THEORETICAL STUDY OF TRANSPORT PROPERTIES OF NANOELECTRONICS FOR SENSOR APPLICATION

IJEOMAH GEOFFREY UGOCHUKWU

Master/Doctor of Philosophy

UNIVERSITI MALAYSIA PAHANG

SUPERVISOR'S DECLARATION

I hereby declare that I have checked this thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Doctor of Philosophy of Engineering.

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(Supervisor's Signature)

Full Name : ASSOC. PROF. IR. DR. FAHMI SAMSURI

Position : ASSOCIATE PROFESSOR

Date : 16 JULY 2018

STUDENT'S DECLARATION

I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

____

(Student's Signature)

Full Name : IJEOMAH GEOFFREY UGOCHUKWU

ID Number : PEL15002

Date : 16 JULY 2018

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IJEOMAH GEOFFREY UGOCHUKWU

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ABSTRAK

Ramalan eksperimen bagi sifat-sifat pengangkutan peranti semikonduktor menghadapi cabaran pada hari ini disebabkan oleh skala peranti berterusan. Memandangkan nanoelektronik berskala untuk skala skala nanometer, persamaan pengangkutan yang dikuasai oleh perlanggaran yang digunakan dalam simulator peranti semasa tidak lagi boleh digunakan. Sebaliknya, penggunaan fungsi Green non-keseimbangan (NEGF) yang lebih baik dan lebih tepat terhalang oleh fakta bahawa ia memerlukan jumlah memori dan masa pengiraan yang melampau. Kerja ini menggunakan Persamaan Pengangkutan Boltzmann (BTE) untuk menyiasat sifat pengangkutan nanoelektronik, yang bertujuan untuk memahami mekanisme penderiaan mereka. Kerja-kerja sebelumnya untuk menyelesaikan BTE telah menggunakan sama ada kaedah anggaran atau kaedah stokastik, yang kedua-duanya tidak mempunyai sifat-sifat yang diperlukan untuk aplikasi peranti praktikal. Oleh itu, kerja ini menerangkan penyelesaian teori langsung BTE untuk nanoelectronics yang boleh digunakan untuk aplikasi praktikal. Ini dicapai dengan menggunakan model teori yang kuat untuk membeza-bezakan BTE baik dalam tenaga dan momentum tanpa membuat perkiraan mengenai fungsi integral atau pengedaran pengangkutan. Pendekatan ini bukan sahaja pantas tetapi juga mempunyai keperluan memori yang rendah kerana ia tidak memerlukan penyimpanan langsung unsur-unsur matriks. Spektrum pengangkutan yang lengkap dalam nanoelectronics yang dilanjutkan dari Ohmic ke medan elektrik yang tinggi melalui transmisi balistik diperiksa untuk menggambarkan kebanyakan jalan masuk purata (mfps). Pengangkutan untuk nilai sewenang-wenang medan elektrik berdasarkan BTE diterapkan pada data eksperimen pada nanoelectronics dari medan rendah hingga tinggi. Dalam had bidang yang rendah, ekspresi mobiliti diperoleh dari segi mfp yang jelas lebih pendek daripada panjang sampel. Hasilnya menunjukkan bahawa nanoelectronics sebahagian besarnya beroperasi dalam rejim kuasi-balistik, di mana pengangkutan pembawa menjadi hampir balistik di seluruh saluran berhampiran sumbernya. Rintangan ohmik didapati dikalkimum dengan nilai 6.453kΩ selaras dengan pemerhatian eksperimen dengan transmisi balistik hampir perpaduan apabila panjang saluran menyusut di bawah mfp yang berselerak. Pembebasan kuantum didapati menurunkan halaju tepu yang bebas dari penyebaran dan oleh itu balistik. Peralihan kepada rejim balistik didapati berlaku apabila panjang saluran dikurangkan di bawah mfp balistik yang ditunjukkan sebagai versi lanjutan dari mfp saluran panjang yang diubah suai melalui suntikan dari kenalan, tetapi pergerakannya merosot. Degradasi mobiliti ini ditunjukkan sebagai punca rintangan kuantum dalam had panjang saluran rendah. Penemuan ini mempunyai implikasi yang luar biasa dalam aplikasi sensor nanoelektronik.

ABSTRACT

Experimental prediction of transport properties of semiconductor devices faces a challenge these days due to continuous device scaling. As nanoelectronics are scaled to nanometre scale lengths, the collision-dominated transport equations used in current device simulators can no longer be applied. On the other hand, the use of a better, more accurate non-equilibrium Green function (NEGF) is hampered by the fact that it requires prohibitive amounts of memory and computation time. This work employs the Boltzmann Transport Equation (BTE) to investigate the transport properties of nanoelectronics, aiming to understand their sensing mechanism. Previous works on solving the BTE have employed either an approximate method or a stochastic method, both of which do not possess the requisite properties for practical device applications. Therefore, this work describes the direct theoretical solution of BTE for nanoelectronics that can be utilized for practical applications. This is achieved by employing powerful theoretical models to discretise the BTE both in energy and momentum without making any approximations on the transport integral or distribution function. This approach is not only fast but also has low memory requirements because it does not require direct storage of matrix elements. The complete spectrum of transport in nanoelectronics extending from Ohmic to high electric field through ballistic transmission is examined to delineate plethora of participating mean free paths (mfps). The transport for arbitrary values of electric field is based on BTE applied to experimental data on nanoelectronics extending from low to high field. In the limit of low field, the mobility expressions are obtained in terms of mfp that is distinctly shorter than the length of the sample. The results indicate that nanoelectronics predominantly operate in quasi-ballistic regime, where carrier transport becomes near ballistic across the channel near the source. The ohmic resistance was found to be quantized with a value of 6.453kΩ consistent with experimental observations with ballistic transmission almost unity as channel length shrinks below the scattering-limited mfp. The emission of a quantum was found to lower the saturation velocity that is independent of scattering and hence ballistic. Transition to ballistic regime was found to occur when channel length is reduced below the ballistic mfp that is shown to be extended version of long-channel mfp modified by injection from the contacts, yet the mobility degrades. This mobility degradation is shown to be the cause of resistance quantum in the low-channel-length limit. These findings have overwhelming implications in nanoelectronics sensor application.

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LIST OF SYMBOLS

Ch	Chiral vector
vF	Fermi velocity
λimp	Elastic mean free path
λe-e	Mean free path between scattering events
μ	Mobility
eV	Electron volt
h	Planck constant
ħ	Inverse Planck constant
kB	Boltzmann constant
G	Conductance
VTH	Thermal threshold
VGS	Gate-source voltage
rc	Reflection coefficient

LIST OF ABBREVIATIONS

NEGF	Non-equilibrium Green function
BTE	Boltzmann Transport Equation
FET	Field effect transistor
CNT	Carbon nanotube
NNTB	Nearest neighbour tight binding
NEADF	Non-equilibrium Arora distribution function
SWCNT	Single-wall carbon nanotube
MWCNT	Multi-wall carbon nanotube
MOSFET	Metal oxide semiconductor field effect transistor
2-D	Two-dimensional
1-D	One-dimensional
TB	Tight binding
RBM	Radial breathing mode
LA	Longitudinal acoustic
LO	Longitudinal acoustic
3-D	Three dimensional
DOS	Density of states
NO2	Nitrogen dioxide
Si	Silicon
NH3	Ammonia
rGO	Reduced graphene oxide
ET	Energy transport
HD	Hydrodynamics
DD	Drift-diffusion
SDP	Shift of Dirac peak
SPICE	Simulation program with integrated circuit emphasis
IoNT	Internet of nano things
NEGF	Non-equilibrium green function
GO	Graphene oxide
GFET	Graphene field effect transistor
SiO_2	Silicon dioxide

C_B	Conduction band
V_B	Valence band
RFID	Radio frequency identification
mfp	Mean free path

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