden. Es wurde ein Simulationsprogramm für Feldeffekt-Transistoren mit Carbon Nanotubes als stromleitendem Kanal entwickelt. Auf Grund der Kleinheit der betrachteten Strukturen wurden quantenmechanische Effekte in vollem Umfang berücksichtigt. Mit Hilfe dieses Programms wurden unterschiedlichste Transistor-Strukturen untersucht. Damit kann das Verhalten dieser Bauelemente so wie verschiedenster Effekte, die in diesen auftreten, besser verstanden und quantitativ beschrieben werden. Damit bildet das Simulationsprogramm ein Werkzeug sowohl für den Entwurf der Bauelemente als auch deren Optimierung. So wurde gezeigt, wie die statischen Eigenschaften eines Carbon Nanotube Feldeffekt-Transistors durch geeignete Wahl der geometrischen Parameter optimiert werden können. Die Streuung der elektronischen Ladungsträger am thermisch angeregten Kristallgitter wurde in dem Modell mitberücksichtigt. Der ausgeprägte Einfluss dieser Streuprozesse auf das dynamische Schaltverhalten des Transistors konnte gezeigt werden. Als ein Sonderbauelement in dieser Klasse wurde der Tunnel-Transistor genauer untersucht. Carbon Nanotubes können auf Grund ihrer speziellen elektronischen Bandstruktur auch als aktive Elemente für optoelektronische Bauelemente verwendet werden. Mit dem entsprechend erweiterten Computermodell wurden auf Carbon Nanotubes basierende Infrarot-Photodioden studiert. Es wurde eine Methode zur Reduktion des Dunkelstroms vorgeschlagen. Auf der theoretischen Seite wurde gezeigt, dass man für die Selbstenergie der Elektron-Photon Wechselwirkung die lokale Näherung nicht verwenden darf, sondern dass die volle Nichtlokalität zu berücksichtigen ist um realistische Ergebnisse zu erhalten. Es wurde der Quantenwirkungsgrad von Nanotubes berechnet und gute Übereinstimmung mit publizierten Messwerten gefunden. Aus Silizium, dem zweiten hier betrachteten Halbleitermaterial, lassen sich Nanodrähte herstellen. In diesem Projekt wurden die thermoelektrischen Eigenschaften von Silizium Nanodrähten näher untersucht. Mit Hilfe des thermoelektrischen Effekts können Temperaturunterschiede direkt in nutzbare elektrische Energie umgewandelt werden. Mit speziell entworfenen Nanodrähten kann ein deutlich höherer Wirkungsgrad als mit den vergleichbaren Bulk-Materialien erzielt werden. Es wurde der Einfluss von Querschnittsfläche, Dotierung und Kristallorientierung des Nanodrahtes auf den Wirkungsgrad genauer untersucht und optimale Parameterbereiche identifiziert.

2. Brief project report of the domestic (sub) project

2.1 Report on the scientific work

2.1.1 Information on the development of the research work

This individual project aimed at the development of a numerical device simulator for semiconductor devices which exhibit quasi-1D transport properties, including carbon nanotube (CNT) and Si nanowire (SiNW) based devices. The goal was to develop a transport module for CNT based devices and one for Si based devices and to integrate these modules with an existing device simulator. Dissipative transport models were to be considered. This goal has been achieved. The transport module for CNT-FETs has been integrated with the general purpose device simulator MINIMOS-NT; that for SiNWs with the in house tool VSP (Vienna Schrödinger-Poisson solver). Instead of a simple effective mass Hamiltonian, as stated in the proposal, tight-binding Hamiltonians have been consistently used for both CNTs and SiNWs.

Next, it was planned to assess the validity of physical models and parameter values by comparing simulation results to measurements of samples fabricated by one of the project partners. Since no measurement data of working devices became available during the project, we changed the direction of this project part. We theoretically investigated additional structures and physical effects, such as optoelectronic devices and thermoelectric devices (see below).

The third objective was to conduct a simulation study of different FET architectures, including CNT and SiNW devices and multi-gate FETs. Again, this objective was accomplished. In addition to FETs the following devices have been investigated: Infrared photodetectors based on CNTs; a resonant tunneling diode made from graphene, and SiNWs for thermoelectric energy conversion

2.1.2 Most important results and brief description of their significance

A program module for field effect transistors with CNTs forming the current-conducting channel has been developed and integrated with MINIMOS-NT. As a transport model the non-equilibrium Green's function (NEGF) technique has been utilized. By means of this program the static and dynamic electrical response of CNT transistors and a variety of effects occurring in these devices have been analyzed. This program represents a tool aiding the design and optimization of CNT FETs. Various transistor structures have been investigated in the course of this project.

Optimization of CNT-FET Performance [7]: We showed that the device characteristics can be optimized by appropriately selecting the geometrical parameters. With increasing gate-drain spacer, the off-current and the gate-drain parasitic capacitance decrease at the expense of a drain current reduction at low bias voltages. With increasing gate-source spacer length, the drain current and gate-source parasitic capacitance decreases. Since the gate delay time is proportional to the parasitic capacitances and inversely proportional to the on-current, there is an optimum value for the gate-source spacer length which minimizes the gate delay time. The optimal point is where the sensitivities of these quantities are equal. As the barrier height at the metal–CNT is reduced, the contribution of thermionic emission to the total current increases and the sensitivity of the on-current with respect to the gate-source spacer length decreases, which results in larger gate-source spacer lengths for optimized performance.

The Effect of Phonon Scattering on the Dynamic Response of CNT-FETs [6, 8]: The effect of the electron-phonon interaction parameters on the performance of CNT-based transistors has been studied numerically, using the NEGF formalism. We showed that elastic back-scattering reduces the on-current effectively, but the strength of this process is weak in CNTs. Inelastic scattering with high-energy phonons reduces the on-current only weakly, but increases the switching time considerably, which can be explained by a charge pile-up in the channel. Scattering with low-energy phonons reduces the on-current more effectively, but has a weaker effect on the switching time. In a CNT at room temperature, the scattering processes are mostly due to electron-phonon interaction with high-energy phonons. Therefore, the on-current of CNT-FETs can be close to the ballistic limit, whereas the switching time is found to be significantly below that limit. This theoretical prediction is confirmed by experimental data on CNT-FET performance from literature.

Numerical Investigation of a Tunnelling CNTFET [5]: Accounting for quantum confinement and band to band tunnelling, the NEGF formalism along with an appropriate band structure gives a suitable model for the analysis of these devices. Simulation results suggest that an asymmetric doping profile reduces the parasitic carrier injection and increases the on-to-off current ratio by several orders of magnitude.

Graphene nanoribbon-based Resonant Tunnelling Diode [25]: As an extension with respect to the original project plan we performed first studies of graphene nanoribbon (GNR) devices. A double barrier resonant tunnelling device can be formed by attached segments of armchair GNRs of different widths. Our results show that the specific device operates as a resonant tunnelling double barrier with resonances determined by the quantum well states. The device characteristics can therefore be constructively engineered by proper design of the layer structure.

CNT Infrared Photo Detectors [13, 14]: Because of their direct band gap, CNTs can also be used as the active elements of optoelectronic devices. In addition to electrical device applications of CNTs considered in the original work plan, we have extended the work to optoelectronic device applications. The self-energy term for electron-photon interaction has been added to the numerical NEGF transport model, and the performance of IR photo detectors based on CNT-FETs has been investigated. The coupled system of transport and Poisson equations was solved self-consistently. In agreement with experimental data, our results indicate that the ratio of the photo-current to the dark-current is relatively low. However, we demonstrated that by employing a dual gate structure the dark-current can be significantly decreased, whereas the photo-current remains nearly unchanged. Our results show that by appropriate selection of the two gate voltages the ratio of the photo-current to the dark-current can be maximized. Furthermore, we have shown that the local scattering approximation, which is widely used in quantum transport simulations, fails to predict the behaviour of devices where electron-photon interaction is present. For accurate simulations a non-local selfenergy must be taken into consideration. With some modifications the model has also been applied to graphene nanoribbon IR detectors [23].

Si Multigate Structures [10, 19, 20, 30, 31]: Our work on multigate devices focused on the calculation of electronic structure and transport in double gate devices. Orientation dependence and strain effects in ultrathin Si films have been studied. A specific outcome is a two-band kp-model for the Si conduction band valleys. We demonstrated that this simple and effective band model gives accurate results for arbitrary strain conditions, crystal orientations, and quantum confinement. In [9] the electron subband structure in thin (100) silicon films is analyzed. For unprimed subbands the dependence of the nonparabolicity parameter on film thickness is obtained. The two-band kp theory gives a thickness dependence of the effective masses for primed subbands. In [30] the effect of uniaxial stress on the electron mobility has been analyzed by means of MC simulations. Experimentally observed mobility data were reproduced for bulk Si and Si inversion layers on (001) and (110) oriented substrates with large and small body thicknesses. Mobility enhancement can be understood from a combination of three effects: (i) subband ladder repopulation, (ii) change in inter-subband scattering, and (iii) stress induced effective mass changes. While repopulation effects can increase the bulk and inversion layer mobilities at relatively large body thicknesses ($T_{\text{soi}} > 20$ nm), the population of higher subband ladders is intrinsically reduced by strong quantum confinement for very small body thickness ($T_{\text{soi}} < 5$ nm). Thus, in the latter case, no mobility enhancement can be expected from stress induced repopulation effects and only the stress induced effective mass change can explain the experimentally observed mobility enhancement. Stress conditions reducing the effective mass in transport direction, such as uniaxial tensile stress along (110), are very beneficial to increase mobility in UTB-MOSFETs.

Si Nanowire Devices [1]: Low-dimensional materials provide the possibility of improved thermoelectric performance due to the additional length scale degree of freedom for engineering their electronic and thermal properties. As a result of suppressed phonon conduction, large improvements in the thermoelectric figure of merit, ZT , have recently been reported in nanostructures, compared to the bulk materials. In addition, low dimensionality changes the electronic structure, offering an additional enhancement in ZT . In this project the $sp^3d^5s^*$ spin-orbit-coupled tight-binding model has been used to calculate the electronic structure of silicon NWs. The Landauer formalism has been applied to calculate an upper limit for the electrical conductivity, the Seebeck coefficient, and the power factor. We examined n-type and p-type nanowires with diameters ranging from 3 nm to 12 nm, in [100], [110], and [111] transport orientations, and at different doping concentrations. Using experimental values for the lattice thermal conductivity in NWs, an upper limit for ZT has been computed. We found that at room temperature, scaling the diameter below 7 nm can at most double the power factor and enhance ZT . Orientations, geometries, and subband engineering techniques for optimized designs have been discussed.

2.1.3 Information on the running of the project, use of the available funding and where appropriate any changes to the original project plan

The project duration is July 2006 through September 2009 (39 months).

Personnel resources requested in the project proposal were 36 PostDoc months and 36 months for a PhD student. The actual funding granted by FWF was 36 PostDoc months.

The following personnel have been funded by the project:

- Dipl.Ing Enzo Ungersboeck PhD-student 100% Jul 2006-Mar 2007 (9PM)
- Dr. Viktor Sverdlov Post-Doc 100% Jun 2007-Aug 2007 (3PM)
- Dr. Mahdi Pourfath Post-Doc 100% Jan 2008-Sep 2009 (21PM)
- Dipl.Ing. Markus Karner PhD-student 50% Aug 2008-Dez 2008 (2.5PM)
- Dr. Neophytos Neophytou Post-Doc 100% Okt 2008-Mar 2009 (6PM)

In total, we spent 30 PostDoc months and 11.5 months for PhD students

2.2. Personnel development – importance of the project for the scientific careers of those involved (including the project leader)

Enzo Ungersboeck finished his PhD study during this project.

Mahdi Pourfath and Neophytos Neophytou gained their first experience as postdoctoral researchers. They both were able to further deepen their expertise gained in their previous PhD projects, and had excellent publication output.

Special possibilities opened by the project are new joint project proposals with European partners. A proposal on graphene research in response to the ESF EuroGraphene call has successfully passed the two stages of the review process, but was finally not supported by one of the national funding agencies. An FP7 proposal on thermoelectric converters has passed the pre-proposal stage. Right now the full proposal is in preparation. A proposal to the Austrian Klima and Energiefonds on thermoelectric nanostructures has been accepted recently. Becoming members of these project consortia would not have been possible without the results and reputation gained from the present project.

2.3 Effects of the project outside the scientific field

The simulator VSP including the new features developed in the project is used in lab exercises for students of the master study “Microelectronics.”

3. Information on domestic 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			PhD students	2	11.5
post-doctoral co-workers			post-doctoral co-workers	3	30
co-workers with "Habilitation" (professorial qualifications)			co-workers with "Habilitation" (professorial qualifications)		
professors	1	4	professors		

4. Attachments

(lists may be as long as required)

List 1

1.a. scientific publications¹

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

**1) N. Neophytou, M. Wagner, H. Kosina, S. Selberherr:
"Analysis of Thermoelectric Properties of Scaled Silicon Nanowires Using an Atomistic Tight-Binding Model";
Journal of Electronic Materials, 1 (2010).**

2) M. Pourfath, H. Kosina:
"Computational Study of Carbon-Based Electronics";
Journal of Computational Electronics, 8 (2009), 427 - 440.

**3) M. Pourfath, H. Kosina:
"Application of the Non-Equilibrium Green's Function Formalism for the Numerical Analysis of Carbon Nanotube FETs"; Journal of Computational and Theoretical Nanoscience, 5 (2008), 1128 - 1137.**

4) M. Pourfath, H. Kosina, S. Selberherr:
"Numerical Study of Quantum Transport in Carbon Nanotube Transistors";
Mathematics and Computers in Simulation, 79 (2008), 1051 - 1059.

5) M. Pourfath, H. Kosina, S. Selberherr:
"Tunneling CNTFETs";
Journal of Computational Electronics, 6 (2007), 243 - 246.

6) M. Pourfath, H. Kosina, S. Selberherr:
"Dissipative Transport in CNTFETs";
Journal of Computational Electronics, 6 (2007), 321 – 324.

7) M. Pourfath, H. Kosina, S. Selberherr:
"Geometry Optimization for Carbon Nanotube Transistors";
Solid-State Electronics, 51 (2007), 1565 – 1571.

**8) M. Pourfath, H. Kosina:
"The Effect of Phonon Scattering on the Switching Response of Carbon Nanotube Field-Effect Transistors";
Nanotechnology, 18 (2007), 424036 - 424041.**

9) V. Sverdlov, E. Ungersböck, H. Kosina, S. Selberherr:
"Current Transport Models for Nanoscale Semiconductor Devices";
Materials Science and Engineering R, 58 (2008), 6-7; 228 - 270.

10) V. Sverdlov, H. Kosina, S. Selberherr:
"Electron Subband Dispersions in Ultra-Thin Silicon Films from a Two-Band k·p

¹ The publication list must mention for each work: all authors; full title; series/journal title; year; volume; and page numbers.

Theory"; Journal of Computational Electronics, 7 (2008), 3; 164 - 167.

11) M. Pourfath, S. Selberherr:

"Modeling Current Transport in Carbon Nanotube Transistors";
Talk: Conference on Electron Devices and Solid-State Circuits (EDSSC),
Hong Kong (invited); 12-08-2008 - 12-10-2008; in: "IEEE International
Conference on Electron Devices and Solid-State Circuit 2008", (2008), 6 p.

12) M. Pourfath, H. Kosina, S. Selberherr:

"Current Transport in Carbon Nanotube Transistors";
Talk: International Conference on Solid State and Integrated Circuit
Technology (ICSICT), Beijing (invited); 10-20-2008 - 10-23-2008; in:
"The 9th International Conference on Solid-State and Integrated-Circuit
Technology", (2008), ISBN: 978-1-4244-2186-2; 361 – 364.

13) M. Pourfath, H. Kosina, S. Selberherr:

"Reduction of the Dark-Current in Carbon Nanotube Photo-Detectors";
Talk: European Solid-State Device Research Conference (ESSDERC),
Edinburgh; 09-15-2008 - 09-19-2008; in: "European Solid-State Device
Research Conference", (2008), 214 – 217.

14) M. Pourfath, H. Kosina:

"Numerical Study of Carbon Nanotube Infra-Red Photo-Detectors";
Talk: International Conference on Simulation of Semiconductor Processes
and Devices (SISPAD), Hakone; 09-09-2008 - 09-11-2008; in:
"International Conference on Simulation of Semiconductor Processes and
Devices 2008", (2008), ISBN: 978-1-4244-1753-7; 81 – 84.

15) N. Neophytou, H. Kosina, S. Selberherr, G. Klimeck:

"Dependence of Injection Velocity and Capacitance of Si Nanowires on Diameter,
Orientation, and Gate Bias: An Atomistic Tight-Binding Study"; Talk: International
Conference on Simulation of Semiconductor Processes and Devices (SISPAD), San
Diego; 09-09-2009 - 09-11-2009;
in: "Proceedings of the International Conference on Simulation of Semiconductor
Processes and Devices", (2009),
ISBN: 978-1-4244-3947-8; 71 - 74.

16) M. Pourfath, S. Selberherr:

"Current Transport in Carbon Nanotube Transistors";
Talk: International Caracas Conference on Devices, Circuits and Systems
(ICCDACS), Cancun (invited); 04-28-2008 - 04-30-2008; in: "Proceedings of
the 7th International Caribbean Conference on Devices, Circuits and
Systems", (2008), ISBN: 978-1-4244-1957-9, 6 p.

17) M. Pourfath, H. Kosina:

"The Effect of Optical Phonon Scattering on the On-Current and Gate Delay Time of
CNT-FETs";
Poster: International Conference on Simulation of Semiconductor Processes and
Devices (SISPAD), Wien; 09-25-2007 - 09-27-2007; in: "International Conference on
Simulation of Semiconductor Processes and Devices 2007", T. Grasser, S.
Selberherr (ed.); Springer-Verlag Wien New York, 12 (2007), ISBN: 978-3-211-
72860-4; 309 - 312.

18) M. Pourfath, H. Kosina, S. Selberherr:
"The Role of Inelastic Electron-Phonon Interaction on the On-Current and Gate Delay Time of CNT-FETs";
Talk: European Solid-State Device Research Conference (ESSDERC), München; 09-11-2007 - 09-13-2007; in: "European Solid-State Device Research Conference", (2007), ISBN: 1-4244-1123-8; 239 - 242.

19) V. Sverdlov, G. Karlowatz, H. Kosina, S. Selberherr:
"Two-Band k.p Model for the Conduction Band in Silicon";
Talk: The European Simulation and Modelling Conference (ESM), Malta; 10-22-2007 - 10-24-2007; in: "Proceedings European Simulation and Modeling Conference (ESM)", (2007), ISBN: 978-90-77381-36-6; 220 – 224.

20) V. Sverdlov, G. Karlowatz, E. Ungersböck, H. Kosina:
"Influence of Uniaxial [110] Stress on the Silicon Conduction Band Structure: Stress Dependence of the Nonparabolicity Parameter";
Poster: International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Wien; 09-25-2007 - 09-27-2007; in: "International Conference on Simulation of Semiconductor Processes and Devices 2007", T. Grasser, S. Selberherr (ed.); Springer-Verlag Wien New York, 12 (2007), ISBN: 978-3-211-72860-4; 329 - 332.

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

References **11) 12) 17)** in List 1

21) M. Pourfath, S. Selberherr:

"Carbon-Based Electronics: A Computational Study";

Talk: International Workshop on the Physics of Semiconductor Devices (IWPSD), New Delhi (invited); 12-15-2009 - 12-19-2009; in: "Proceedings of the International Workshop on the Physics of Semiconductor Devices (IWPSD)", (2009).

22) M. Pourfath, H. Kosina:

"Carbon Based Electronics: A Computational Study";

Talk: Quantum Systems and Devices: Analysis, Simulations, Applications, Beijing (invited); 04-20-2009 - 04-24-2009; in: "Quantum Systems and Devices: Analysis, Simulations, Applications", (2009), 18.

2.2. Conference participations - lectures

References **11) 12) 13) 14) 15) 16) 18) 19)** from List 1

23) M. Pourfath, O. Baumgartner, H. Kosina, S. Selberherr:

"Performance Evaluation of Graphene Nanoribbon Infrared Photodetectors"; Talk: Numerical Simulation of Optoelectronic Devices (NUSOD), Gwangju; 09-14-2009 - 09-17-2009; in: "Proceedings of the 9th International Conference on Numerical Simulation of Optoelectronic Devices", (2009), ISBN: 978-1-4244-4180-8; 13 – 14.

24) H. Kosina: "Transport Modeling for Nanowires and Nanotubes";

Talk: Final FoNE Conference, Miraflores de la Sierra, Madrid; 09-09-2009 - 09-13-2009; in: "Proceedings of the Final FoNE Conference", (2009), 35.

25) A. Yazdanpanah, M. Pourfath, M. Fathipour, H. Kosina, S. Selberherr:

"A Numerical Study of Graphene Nano-Ribbon based Resonant Tunneling Diodes"; Talk: International Symposium on Graphene Devices: Technology, Physics, and Modeling (ISGD), Japan; 11-17-2008 - 11-19-2008; in: "International Symposium on Graphene Devices: Technology, Physics, and Modeling", (2008), 66 – 67.

26) M. Pourfath, O. Baumgartner, H. Kosina:

"On the Non-locality of the Electron-Photon Self-Energy: Application to Carbon Nanotube Photo-Detectors";

Talk: Numerical Simulation of Optoelectronic Devices (NUSOD), Nottingham; 09-01-2008 - 09-04-2008; in: "Proceedings of the 8th International Conference on Numerical Simulation of Optoelectronic Devices", (2008), ISBN: 978-1-4244-2307-1; 99 - 100.

27) N. Neophytou, M. Wagner, H. Kosina, S. Selberherr:

"Analysis of Thermoelectric Properties of Scaled Silicon Nanostructures using an Atomistic Tight-Binding Model";

Talk: 28th International Conference/7th European Conference on Thermoelectrics, Freiburg; 07-26-2009 - 07-30-2009; in: "Book of Abstracts", (2009), 91.

28) M. Pourfath, V. Sverdlov, H. Kosina:
"On the Role of Off-Diagonal Dephasing in Carbon Nanotube Based Photo-Detectors"; Talk: 1st FoNE Conference Nanoelectronics 2008, Taormina, Italy; 06-29-2008 - 07-03-2008; in: "1st Fone Conference Nanoelectronics 2008", (2008), 41.

29) M. Pourfath, H. Kosina, S. Selberherr:
"Carbon Nanotube Based Transistors: A Computational Study";
in: "28th International Conference on the Physics of Semiconductors", American Institute of Physics, 2007, ISBN: 978-0-7354-0397-0, 1041 – 1042.

30) E. Ungersböck, V. Sverdlov, H. Kosina, S. Selberherr:
"Low-Field Mobility in Strained Silicon Inversion Layers and UTB MOSFETs for Different Substrate Orientations";
in: "28th International Conference on the Physics of Semiconductors", American Institute of Physics, 2007, ISBN: 978-0-7354-0397-0, 1389 – 1390.

2.3. Conference participations - posters

References **17) 20)** from **List 1**

31) V. Sverdlov, H. Kosina:
"Electron Subband Dispersions in Ultra-Thin Silicon Films from a Two-Band k·p Theory";
Poster: International Workshop on Computational Electronics (IWCE), Amherst; 10-08-2007 - 10-10-2007; in: "12th International Workshop on Computational Electronics", (2007), 92 – 93.

2.4. Conference participations - other

List 3 Development of collaborations

Indication of the most important collaborations (maximum 8), 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 (national); E (European); I (other international cooperation)
↓	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	D within the discipline T transdisciplinary

N	E	D	Collaboration partner / content of the collaboration
	E2		1) Name: Udo Schwalke Title: Prof. Institution: TU Darmstadt Content: FP7 full proposal on graphene devices; ESF EuroGraphene proposal
	E2		2) Name: Thomas Zimmer Title: Prof. Institution: University of Bordeaux Content: FP7 full proposal on graphene devices; ESF EuroGraphene proposal
			3) Name: Title: Institution: Content:
			4) Name: Title: Institution: Content:
			5) Name: Title: Institution: Content:
			6) Name: Title: Institution: Content:

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

List 4 “Habitations” (professorial qualifications) / PhD theses / diploma theses
with an indication of the status (in progress / completed)

4.1. Professorial Qualifications

4.2. PhD Theses

1) Enzo Ungersboeck: “Advanced Modeling of Strained CMOS Technology”,
Reviewer: H. Kosina, E. Bertagnolli; Institute for Microelectronics, TU Vienna (2007)

4.3. Diploma Theses

1) Zlatan Stanojevic: “Simulation of Carrier Transport in Ultra-Thin-Body Devices”,
Institute for Microelectronics, TU Vienna (2009)

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

Sections of the list:

- 5.1. **Organization of scientific events**
- 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

with an indication of the status (submitted / approved) and the funding organization.

6.1 Applications for follow-up projects (FWF projects)

1) Analysis of Graphene-based Electronic Devices
FWF stand-alone project, submitted Feb. 2010

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

(e. g. FFG, CD Laboratory, a K-plus Centre, funding from the Austrian National Bank, the Federal Government, the provincial government or similar)

1) Analysis of Thermoelectric Nanostructures (ATHENS)
Approved Dec. 2009
Neue Energien 2020 – 3.Ausschreibung, Klima und Energiefonds des Bundes,
managed by FFG.

6.3 Applications for follow-up projects (International projects)

(eg. ERA project, ESF)

1) Electrical and Optoelectronic Graphene Devices (ELOGRAPH)
ESF EuroGraphene call
Approved by ESF, funding rejected by one of the national partners