Advanced Boundary Condition Method in Quantum Transport and its Application in Nanodevices

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Overview of my phD works

Software Development and Optimization:
RGF, QTBM,
contact self-energy,
interface roughness,
phonon scattering,
……

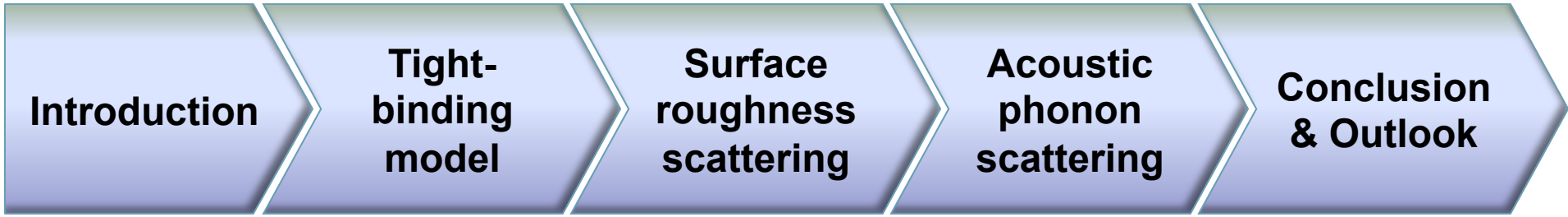
Algorithm Development:
Low Rank Approximation
General lead algorithm
Surface passivation model

Transistor Physics:
GaSb/InAs TFET
MoS_2 heterostructure
Black phosphorus transistor

Other Projects:
Graphene
Phonon and heat transport
Transport in Bi_2Te_3
……

Today's focus: transport study of black phosphorus

Outline

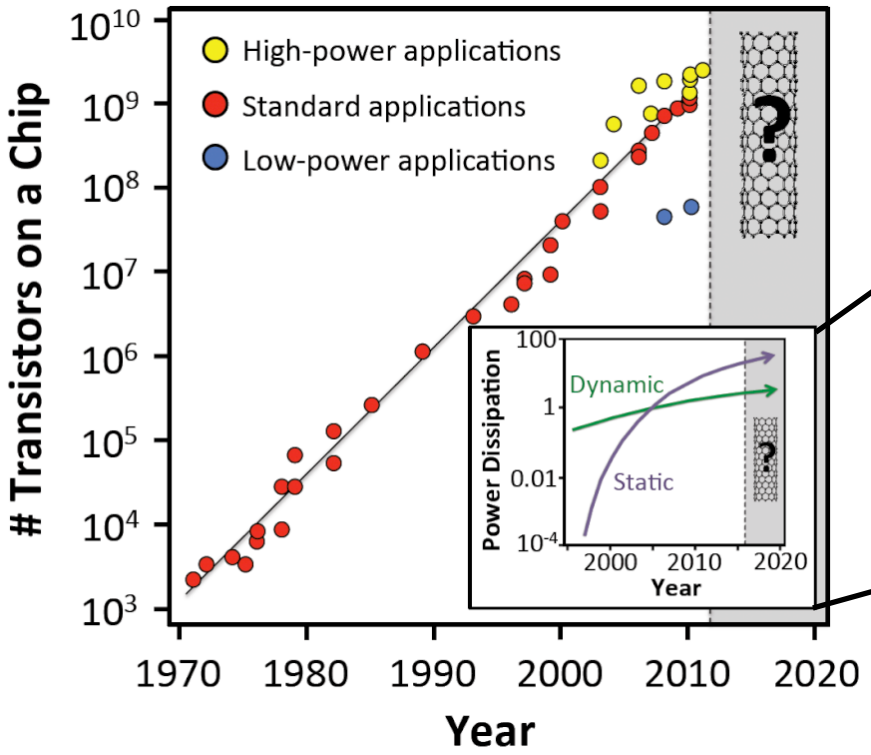

Introduction
Tight-binding model
Surface roughness scattering
Acoustic phonon scattering
Conclusion & Outlook

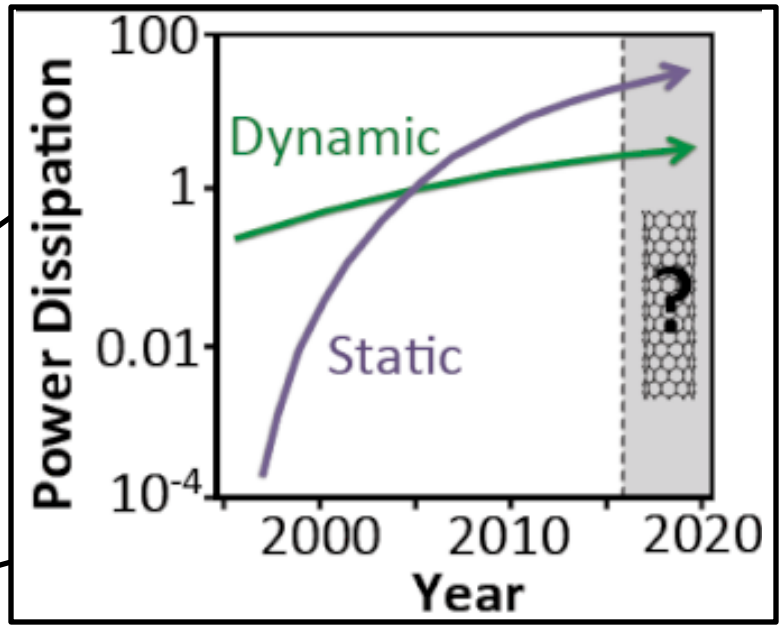
Outline

Introduction | Tight-binding model | Surface roughness scattering | Acoustic phonon scattering | Conclusion & Outlook

- Why do we study black phosphorus?
- Open questions in black phosphorus

Challenges in transistors





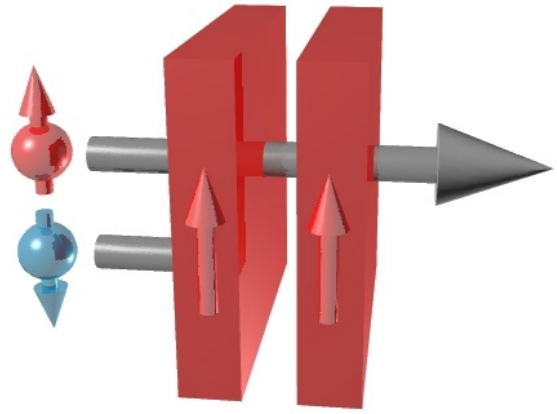
http://www.eeweb.com/blog/aaron_franklin

Challenges:
Power consumption
Leakage current
Short channel effect
Quantum effect
……

Research efforts to solve these challenges

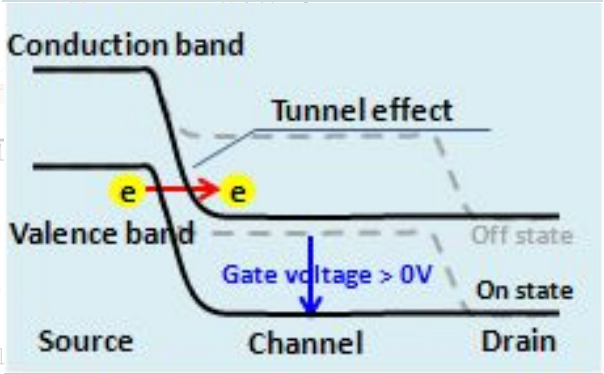
Transistor concept/design

Spintronics



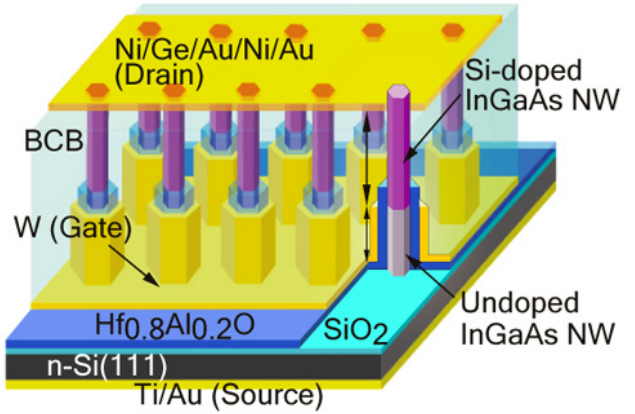
http://bestlegalsteroidsarea212.rhcloud.com/tag/spintronics

Operation mechanism: tunneling FET



http://phys.org/news/2012-11-compact-tunnel-field-effect-transistors.html

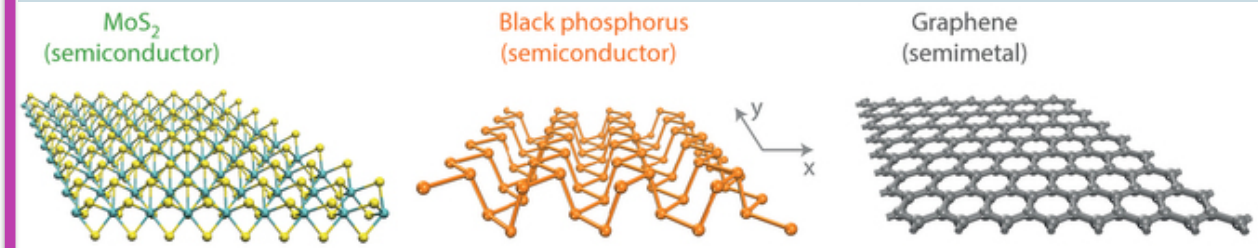
Geometry: vertical transistor



http://physicsworld.com/cws/article/news/2012/aug/02/nanowires-give-vertical-transistors-a-boost

Beyond traditional materials

2D materials

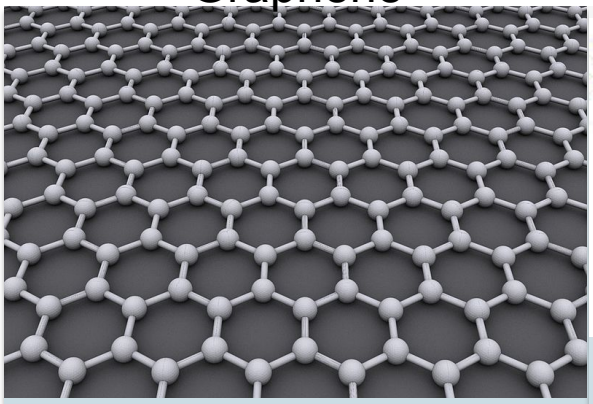


http://www.nature.com/nphoton/journal/v8/n12/fig_tab/nphoton.2014.271_F1.html

2D materials timeline

2004 → 2011 → 2014

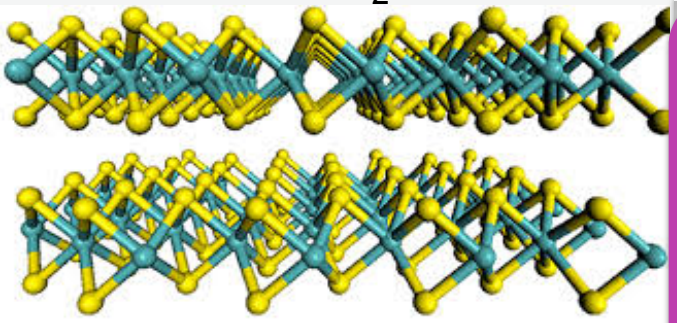
Graphene



- 2D plane structure honeycomb shape
- High carrier mobility ~$10^5 cm^2/Vs$
- Semi-metal, no intrinsic band gap
- Nanoribbon, nanomesh

https://en.wikipedia.org/wiki/Graphene

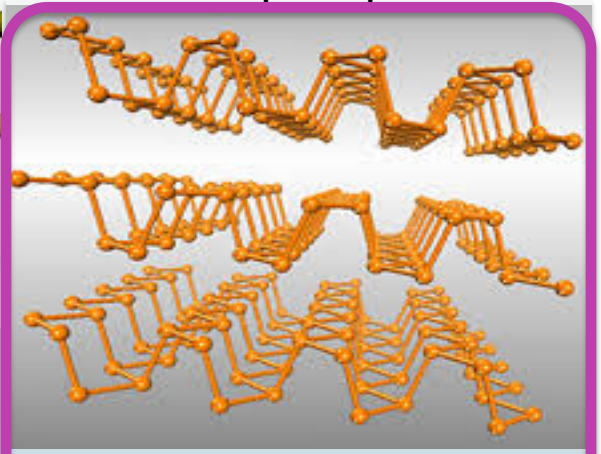
MoS_2



- TMDC (transition metal dichalcogenide)
- Stacked layer structure
- Intrinsic band gap
- Comparably low mobility 200~400cm^2/Vs <<graphene

https://en.wikipedia.org/wiki/Molybdenum_disulfide

Black phosphorus



- Stacked layer structure
- Intrinsic band gap
- Potential candidate in transistor application
- Many unknowns

L Li et al, Nature Nanotechnol. 9, 372 (2014).

Explore black phosphorus and its transport features

First black phosphorus transistor shows promising performance

ARTICLES
PUBLISHED ONLINE: 2 MARCH 2014 | DOI: 10.1038/NNANO.2014.35
nature nanotechnology

Black phosphorus field-effect transistors

Likai Li[1], Yijun Yu[1], Guo Jun Ye[2], Qingqin Ge[1], Xuedong Ou[1], Hua Wu[1], Donglai Feng[1], Xian Hui Chen[2]* and Yuanbo Zhang[1]*

We have succeeded in fabricating p-type FETs based on few-layer phosphorene. Our samples exhibit ambipolar behaviour with drain current modulation up to $\sim 10^5$, and a field-effect mobility

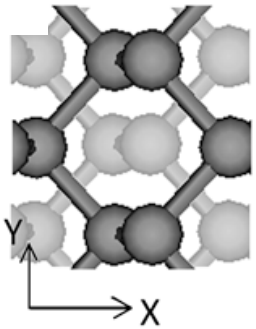
measured as a function of gate voltage for devices with different thicknesses: 10 nm (black solid line), 8 nm (red solid line) and 5 nm (green solid line), with field-effect mobility values of 984, 197 and 55 $cm^2 V^{-1} s^{-1}$, respectively. Field-effect mobilities were extracted from the line fit of the

Promising performance motivates further exploration of black phosphorus

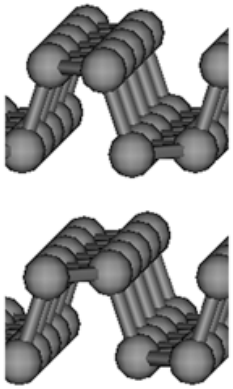
Why is black phosphorus good for transistor?
Intrinsic direct band gap

Black phosphorus structure

top view



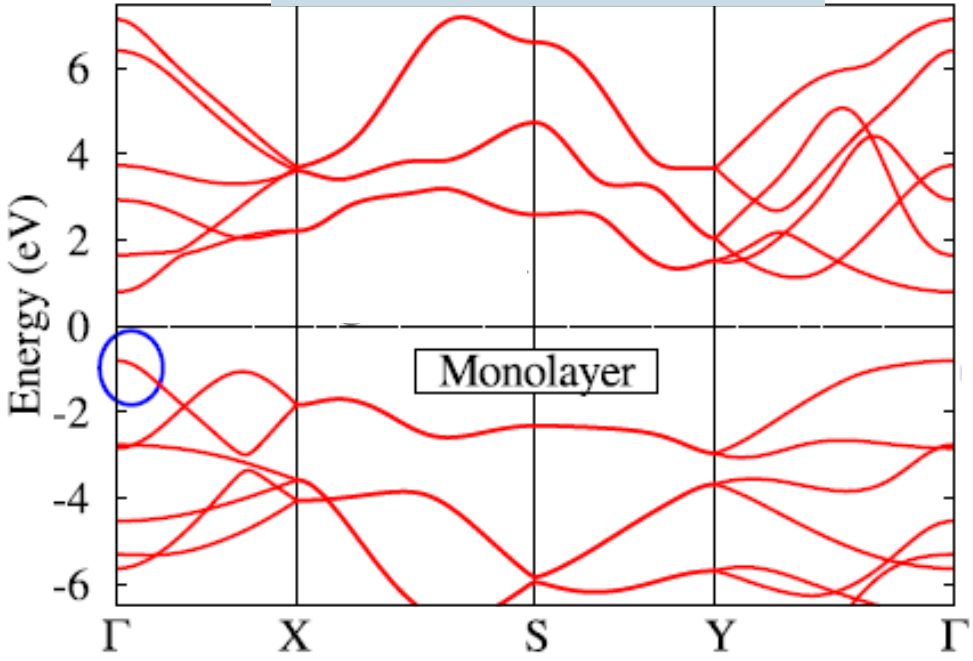
side view



X: armchair
Y: zigzag

- Stacked layer
- Honeycomb shape top view
- Different bond length

DFT-GW band structure



A Rudenko et al, Phys. Rev. B 89, 201408 (2014)

- Intrinsic direct E_g → superior to graphene
- Direct E_g thickness (layer) dependent → optoelectronics
  - ✓ monolayer ~1.5eV, bulk ~0.3eV

Why is black phosphorus good for transistor?

High mobility

CrossMark click for updates

Cite this: *Chem. Soc. Rev.*, 2015, 44, 2732

Semiconducting black phosphorus: synthesis, transport properties and electronic applications

Han Liu, Yuchen Du, Yexin Deng and Peide D. Ye*

out to be an impurity dominated semiconductor. A band gap of 0.31 eV was estimated. Carrier mobilities extracted from the magnetoresistance coefficients gave the values of 2.7 × 10^4 cm^2 V^{-1} s^{-1} at 77 K and 1.5 × 10^4 cm^2 V^{-1} s^{-1} at 294 K, respectively, which are roughly one order of magnitude higher

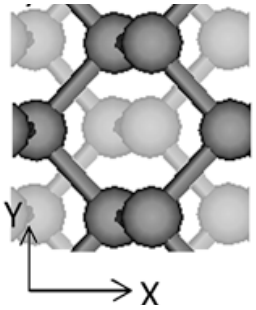
Hall effect measurement for bulk black phosphorus

DFT calculation

$$\mu_{2D} = \frac{e\hbar^3 C_{2D}}{k_B T m_e^* m_d (E_1^i)^2}$$

	μ_{x_2D} (10^3 cm^2 V^{-1} s^{-1})	μ_{y_2D} (10^3 cm^2 V^{-1} s^{-1})	
Hole mobility	0.64-0.70	10-26	1L
	2.6-2.8	1.3-2.2	
	4.4-5.2	2.2-3.2	
	4.4-5.2	2.6-3.2	
	4.8-6.4	3.0-4.6	5L

J Qiao et al, Nature Comm. 5, 4475



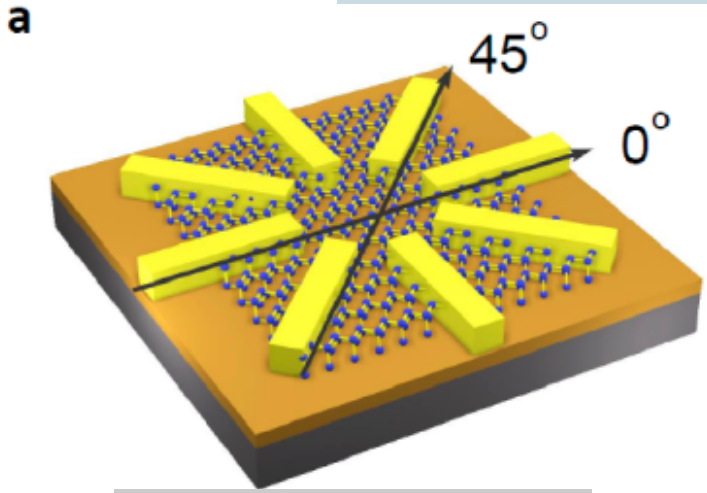
X: armchair
Y: zigzag

Hole mobility ~10^4 cm^2/Vs

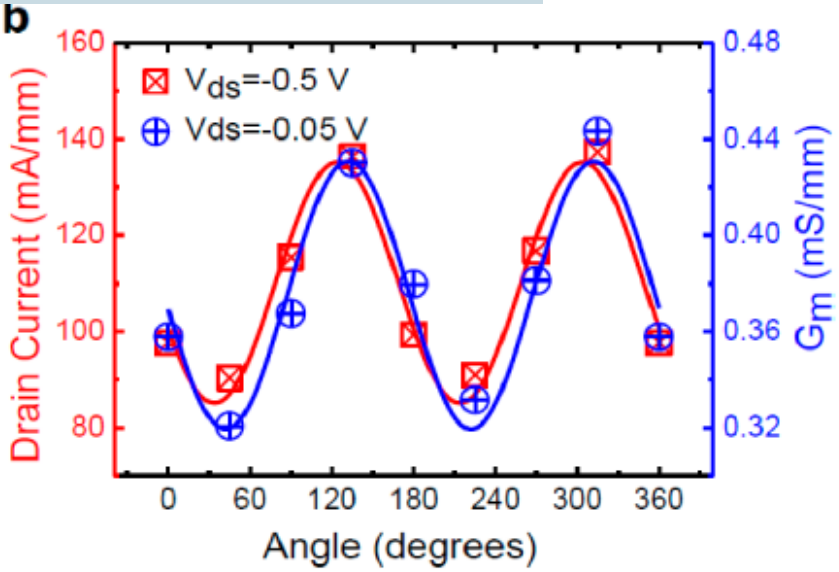
Why is black phosphorus good for transistor?

Anisotropic transport

Measured current along different directions



H Liu et al, ACSnano 8, 4033 (2014)



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Cite this: *Chem. Soc. Rev.*, 2015, 44, 2732

Semiconducting black phosphorus: synthesis, transport properties and electronic applications

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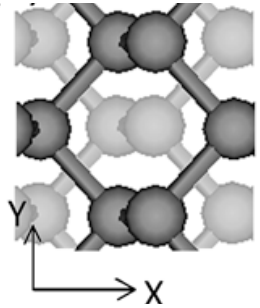
demonstrated. In principle, we can design the transport along *x*-direction, which provides highest mobility, and channel width along *y*-direction, which has the highest density of states and where density of states remains the same determined by $(m_x m_y)^{1/2}$.[56] It is superior over other conventional III–V semiconductors, which has high electron mobility but low density of states. We can also design



Anisotropy: high mobility and DOS

Existing transport simulation
ballistic, qualitatively shows anisotropic feature

- Many theoretical studies in dispersion level (electronic and phonon) using DFT
- One NEGF Ballistic transport
  1L BP, n-type, 4-band tight binding

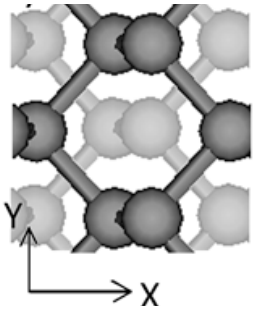
F Liu et al, IEEE Trans. Electron. Dev. 61, 3871 (2014)

IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 61, NO. 11, NOVEMBER 2014

Ballistic Transport in Monolayer Black Phosphorus Transistors

Fei Liu, Yijiao Wang, Xiaoyan Liu, Jian Wang, and Hong Guo

The drain current density in AD can reach $3.1 \times 10^3 \mu A/\mu m$ at $V_G = 1.0$ V. The current in ZD, on the other hand, is lower by about $1.4 \times 10^3 \mu A/\mu m$, i.e., ~45.2% of that in AD. The



X: armchair
Y: zigzag

Measurement

H Liu et al, ACSnano 8, 4033 (2014).

channel length display a high on-current of 194 mA/mm,

Qualitatively reproduces anisotropic transport

Quantitatively differs from measurement

Measurement is far from ballistic
→ scattering exists

Open question
Mobility << expected

DFT calculation

$$\mu_{2D} = \frac{e\hbar^3 C_{2D}}{k_B T m_e^* m_d (E_1^i)^2}$$

	μ_{x_2D}	μ_{y_2D}
	$(10^3\ cm^2\ V^{-1}\ s^{-1})$	
Hole mobility	0.64-0.70	10-26
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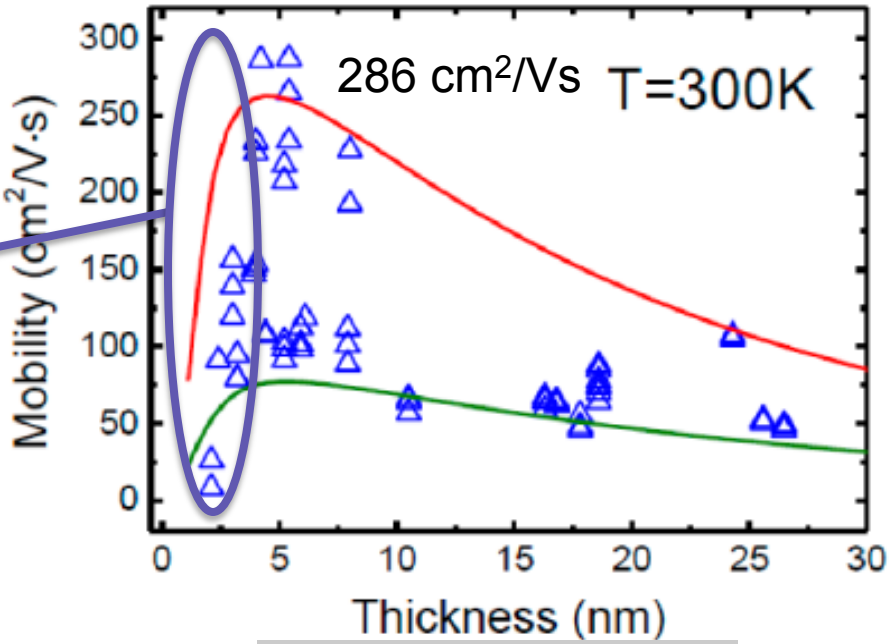
	4.4-5.2	2.6-3.2
	4.8-6.4	3.0-4.6

1L ↓ 5L

J Qiao et al, Nature Comm. 5, 4475 (2014)

Measured hole mobility



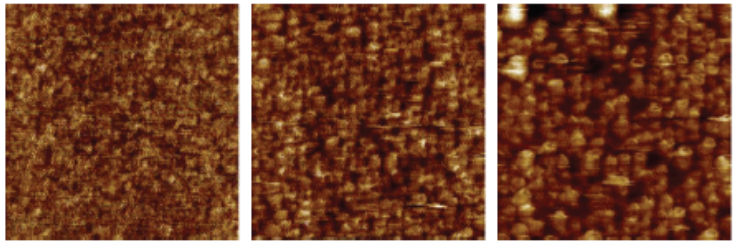
H Liu et al, ACSnano 8, 4033 (2014).

- Transport measured mobility 286cm²/Vs<< expected 10^4cm²/Vs → scattering
- Possible scattering mechanism
  - Phonon, roughness, defect, impurity …

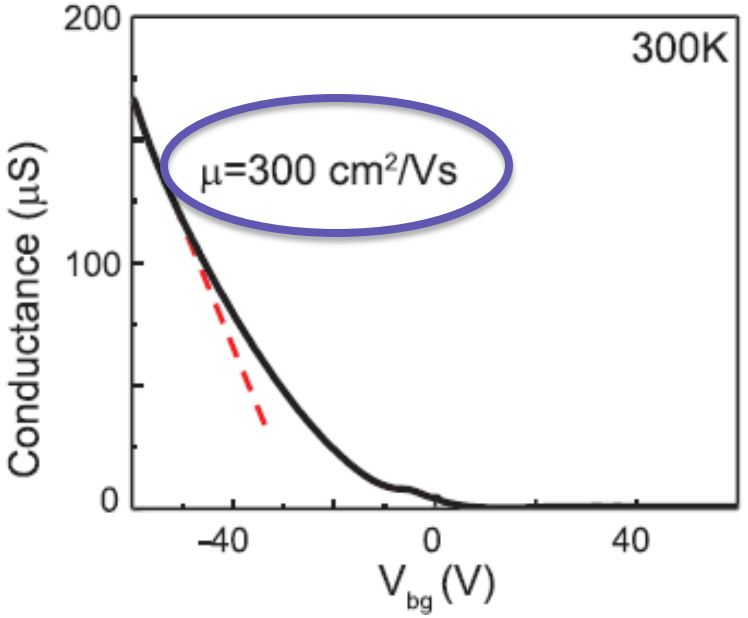
Understand the dominating scattering mechanism through transport study is critical

Open question
Does surface roughness dominate?

Surface roughness in black phosphorus samples



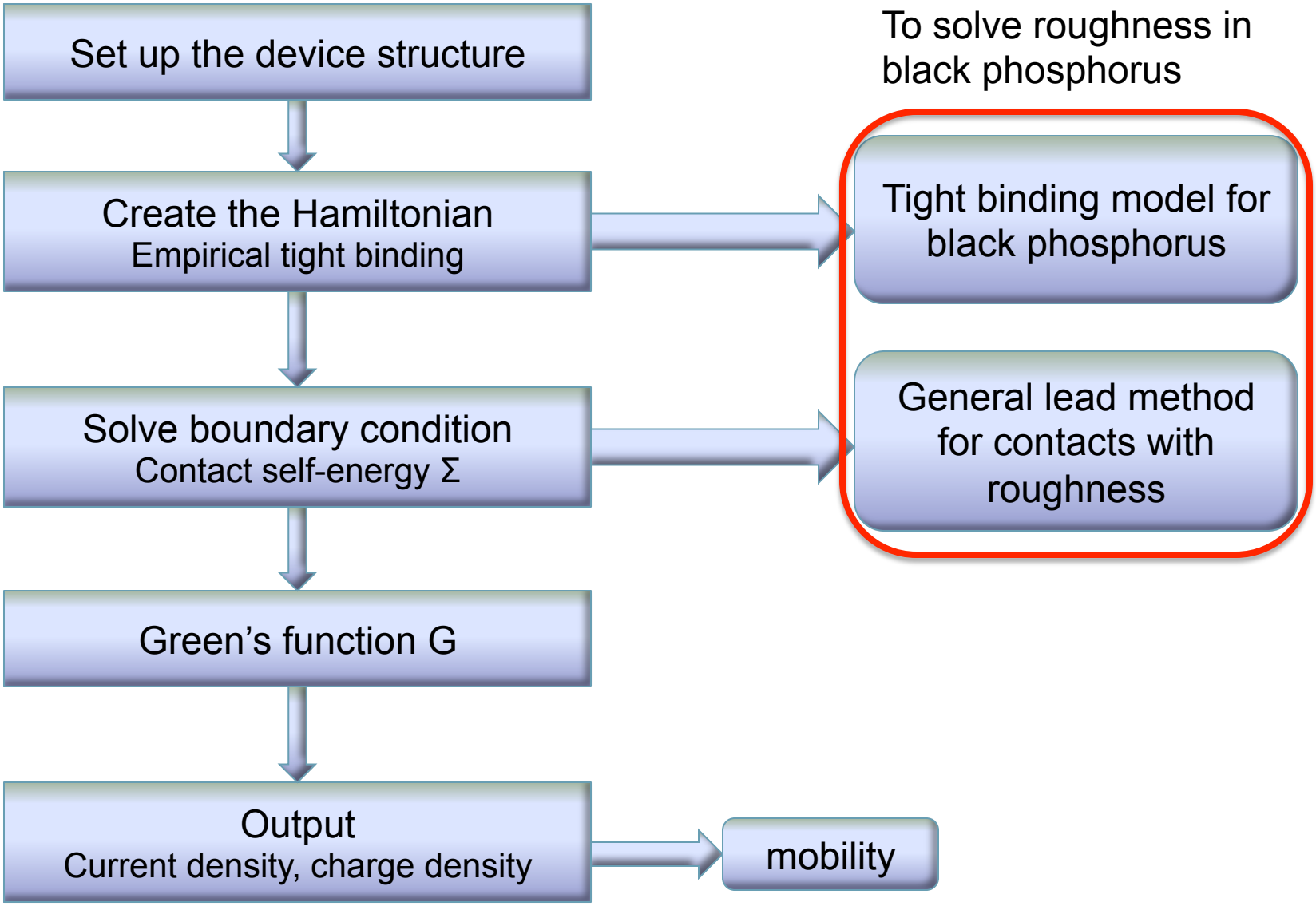
S Koenig et al, Appl. Phys. Letts. 104, 103106 (2014)



- Surface roughness observed in experiment
- Measured mobility from rough sample is ~300cm^2/Vs
- Does roughness scattering dominate?

Understand the impact of roughness scattering through transport study

Transport (NEGF) simulation flow



Outline

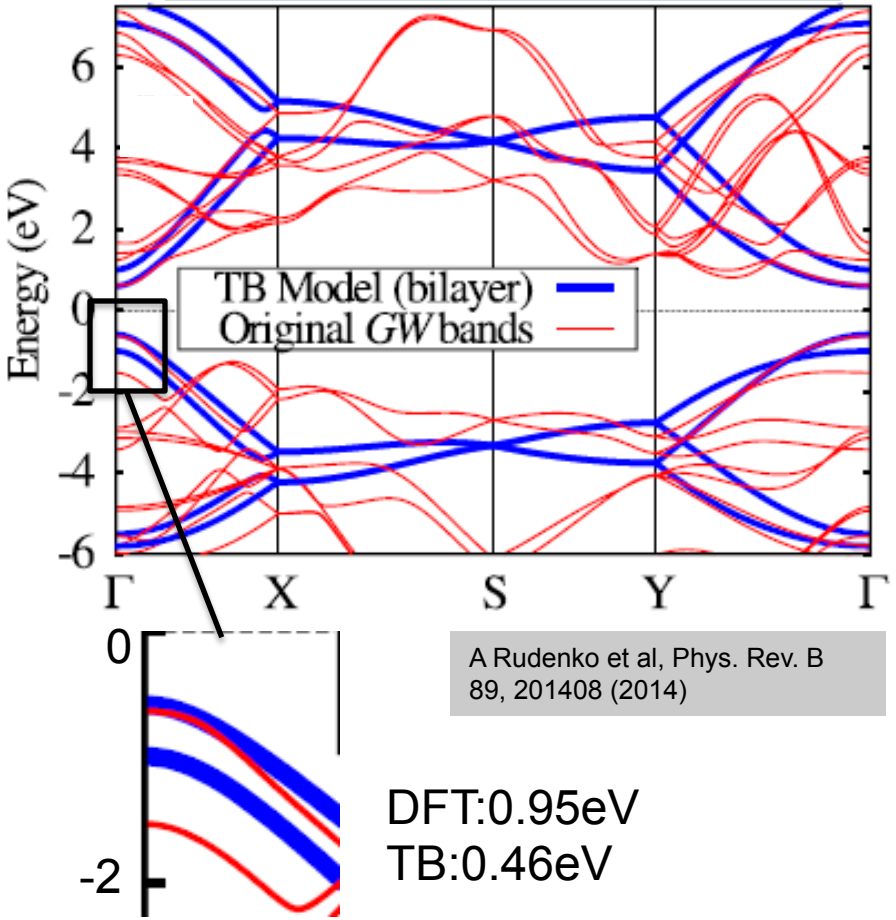
Introduction → **Tight-binding model** → Surface roughness scattering → Acoustic phonon scattering → Conclusion & Outlook

- Problem of existing 4-band model
- 10-band model and parameterization

Problem of the four band TB model
Underestimate band splitting

- 4-band TB underestimates E_v splitting by ~50%
- DFT splitting smaller in more layers
  →3L:0.4eV; 4L:0.2eV;
  4-band model close to degenerate
- Would change hole distribution
- Worse if scattering exists

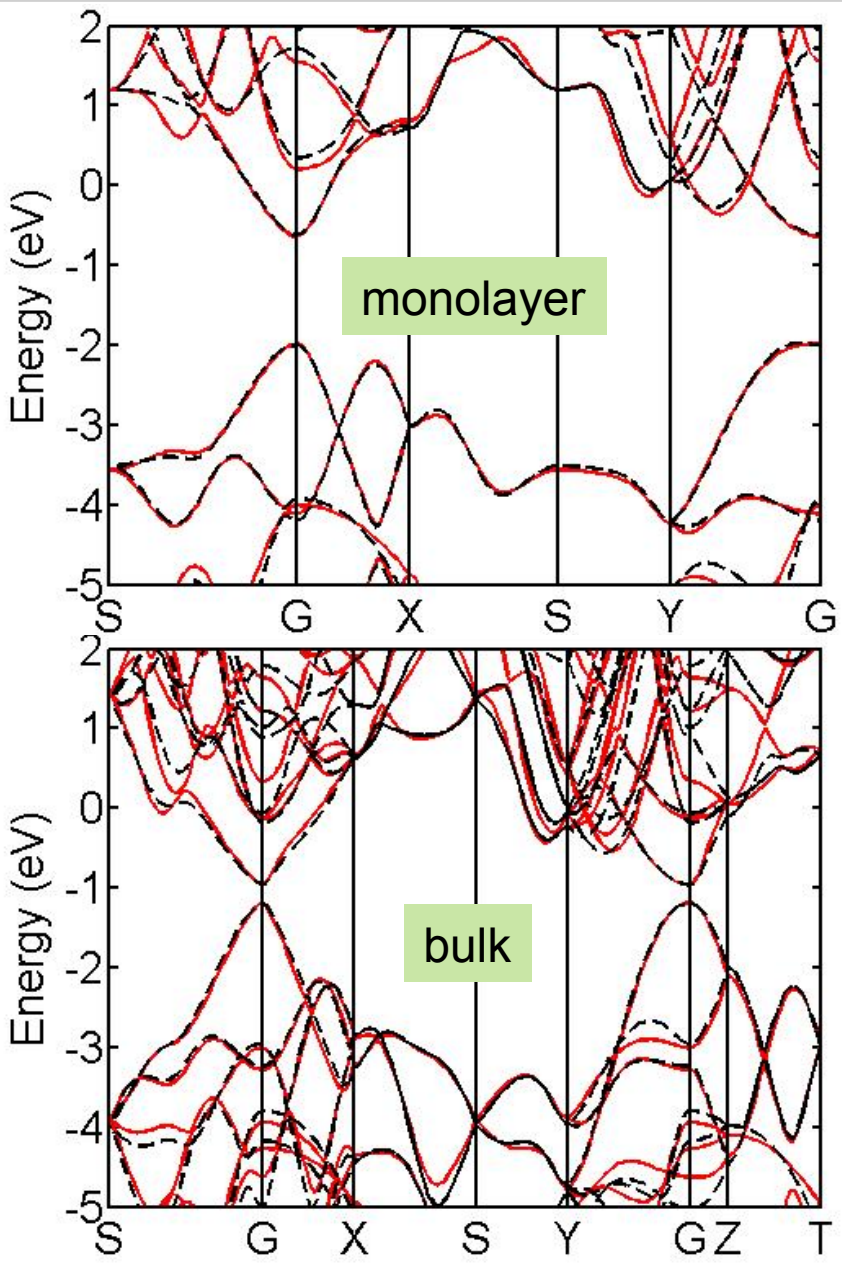
Band structure for bilayer (2L) black phosphorus

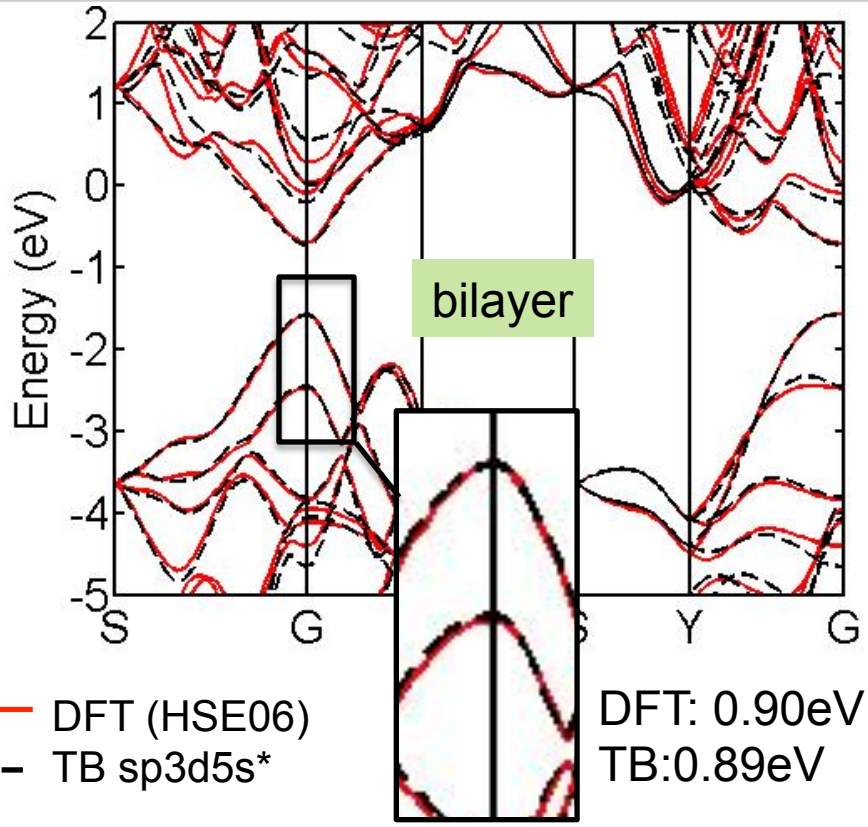


A Rudenko et al, Phys. Rev. B 89, 201408 (2014)

Better TB model is required for quantitative simulation

Ten-band (sp3d5s*) TB model





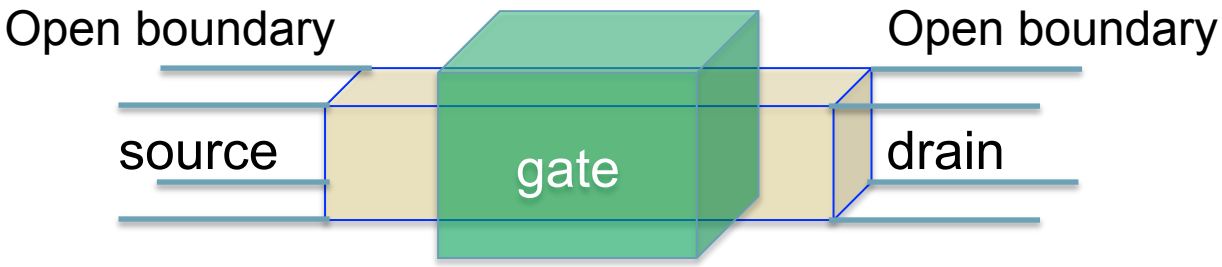
- DFT HSE06 band structure is nicely reproduced with 10-band TB.
- Band splitting is well captured.
- Generic model for arbitrary layers.

Outline

Introduction → Tight-binding model → **Surface roughness scattering** → Acoustic phonon scattering → Conclusion & Outlook

- Challenges in solving rough contacts
- New algorithm: general lead method
- Benchmark and application
- General lead method applied to roughness in black phosphorus

Physical distinction between contact and device



Device:

- Where the critical physics do not change
  e.g. for a homogeneous device structure, the transmission is length independent in ballistic calculation

Contact:

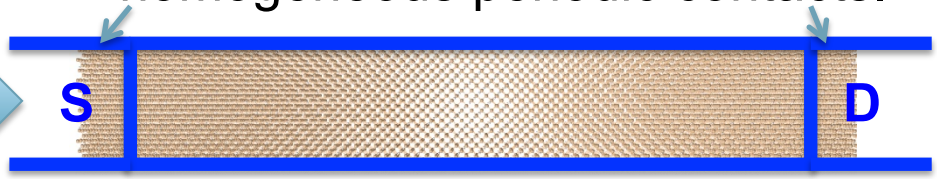
- Serve as the boundary condition of the device
- Have specific DOS and carrier distribution
- Semi-infinite extension of the device at its boundary
  →homogeneous (periodic) , reserve the critical physics of the device

Critical physics of the device should be reserved with proper contact treatment

Challenges in the existing contact treatment
only solve homogeneous (periodic) contacts

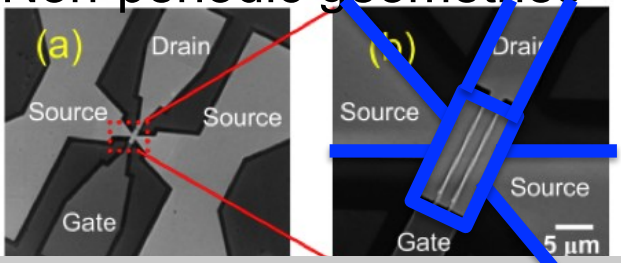
Common contact methods: Sancho Rubio, transfer matrix

homogeneous periodic contacts.



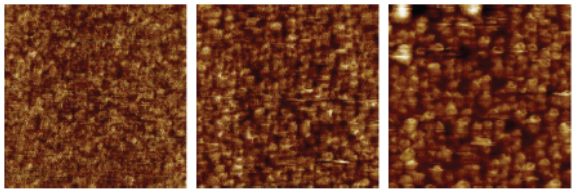
But in the real world…

Non-periodic geometries



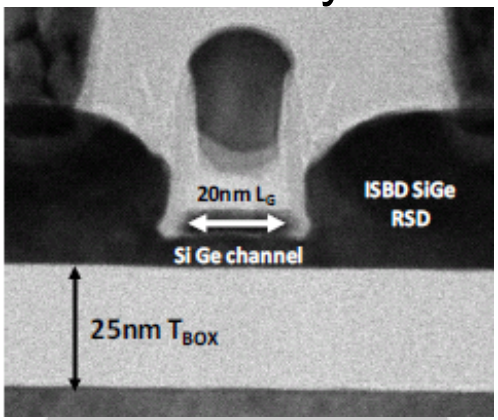
http://www.electroiq.com/articles/sst/2010/12/iedm-reflections_.html

Roughness



S. Koenig et al, Appl. Phys. Lett, Vol. 104, pp. 103106, 2014

Random alloy

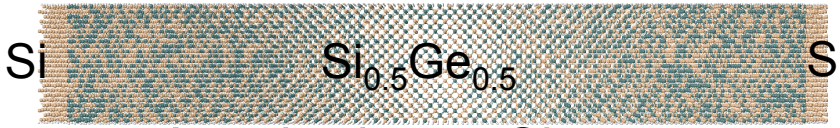


Q. Liu, et al, IEDM p.229 2013

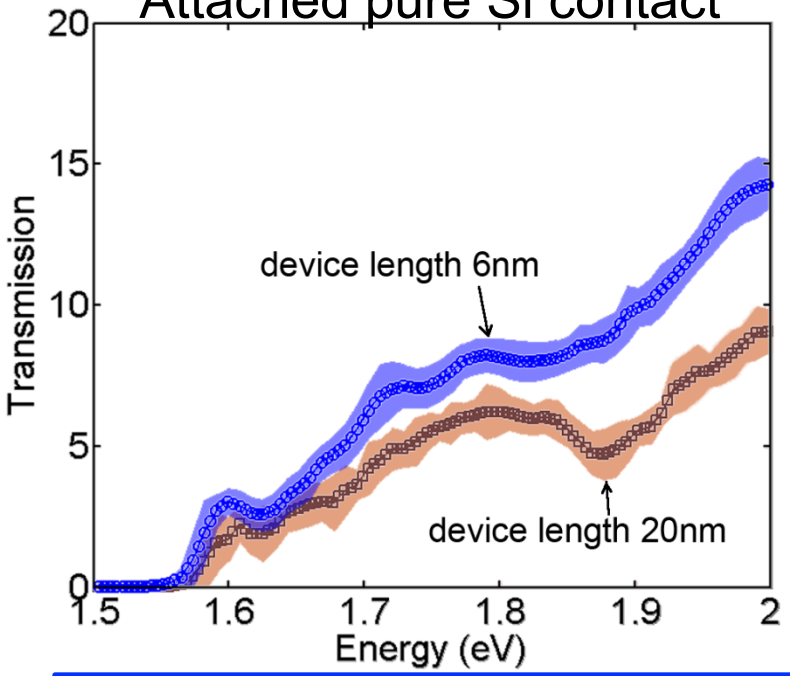
With disorder in the device, homogeneous (periodic) contact cannot reserve the device physics

Alloyed device with periodic contacts

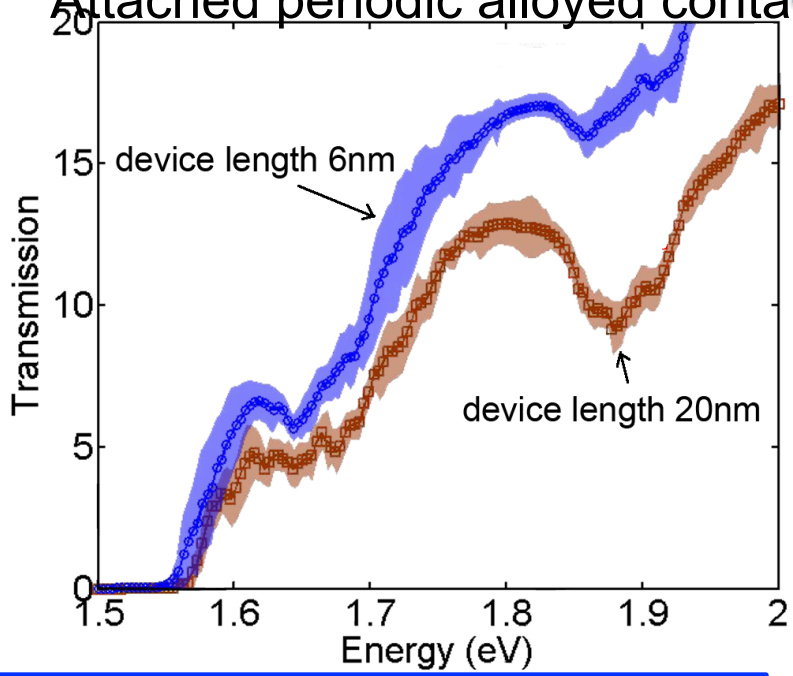
3nm diameter $Si_{0.5}Ge_{0.5}$ nanowire



Attached pure Si contact



Attached periodic alloyed contact



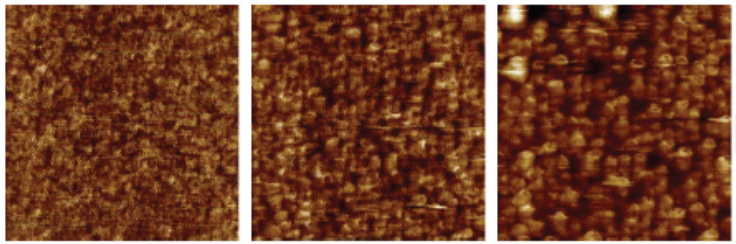
With periodic contacts, alloy device's transmission in ballistic calculation is 1) length dependent, and 2) relied on contact materials

→ DOS mismatch between periodic contacts and alloy device

- Critical device physics change with contact
- Possible solution: have disorder contact treatment

Solve NEGF with surface roughness
roughness exists in both device and contacts

Roughness in experiment



S Koenig et al, Appl. Phys. Letts. 104, 103106 (2014)

Roughness in simulation

- Randomly distribute atoms at the surfaces
- Distribution follows autocovariance function

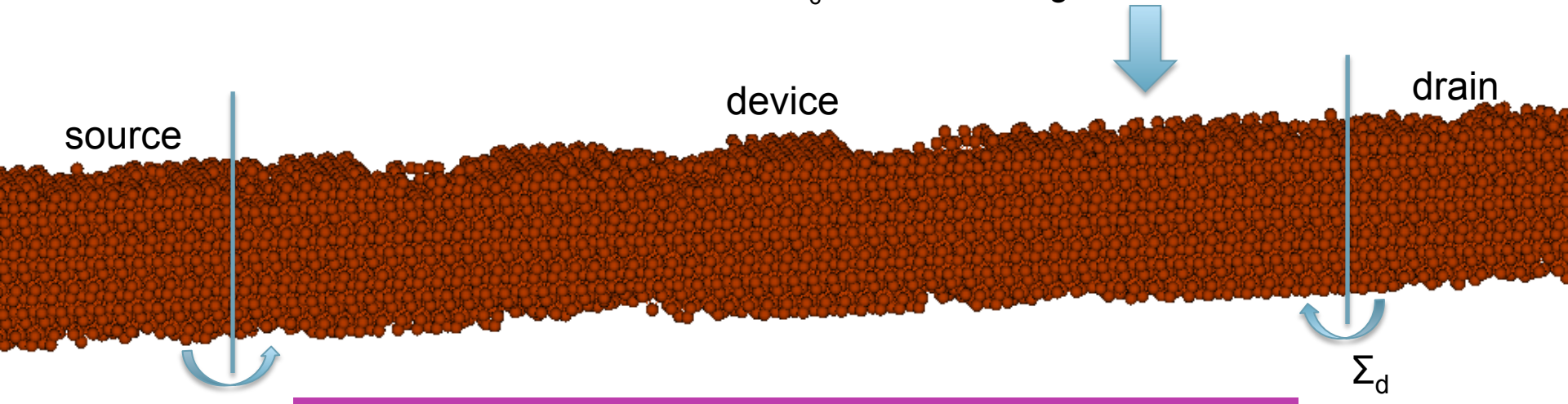
$$ACVF_{ij} = \Delta^2 \exp(-\sqrt{2}\,|\,r_i - r_j\,|\,/\,L_c)$$

Kim et al, IEEE Trans. Elect. Dev. 58, 1371 (2011).

r_i, r_j the coordinates of surface atoms i, j

[?] root mean square of roughness

L_c correlation length

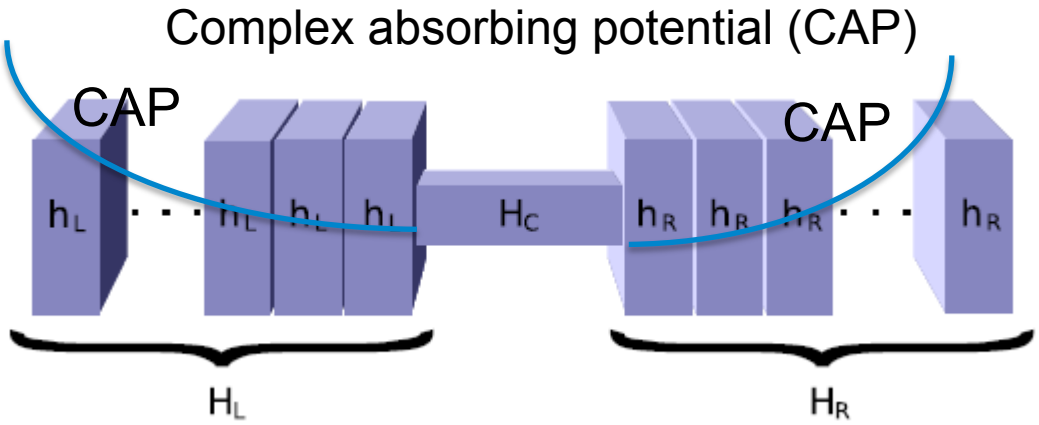


To correctly capture the physics of rough device, contact treatment with roughness is needed.

Method: problem & idea

Problem:

- No exact solution for semi-infinite systems if not assume periodicity;
- Approximate solution
  - ✓ Physically correct
  - ✓ Numerically solvable for arbitrary contact structures

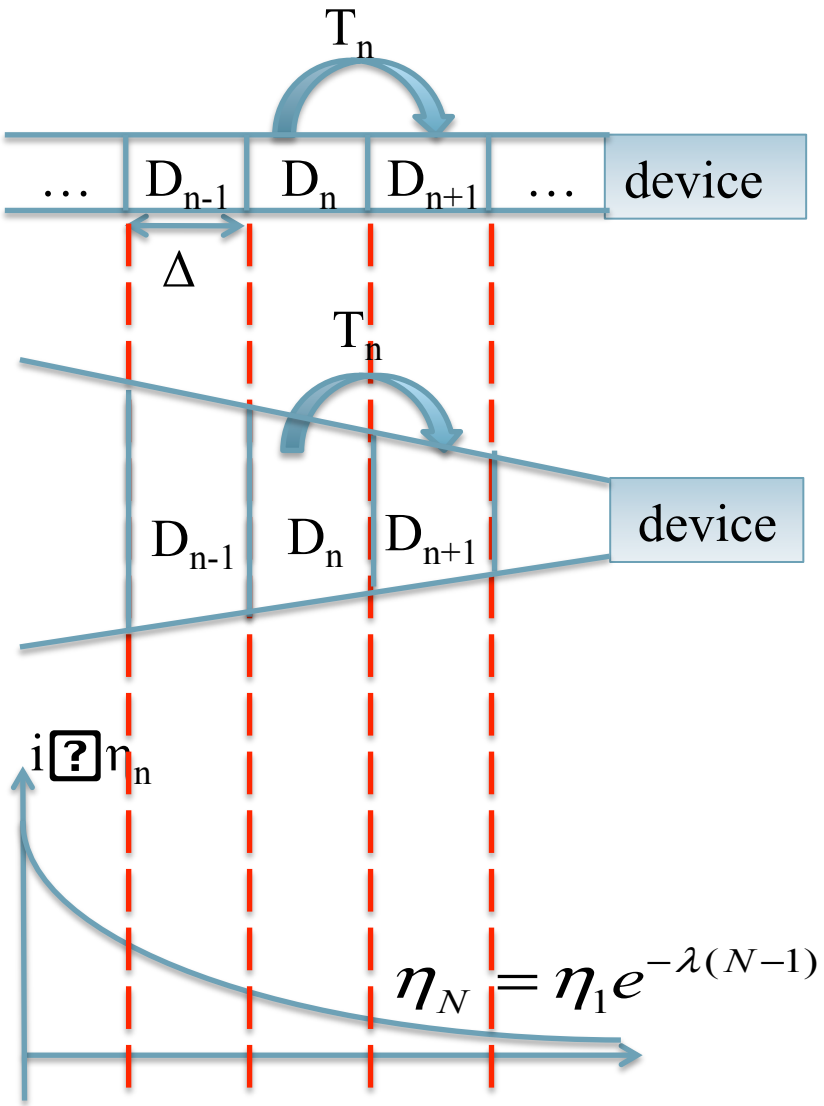


J. Driscoll et al, Phys. Rev. B. Vol. 78, pp. 245118, 2008

Idea: extend complex absorbing potential (CAP) method

- **Non-periodic contact** : Hamiltonian for explicit contact segments
- **CAP serves as scattering** : physical assumption of contacts
- **Efficient, memory thin** : converge within finite iterations

Method: general lead approach detail



Known: direct iterative method

$$\Sigma_n = T_n \, g_{n-1} \, T_n^{\dagger}$$
$$g_n = (D_n - \Sigma_n)^{-1}$$

convergence issues: initial guess propagates ballistically (>10^3 iterations)

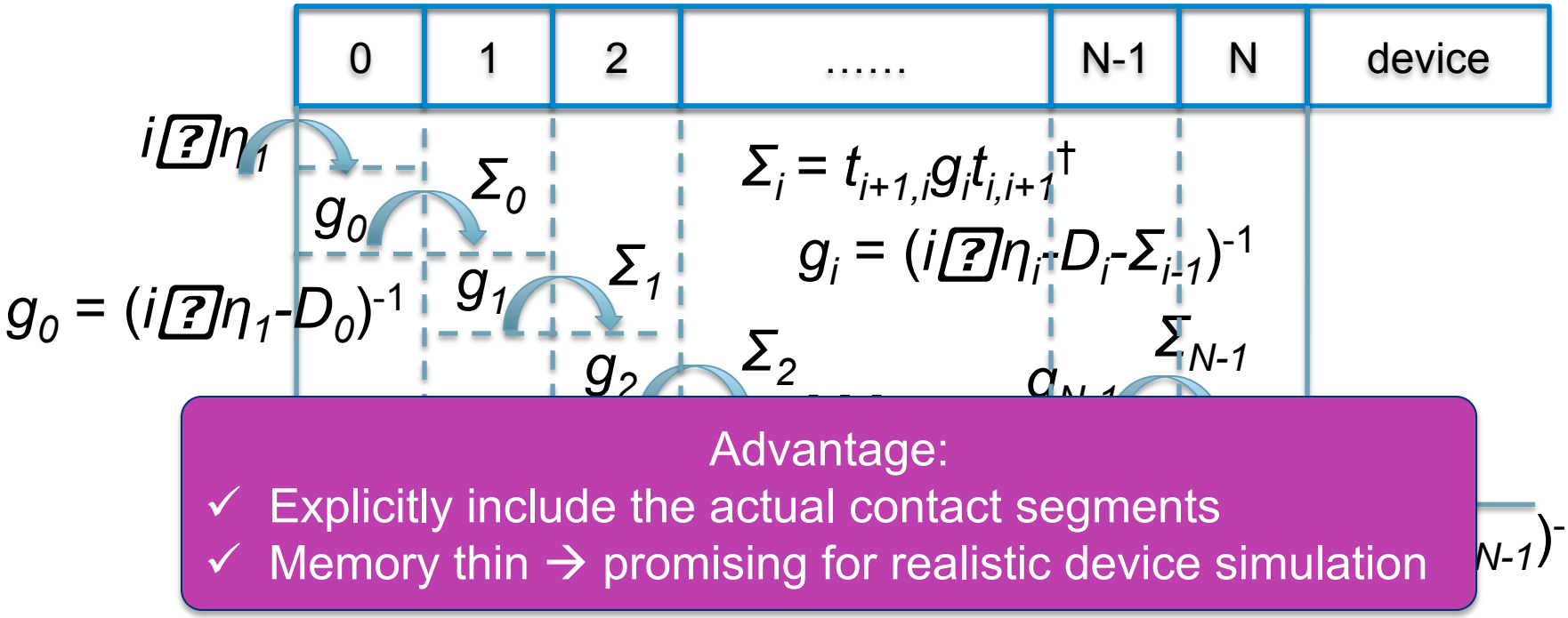
General lead approach: CAP i η

$$\Sigma_n = T_n \, g_{n-1} \, T_n^{\dagger}$$
$$g_n = (D_n + i\,\eta_n - \Sigma_n)^{-1}$$

Basic rules to choose η:

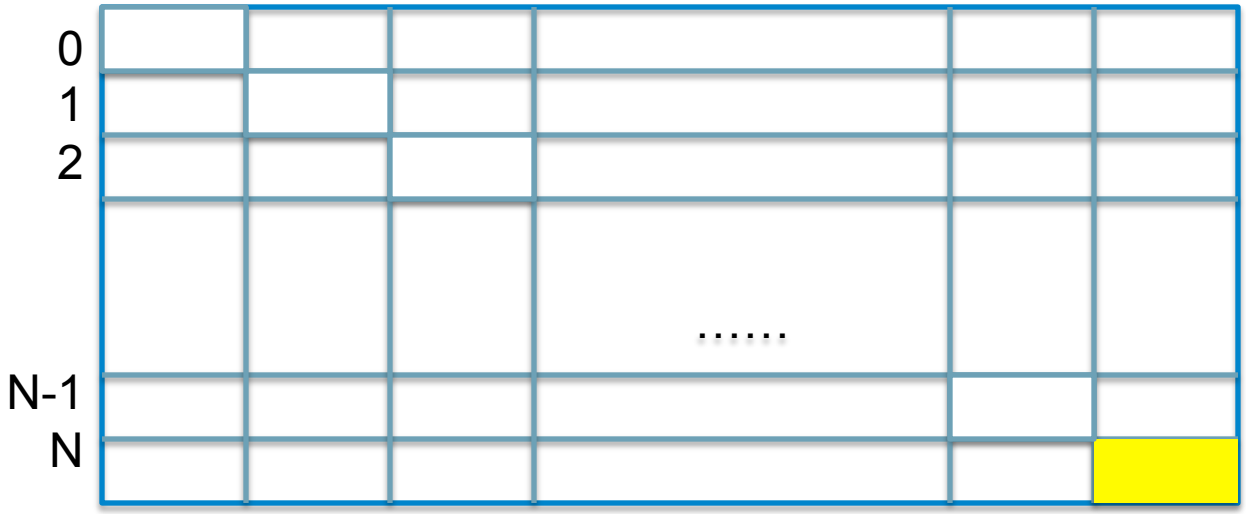
- Big initial value → blurs interference far away
- Ballistic close to the interface → matches device DOS
- Fast convergence (within 200 iterations)

General lead approach algorithm flow

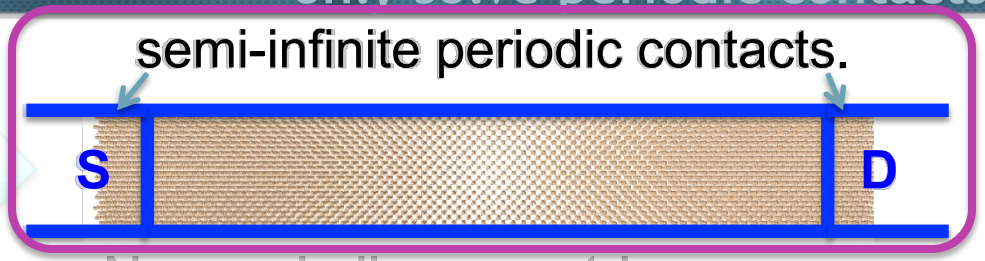


Advantage:

- ✓ Explicitly include the actual contact segments
- ✓ Memory thin → promising for realistic device simulation



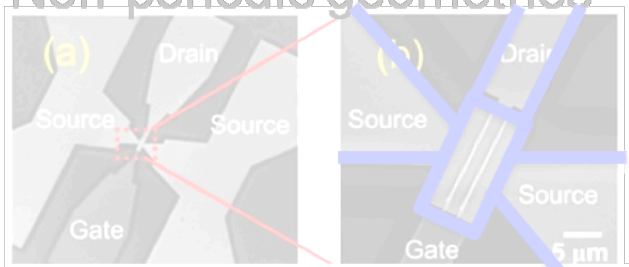
Challenges in existing self-energy methods
only solve periodic contacts



Common self-energy methods Sancho Rubio, transfer matrix

But in the real world…

Non-periodic geometries

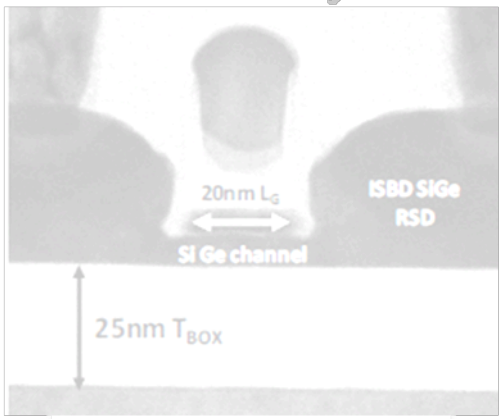


http://www.electroiq.com/articles/sst/2010/12/iedm-reflections_.html

Roughness

S. Koenig et al, Appl. Phys. Lett, Vol. 104, pp. 103106, 2014

Random alloy



Q. Liu, et al, IEDM p.229 2013

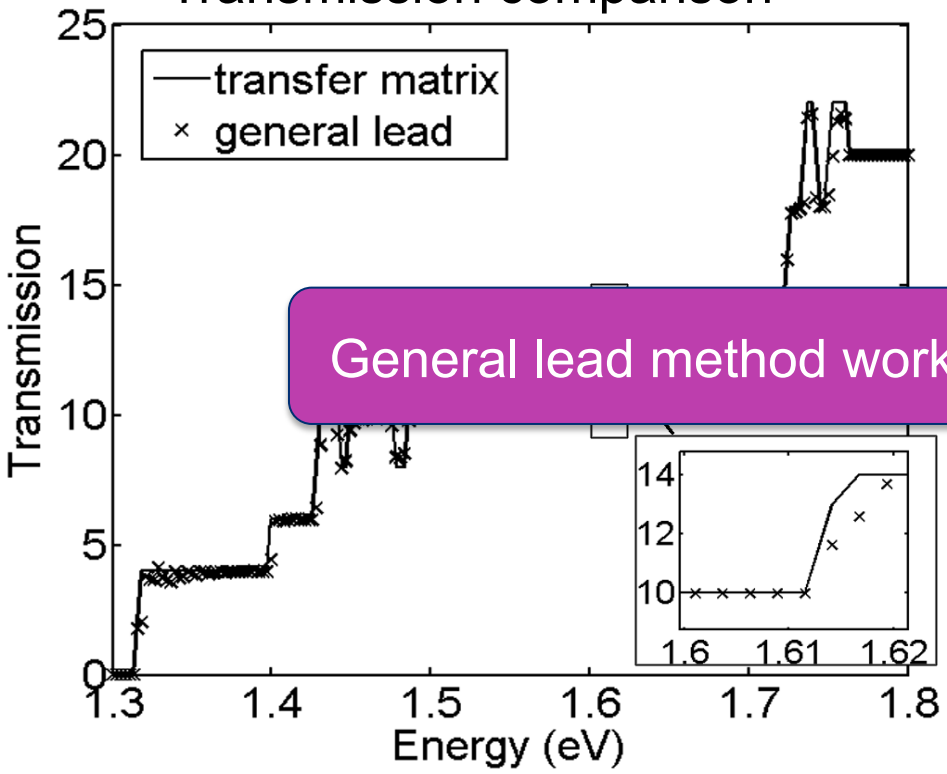
- Periodic assumption contradicts realistic contacts
- Method applicable for non-periodic contacts is required

Benchmark on periodic contacts

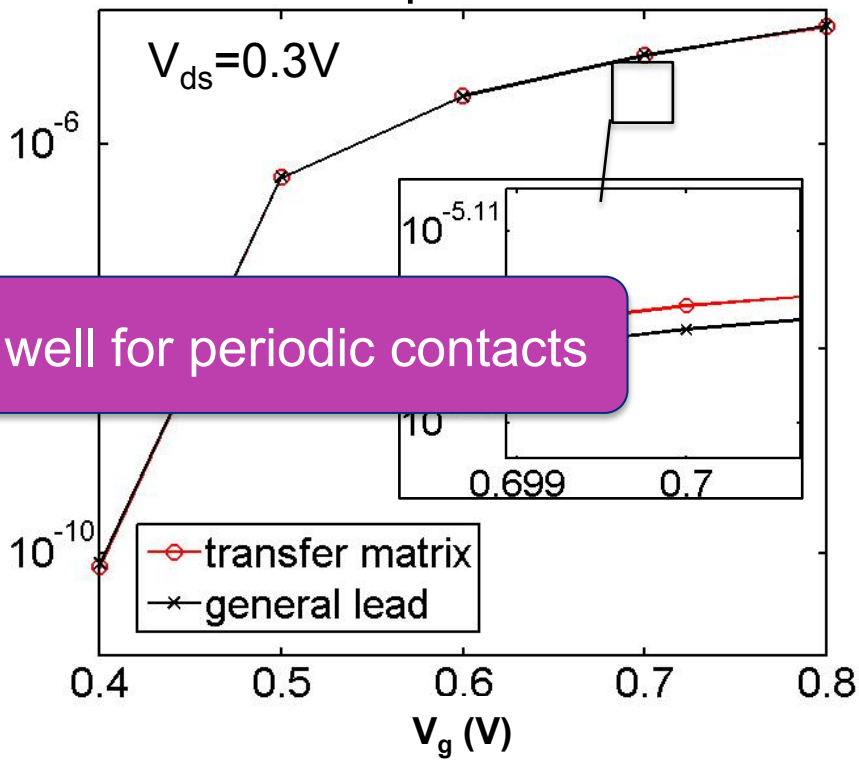
Example:
Regular 3x3x20nm Si nanowire in $sp^3d^5s^*$ tight binding
Pure Si contact

Damping details:
η_1 = -0.5 eV,
$\eta_i = \eta_1 \exp(-\lambda ? i)$
λ = 0.1, i = 0…155

Transmission comparison



IV comparison



General lead method works well for periodic contacts

Timing for Σ solution
Transfer matrix: 9.6s
General lead: 50.8s

- Transmission agrees with common method
- Deviations observed only close to van Hove singularities
- I-V curve agrees well

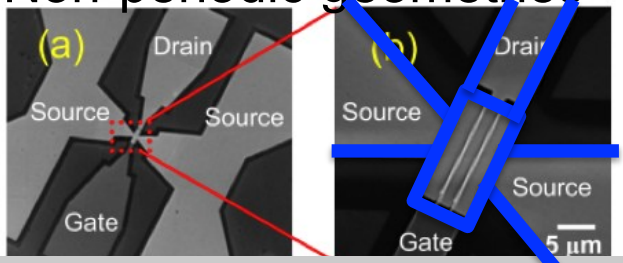
Challenges in existing self-energy methods
only solve periodic contacts

semi-infinite periodic contacts.

Common self-energy methods Sancho Rubio, transfer matrix

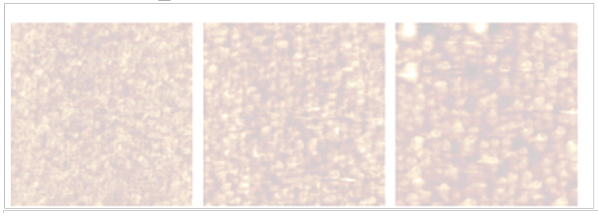
But in the real world…

Non-periodic geometries



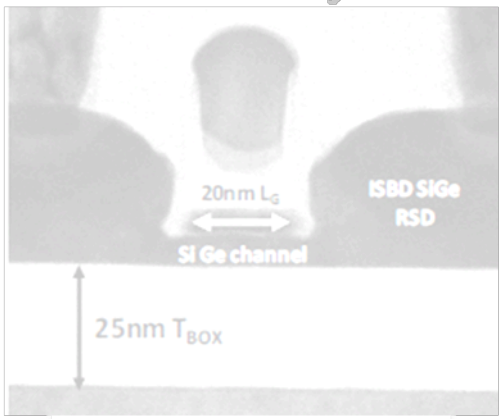
http://www.electroiq.com/articles/sst/2010/12/iedm-reflections_.html

Roughness



S. Koenig et al, Appl. Phys. Lett, Vol. 104, pp. 103106, 2014

Random alloy

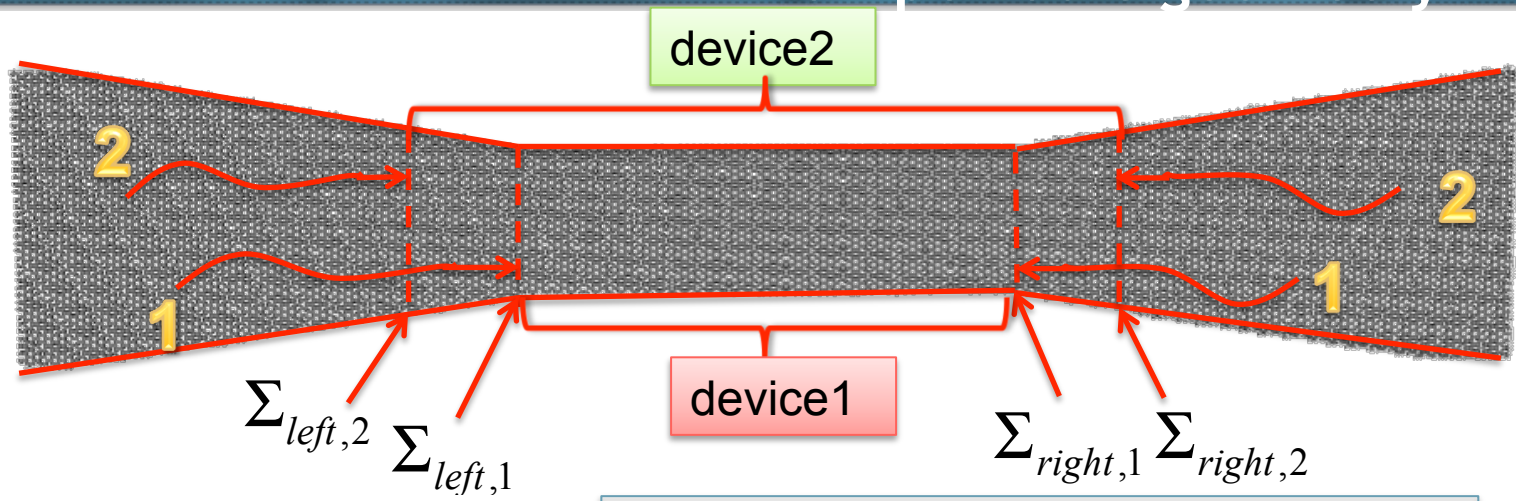


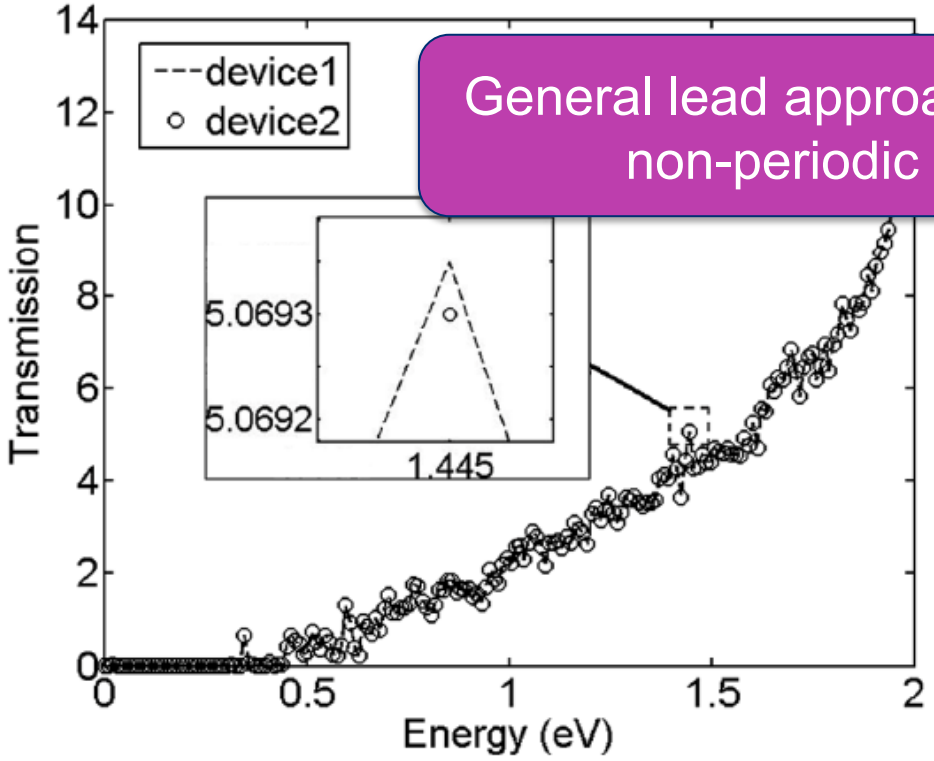
Q. Liu, et al, IEDM p.229 2013

- Periodic assumption contradicts realistic contacts
- Method applicable for non-periodic contacts is required

Application: Contacts with non-periodic geometry

Example:
20x10nm GNR with trumpet shaped contacts, Electrons in PD tight binding





General lead approach is able to represent non-periodic contact geometries

Verification of irregular lead

e 2 are numerical different but physically equivalent

- Equilibrium results of device 1 and 2 have to agree

✓ Identical transmission for device 1 and device 2

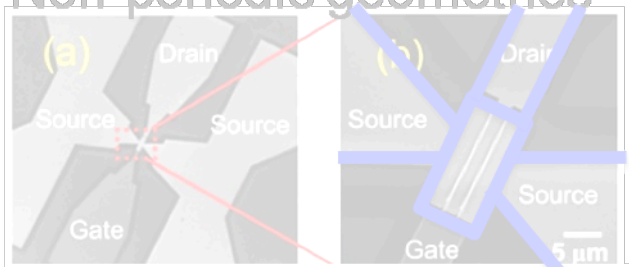
Challenges in existing self-energy methods
only solve periodic contacts

Common self-energy methods Sancho Rubio, transfer matrix

semi-infinite periodic contacts.

But in the real world…

Non-periodic geometries



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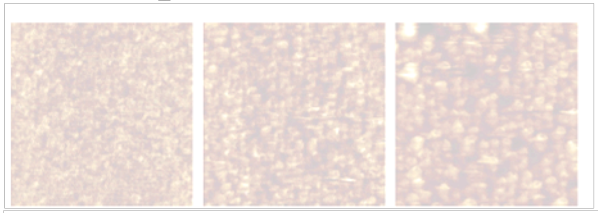
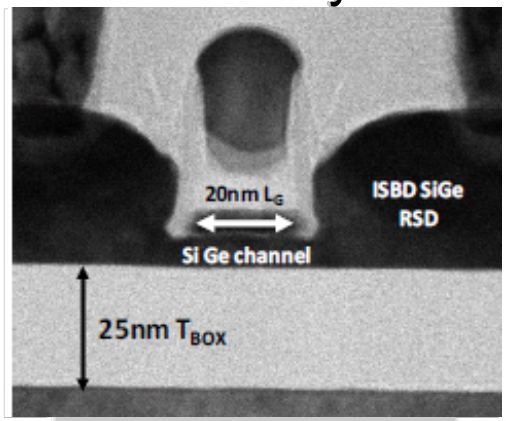


S. Koenig et al, Appl. Phys. Lett, Vol. 104, pp. 103106, 2014

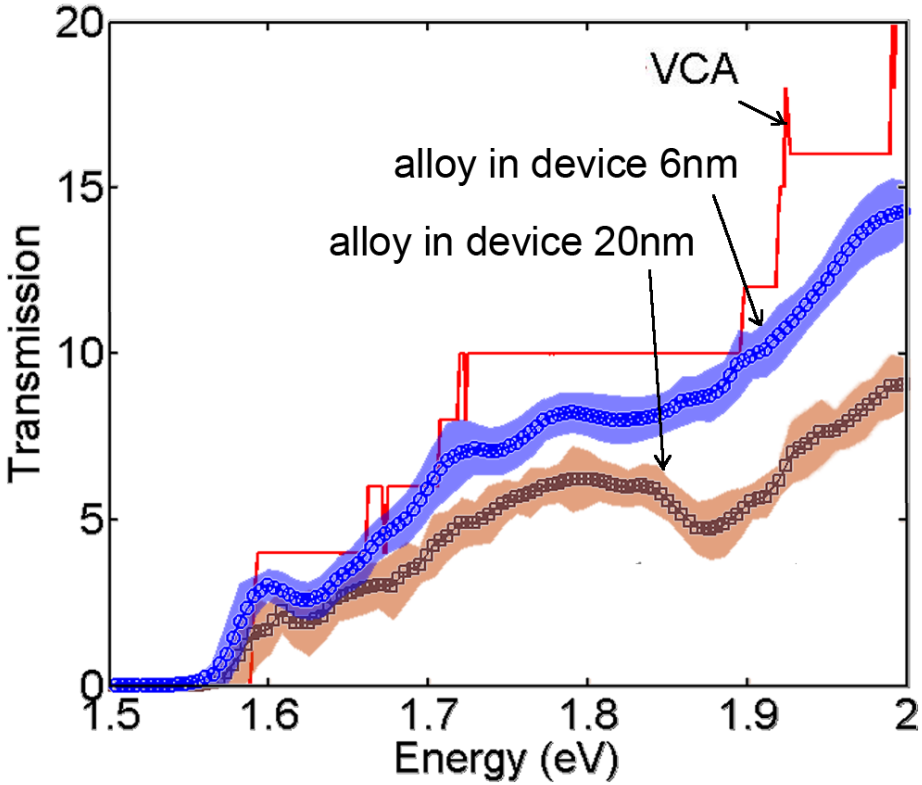
Random alloy



Q. Liu, et al, IEDM p.229 2013

- Periodic assumption contradicts realistic contacts
- Method applicable for non-periodic contacts is required

Application: SiGe random alloy

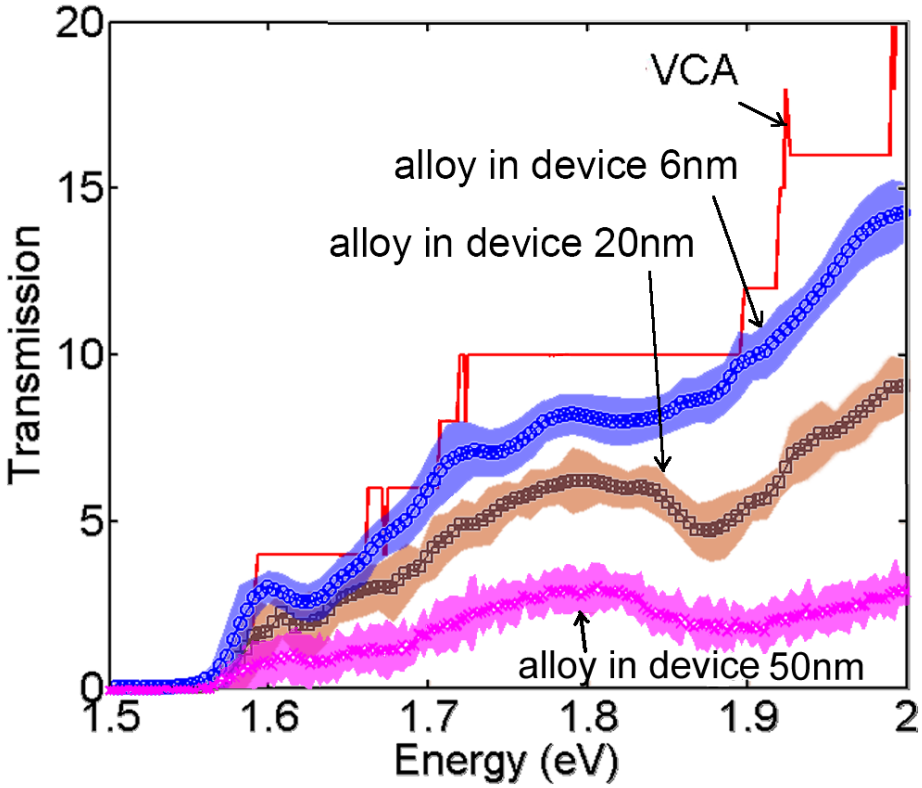


Example:
3x3nm $Si_{0.5}Ge_{0.5}$ nanowire in sp3d5s* tight binding
Device length 20nm and 6nm
Results averaged over 50 samples
Relaxed using Keating strain model

Keating, Phys. Rev., Vol. 145, pp. 637, 1966

DOS mismatch between alloy device and periodic contacts → longer device, less electrons tunnel through

Application: SiGe random alloy



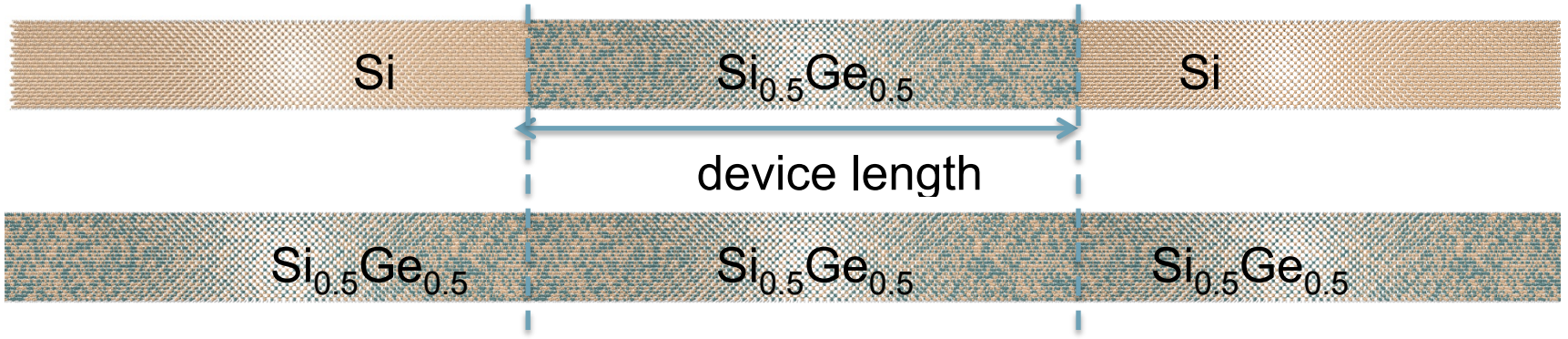
Example:
3x3nm $Si_{0.5}Ge_{0.5}$ nanowire in sp3d5s* tight binding
Device length 20nm and 6nm
Results averaged over 50 samples
Relaxed using Keating strain model

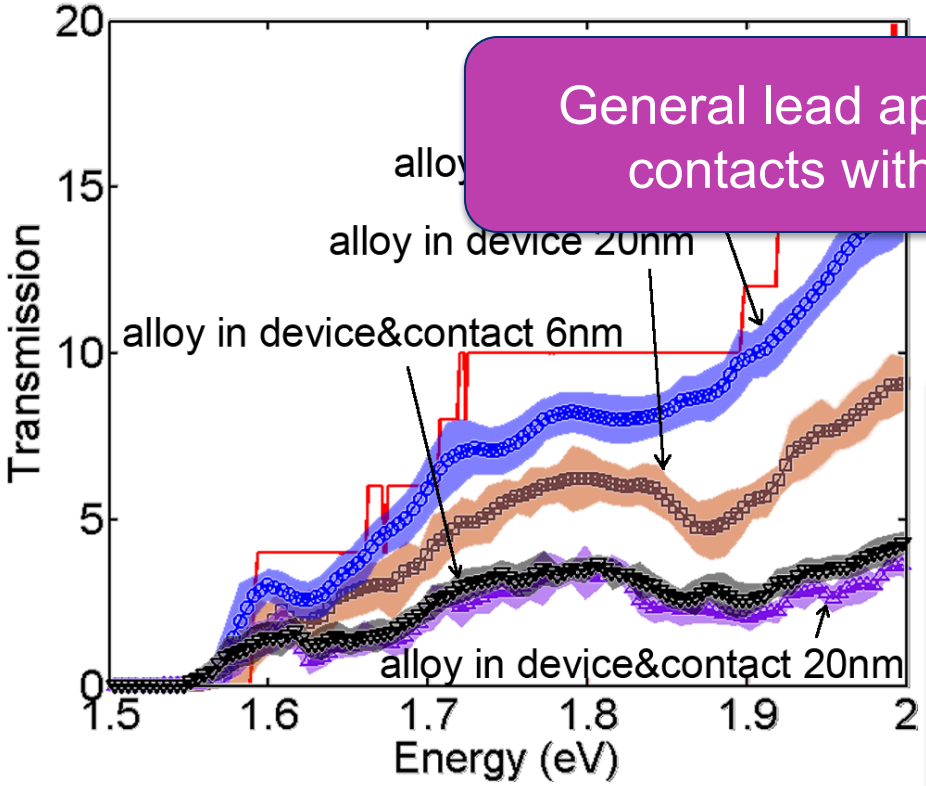
Keating, Phys. Rev., Vol. 145, pp. 637, 1966

DOS mismatch between alloy device and periodic contacts → longer device, less electrons tunnel through

Continue to extend the device length → transmission starts to vanish

Application: SiGe random alloy



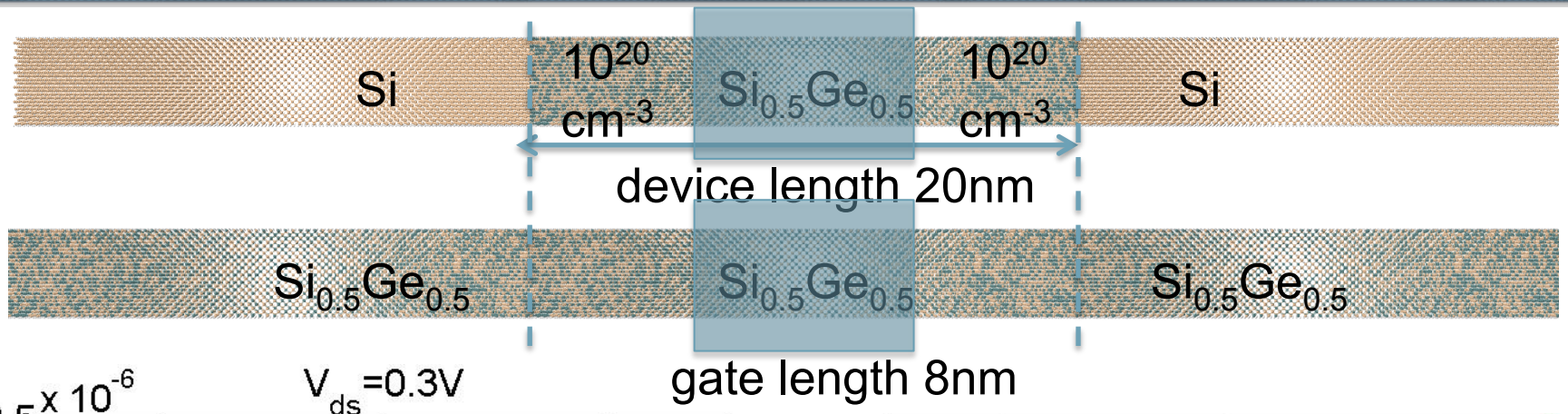


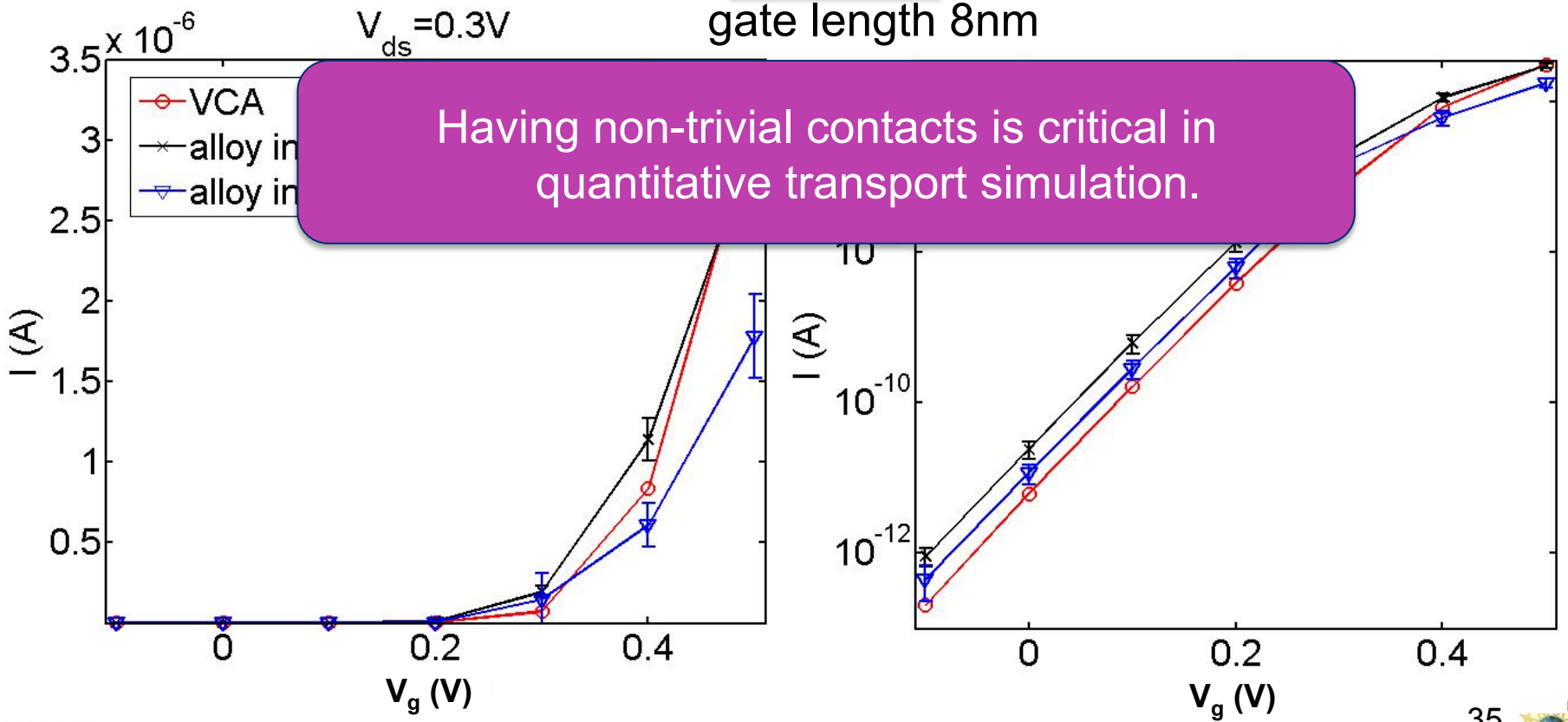
General lead approach works well for contacts with alloy randomness

yed disorder
smission has
weak dependence of device length

- ✓ Alloyed contact yield virtually device length independent transmission
- ✓ DOS of contacts match device better → less reflections of electrons
- ✓ Device physics well reserved with disorder contact treatment

Application: SiGe random alloy





Having non-trivial contacts is critical in quantitative transport simulation.

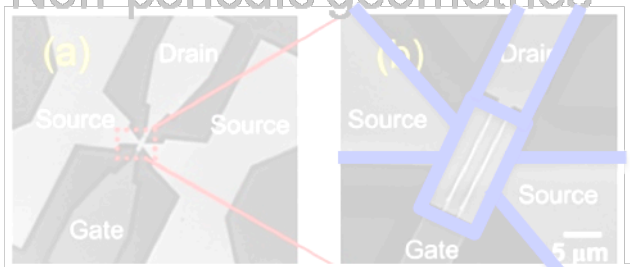
Challenges in existing self-energy methods
only solve periodic contacts

Common self-energy methods Sancho Rubio, transfer matrix

semi-infinite periodic contacts.

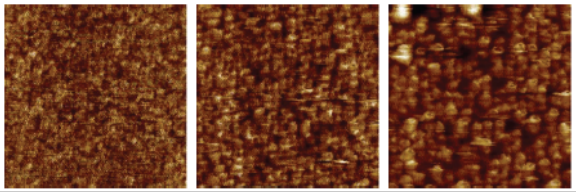
But in the real world…

Non-periodic geometries



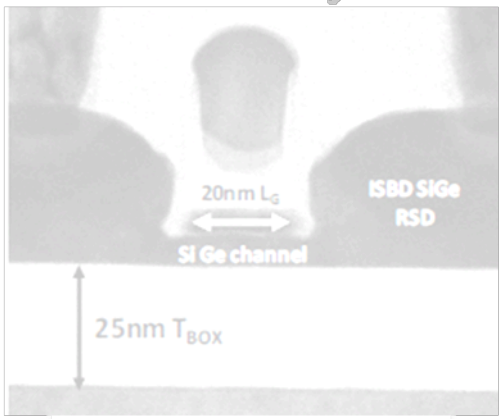
http://www.electroiq.com/articles/sst/2010/12/iedm-reflections_.html

Roughness



S. Koenig et al, Appl. Phys. Lett, Vol. 104, pp. 103106, 2014

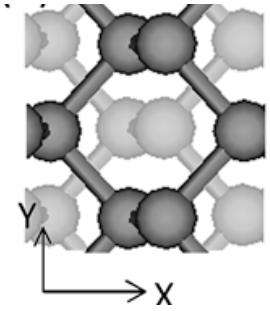
Random alloy



Q. Liu, et al, IEDM p.229 2013

- Periodic assumption contradicts realistic contacts
- Method applicable for non-periodic contacts is required

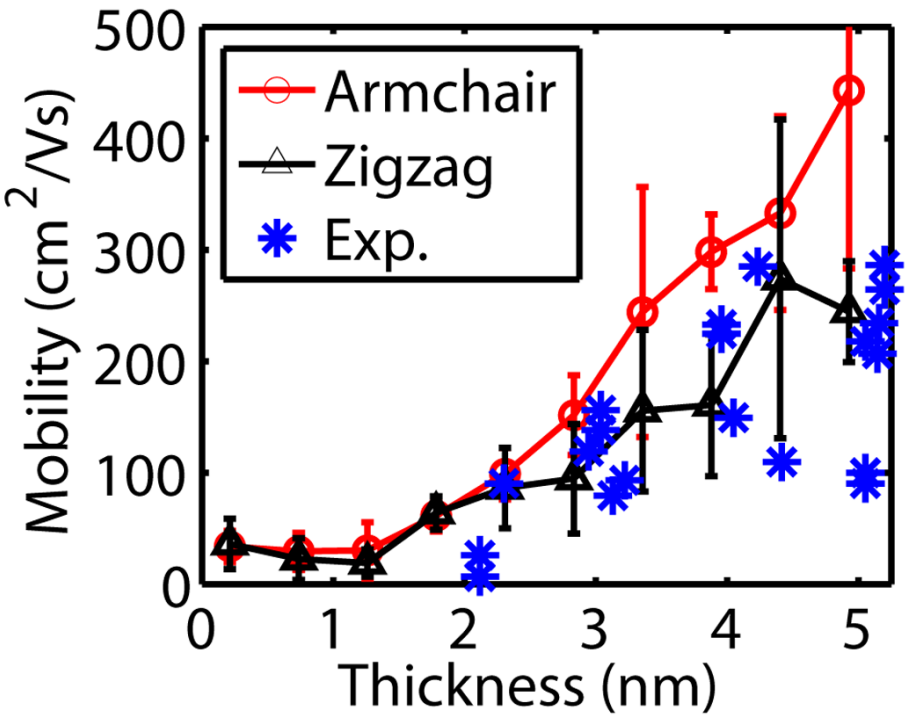
Results: Surface roughness in black phosphorus
Mobility



Roughness
- ✓ L_c=1.1nm, ?=0.2nm
- ✓ Average over 50 samples

NEGF+general lead

X: armchair
Y: zigzag



Exp. data taken from H Liu et al, ACSnano 8, 4033 (2014)

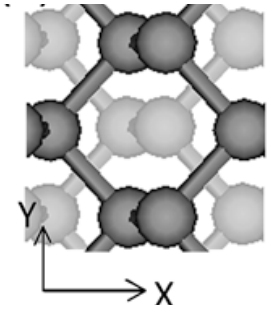
- Anisotropic transport behavior is observed for thickness>2nm (5L)
  - ✓ Armchair > zigzag
  - ✓ Impact of roughness scattering is weaker in thicker layer
- Ballistic mobility ~10^4 cm^2/Vs
- Roughness scattering reduces mobility down to ~10^2 cm^2/Vs
- Mobility due to roughness agrees with measurement

H Liu et al, ACSnano 8, 4033 (2014)
S Koenig et al, Appl. Phys. Letts. 104, 103106 (2014)

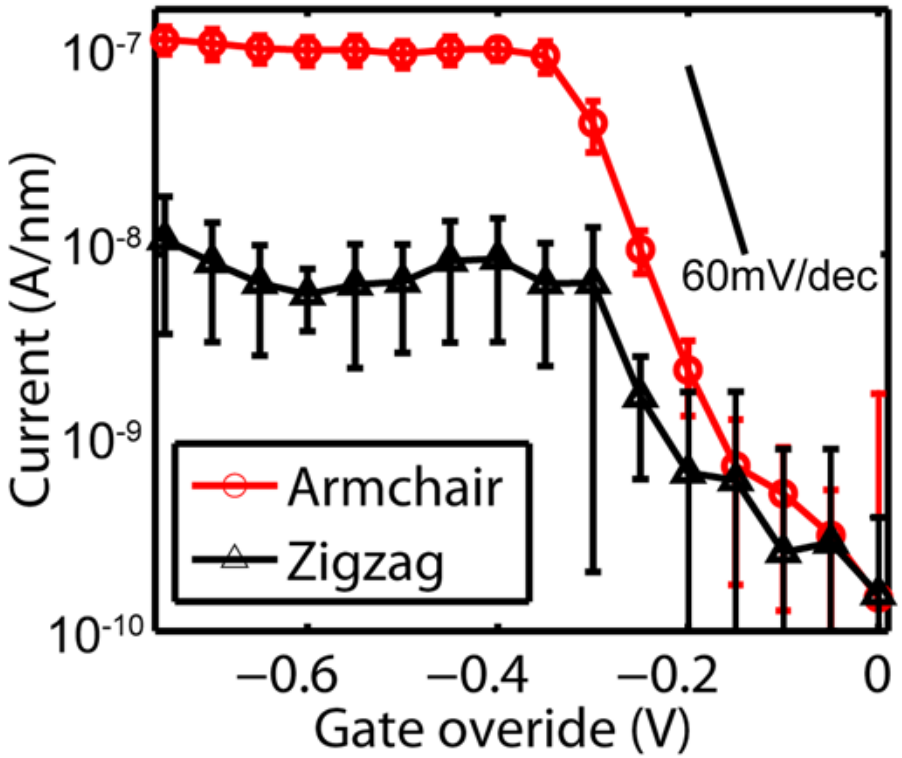
Surface roughness reduces mobility from ballistic ~10^4 to measurement ~10^2 cm^2/Vs → might be one of the dominating mechanisms

Results: Surface roughness in black phosphorus
I-V characteristics

- Roughness
  - ✓ L_c=1.1nm, [?]=0.2nm
  - ✓ Average over 50 samples
- ITRS 2020 transistor target
  - ✓ L=8.5nm, D=3.4nm
  - ✓ $I_{off}=10^{-10}$A/nm
  - ✓ V_{ds}=0.75V



X: armchair
Y: zigzag



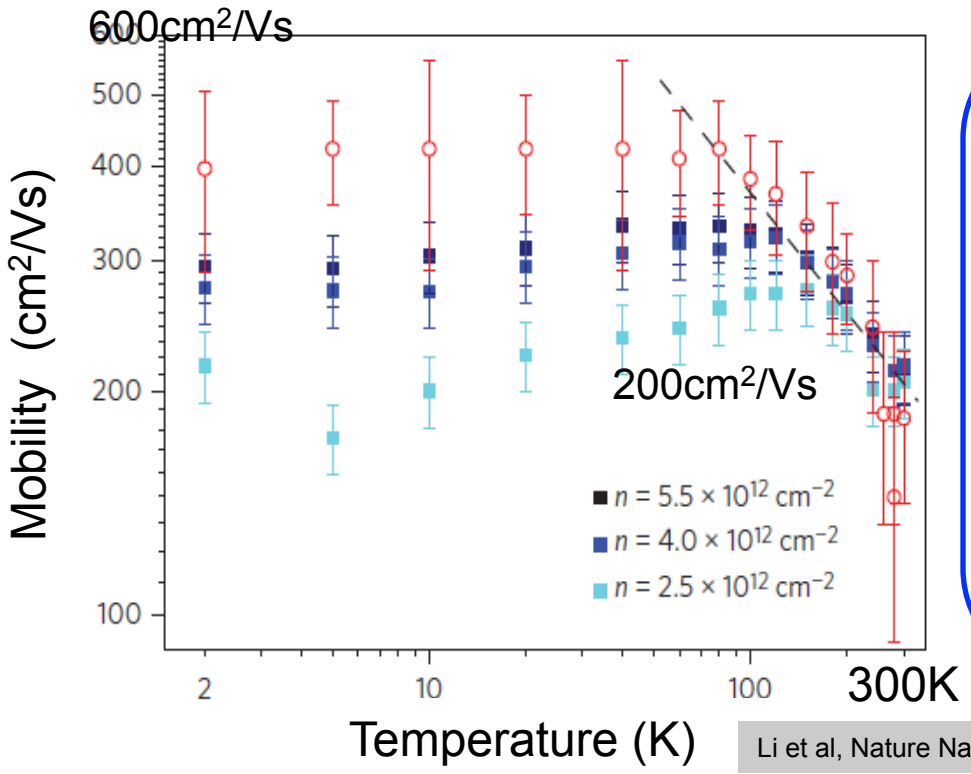
- ➢ Armchair SS 76mV/dec, ON/OFF ratio ~1400
- ➢ Zigzag SS 82mV/dec, ON/OFF ratio ~130

- Armchair direction outperforms zigzag
  - ✓ $m_{h\_X}<m_{h\_Y}$
- ON/OFF ratio lower than ITRS requirement ~10^4

Outline


Introduction
Tight-binding model
Surface roughness scattering
Acoustic phonon scattering
Conclusion & Outlook

Temperature dependence of mobility



- Mobility shows temperature dependence, with values 200cm²/Vs~400cm²/Vs
- Temperature dependence not attributed to roughness scattering
- Matthiessen's rule

$$\frac{1}{\mu_{tot}} = \frac{1}{\mu_{SR}} + \frac{1}{\mu(T)}$$

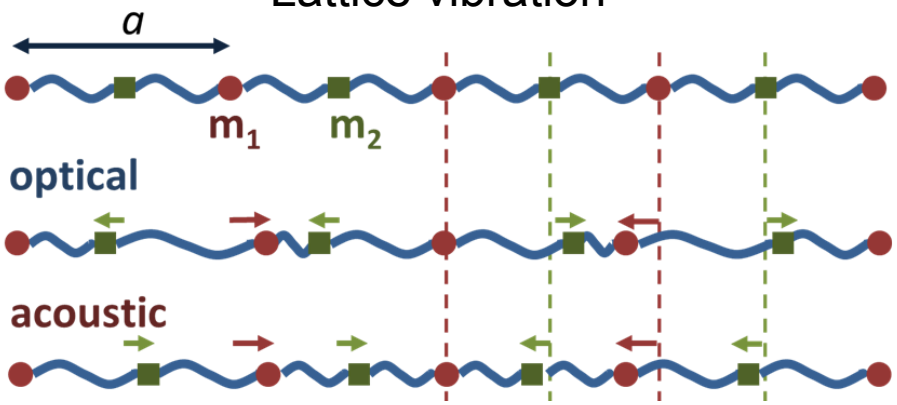
Li et al, Nature Nanotechnol. 9, 372–377 (2014)

Possible scattering mechanism for temperature dependent mobility → phonon, impurity, …

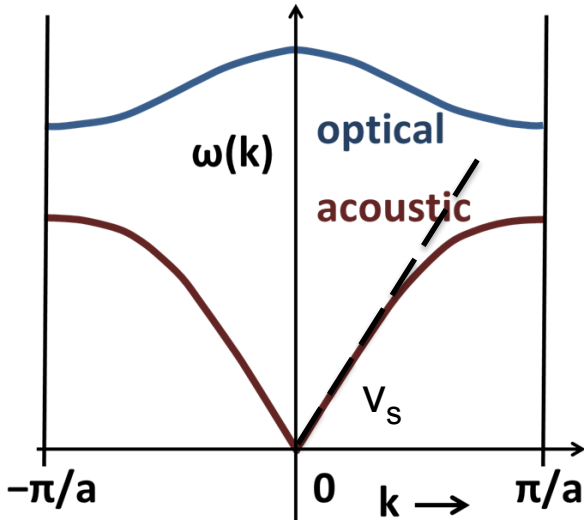
Electron-phonon scattering

https://en.wikipedia.org/wiki/Phonon

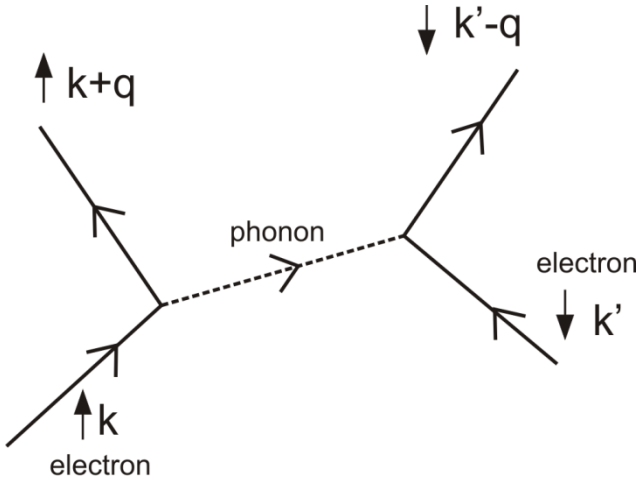
Lattice vibration



Phonon dispersion



Electron-phonon scattering



- Lattice vibration denoted by phonons (acoustic and optical)
- Electrons exchange momentum and energy with phonons
- Only acoustic phonon is considered here, optical branch is not included due to lack of parameters

Mobility due to acoustic phonon scattering

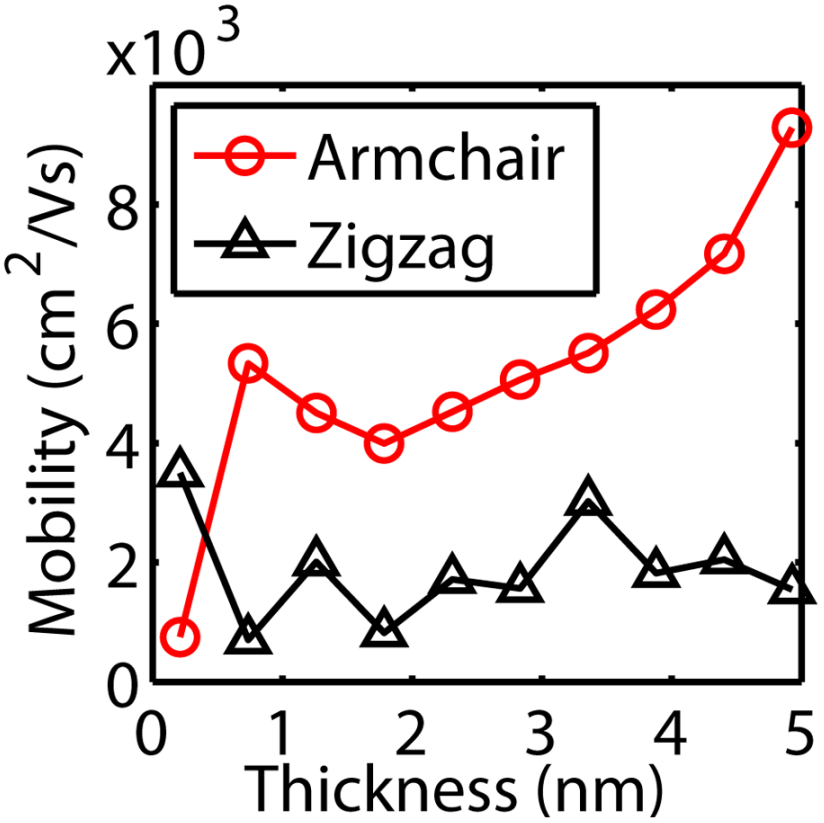
- Linear phonon dispersion is assumed
  - ✓Material density 2.69 g/cm^3

    H Liu et al, Chem. Soc. Rev. 44, 2732 (2015)
  - ✓Deformation potential: thickness dependent

    J Qiao et al, Nature Comm. 5, 4475 (2014)
  - ✓Sound velocity 3.8km/s armchair direction, 7.8km/s zigzag direction

    Z Zhu et al, Phys. Rev. Lett. 112, 176802 (2014)
- Low energy, room temperature assumed
- Acoustic phonon scattering denoted by scattering self-energy, solved with self-consistent Born approximation

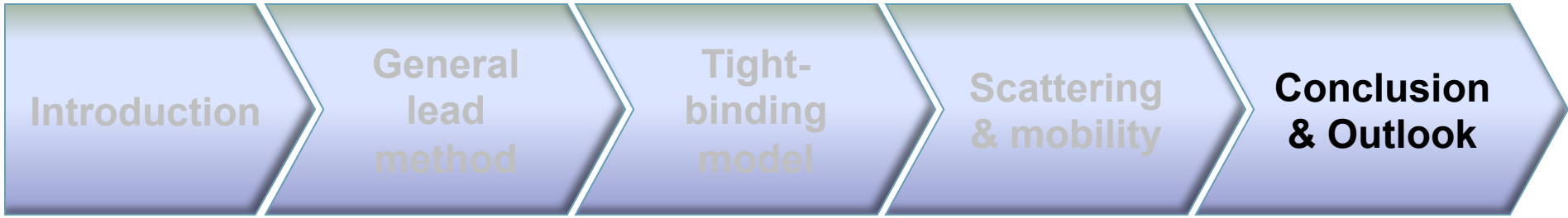
  Lake et al, J. Appl. Phys. 81, 7845 (1997)



- ➢ Mobility shows anisotropic transport behavior
  - ✓$m_{h\_X} < m_{h\_Y}$
  - ✓Deformation potential for 1L zigzag very small (0.15eV)
- ➢ Phonon mobility ~10^3 cm^2/Vs >> measured values ~200 cm^2/Vs (T=300K)

Room temperature mobility >> measurement → acoustic phonon does not dominate the temperature dependent mobility

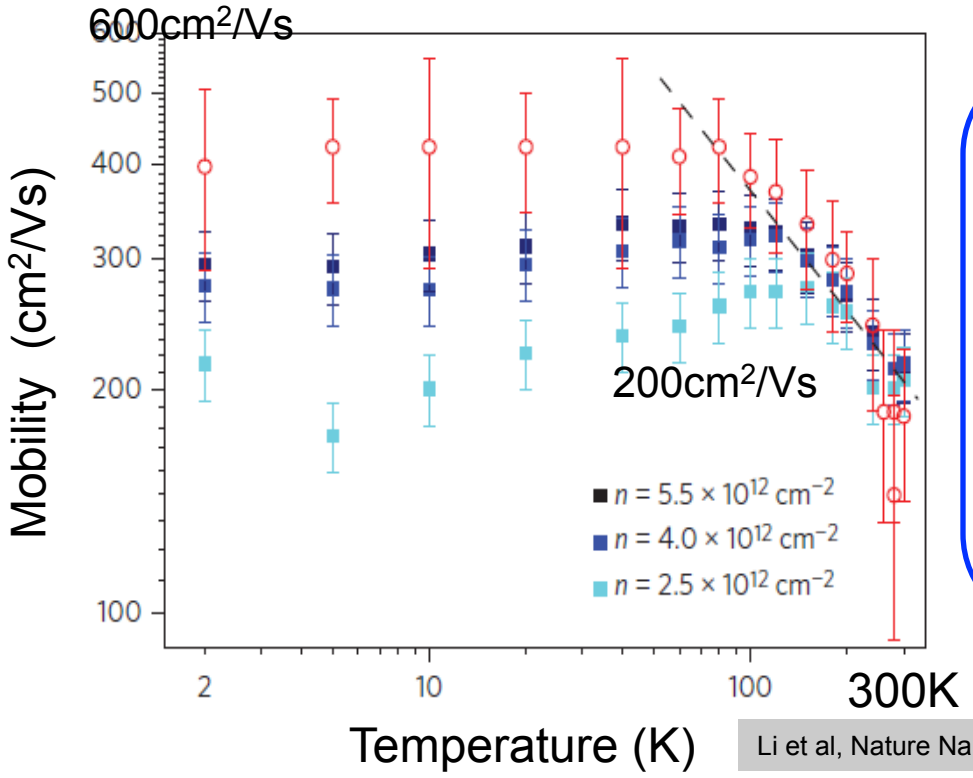
Outline


Introduction
General lead method
Tight-binding model
Scattering & mobility
Conclusion & Outlook

Conclusion

- Measured mobility of black phosphorus transistor is lower than expected; surface roughness observed experimentally but its impact is not fully understood.
- A 10-band TB model for black phosphorus is developed.
- General lead method is developed for contact self-energy calculations of non-periodic non-ideal contacts (e.g. roughness, alloy, etc).
- Mobility due to surface roughness agrees well with measurement.
- IV characteristic based on ITRS 2020 target transistor using black phosphorus shows anisotropic properties; yet ON/OFF ratio is lower than requirement.
- Acoustic phonon scattering in black phosphorus is studied and found to be not dominating the mobility.

Outlook



Li et al, Nature Nanotechnol. 9, 372–377 (2014)

- Mobility shows temperature dependence, with values 200cm²/Vs~400cm²/Vs
- Acoustic phonon assisted mobility >10³cm²/Vs >> measured values → not dominate temperature dependence

- Possible mechanism that dominates the temperature dependent mobility might be optical phonon scattering
- NEGF with optical phonon scattering might provide the answer
- Require optical phonon energy and deformation potential from either DFT calculation or experiment

Tunnel Field-Effect Transistors in 2D Transition Metal Dichalcogenide Materials

Hesameddin Ilatikhameneh[1], Yaohua Tan[1], Bozidar Novakovic[1], Gerhard Klimeck[1], Rajib Rahman[1], and Joerg Appenzeller[2]

The simulation results show that WTe_2 TFETs can provide highest performance in terms of ON-current and SS in comparison to the other TFETs. Since WTe_2 has the smallest band gap and effective mass compared to the other TMDs, its ON-current is significantly higher. No-

H. Ilatikhameneh, Exploratory Solid-State Computational Devices and Circuits, IEEE Journal on, vol. 1, pp. 12, 2015.

$$I \propto \exp\left(\frac{-4\Lambda\sqrt{2m_r^* E_g}}{3\hbar}\right) \qquad \eta = \Lambda\sqrt{m_r^* E_g}$$

Material	I_{ON}	Eg	m_r^*	λ	Λ	η
WTe_2	127	0.75	0.17	0.45	2.45	3.15

- ON-state current of TFET depends on effective masses and band gap
- Black phosphorus can be a nice candidate to explore
  - ✓Armchair direction gives small effective masses
  - ✓Band gaps decrease fast with number of layers

	1L	2L	3L	4L	5L
m_r^*	0.0927	0.0851	0.0719	0.0657	0.0620
E_g	1.374	0.8419	0.573	0.466	0.41

Acknowledgement

- Prof. Klimeck
- Prof. Datta, Prof. Rokhinson, Prof. Kubis

- Prof. M. Povolotskyi, Dr. J. Fonseca, Dr. B. Novakovic, Dr. J. Huang, Dr. L. Zeng, Dr. G. Hegde, Dr. S. Mehrotra, Dr. S. Park, Dr. S. Kim, Dr. H. Park, Dr. A. Ajoy, Dr. S. Steiger

- **NCN people:** Z. Jiang, J. Geng, Y. Tan, D. Mejia, K. Miao, Y. Hsueh, M. Salmani, X. Wang, H.Ilatikhameneh, D.Lemus, P. Long, F. Chen, Y. Wang and P. Sarangapani , all other sutdents in NCN.
- **NCN Staff members:** V. Johnson, C. Heins, L. Schumacher, A. Buckles
- **NEMO5 core team:** Prof. M. Povolotski, Prof. T. Kubis, Prof. R. Rahman, Dr. J. Fonseca, Dr. B. Novakovic , Dr. J. Huang

Related publications

Related Publications

- Yu He, Yaohua Tan, James Charles, Gerhard Klimeck, and Tillmann Kubis, “Transport in few-layer black phosphorus with empirical tight binding”, under preparation.

- Yu He, Yaohua Tan, Zhengping Jiang, Michael Povolotskyi, Gerhard Klimeck, and Tillmann Kubis, “Surface passivation in empirical tight binding”, submitted to *IEEE Trans. Electr. Dev.*, 2015.

- Yu He, Yu Wang, Gerhard Klimeck, and Tillmann Kubis, “Nonequilibrium Green’s Function Method: Non-trivial and disordered leads”, *Appl. Phys. Lett.*, Vol. 105, pp. 213502, 2014.

- Yu He, Tillmann Kubis, Michael Povolotskyi, Jim Fonseca, and Gerhard Klimeck, “Quantum transport in NEMO5: algorithm improvements and high performance implementation”, *2014 International Conference on Simulation of Semiconductor Processes and Devices*, Yokohama, Japan, 2014.

List of projects

Low Rank Approximation in NEGF

Yu He, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck

Objective:

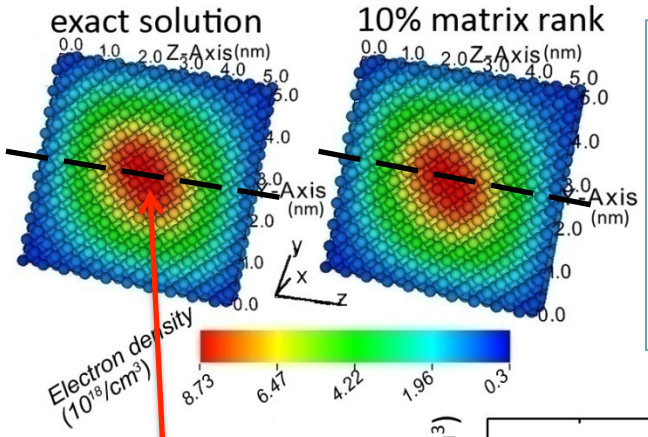
- Quantum transport is numerically very expensive for realistic devices
  - ➢ Realistic device requires huge simulation domain → huge computational resources
  - ➢ Operation of large Matrices with the size of device Hamiltonian

Method:

- Non-equilibrium Green's functions in atomistic tight binding representation
- Low rank approximation in appropriate basis set
  - ➢ Transform the system into a reduced space with much smaller size
  - ➢ Perform all operations in the reduced space

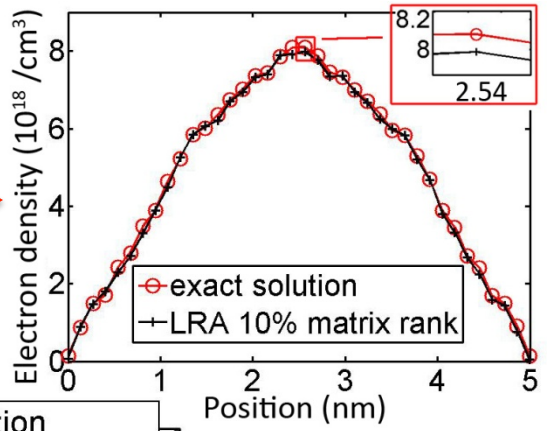
Impact:

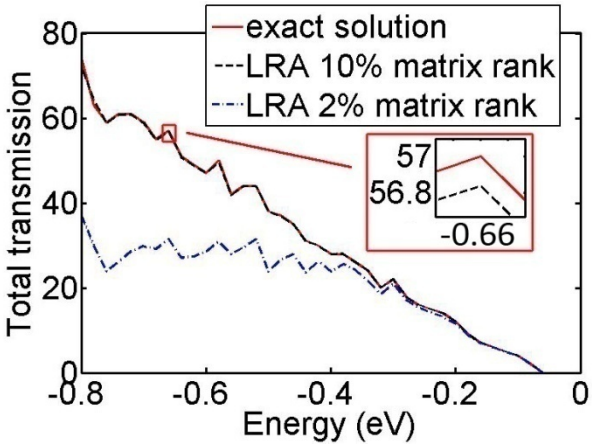
- 5nm diameter Si nanowire
- 10% of original matrix size (rank)
- Speed up by 8 times achieved
- With almost no loss in transmission and electron density



- Si nanowire 5nm diameter
- Sp3d5s* TB model
- Transport along x-axis

Electron density along the black dashed lines





LRA applied to Band-To-Band Tunneling FET

Yu He, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck

Objective:

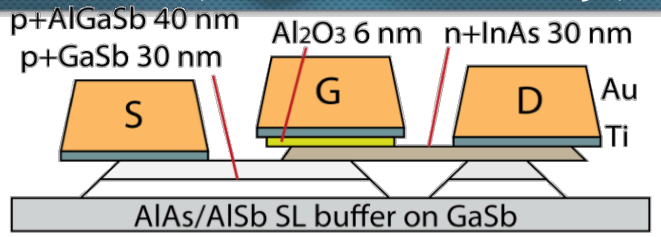
- Real BTBT device → Huge simulation domain requires huge computational resources

Method:

- Low rank approximation in NEGF with Tight binding representations
- Extract critical elements from computational domain → reduce problem size to save resources

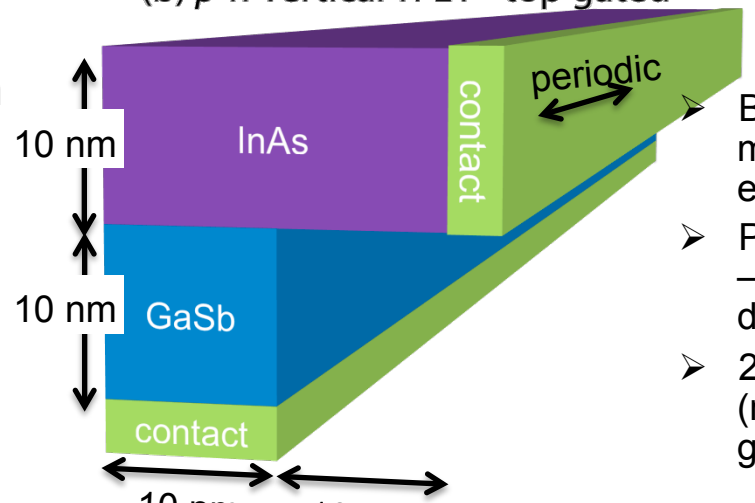
Impact:

- Use only 5% of full basis in L-shape GaSb-InAs BTBT, with almost no loss in accuracy
- Reduce matrix operations by $(1/0.05)^3$=8,000 times
- Open a way to simulate realistic BTBT devices

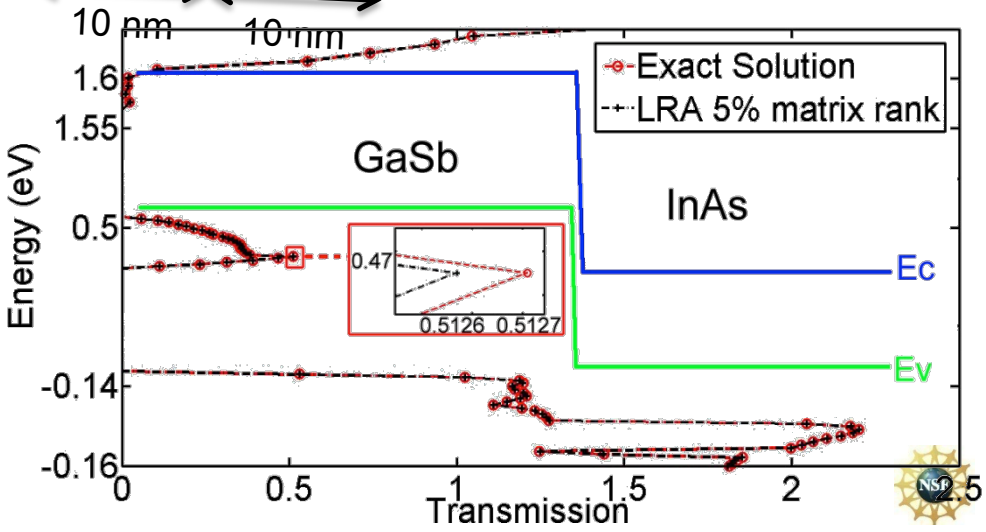


L-shape GaSb-InAs tunneling FET

(b) *p-n* vertical TFET - top gated



- Broken gap – mixture of electrons/holes
- Periodic direction – momentum dependent basis
- 2D transport (nonlinear geometry)



Low Rank Approximation in effective mass

Lang Zeng, Yu He, Tillmann Kubis,
Michael Povolotskyi, Xiaoyan Liu, Gerhard Klimeck

Objective:

- NEGF transport with phonon scattering is expensive → self consistent Born solution ~100x to ballistic calculation.

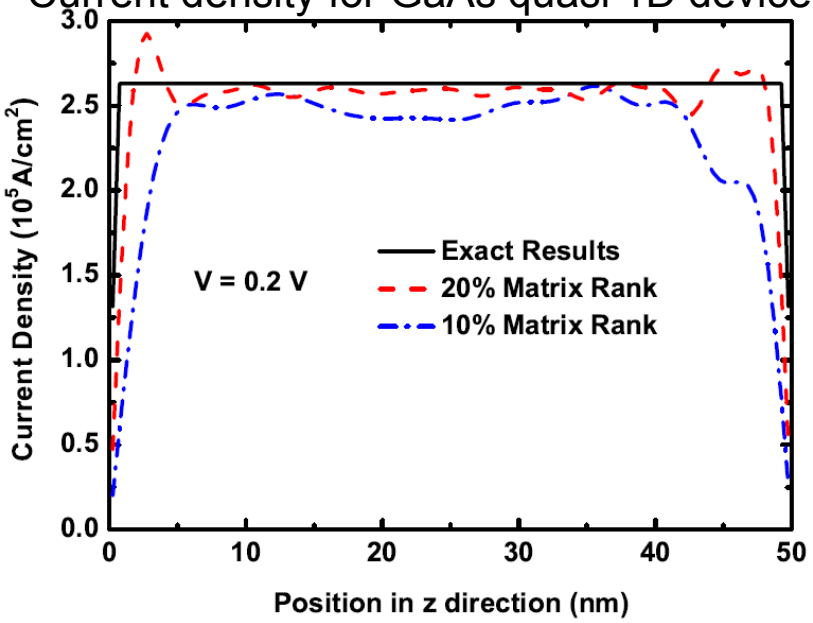
Method:

- Construct reduced real space basis in the relevant states only.
- Transform original NEGF equation into reduced space with the obtained basis.
- Solve NEGF+scattering in the reduced space.
- Transform back into original space to calculate the observables.

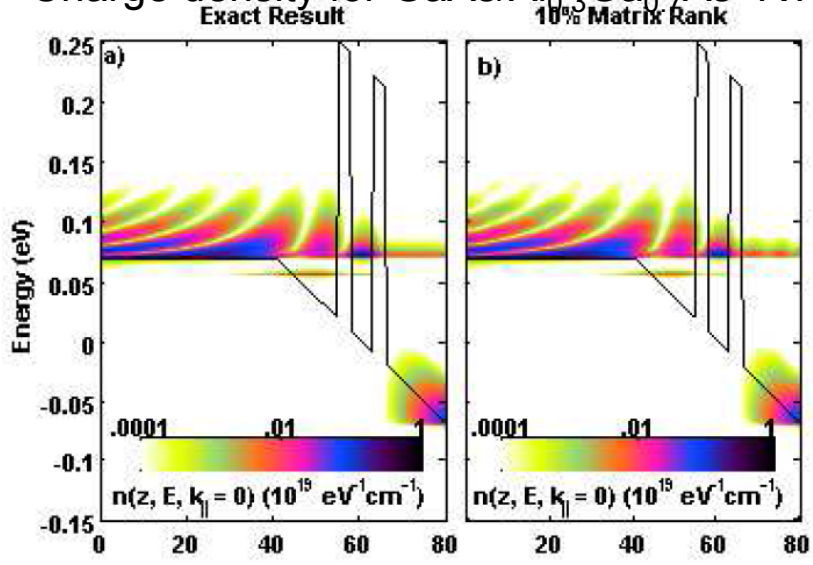
Impact:

- With 10% of original matrix rank the charge density and current density is well reproduced.
- Speed up >100x is achieved.

Current density for GaAs quasi 1D device



Charge density for GaAs/$Al_{0.3}Ga_{0.7}As$ RTD



LRA applied in 1μm GaAs layer

Lang Zeng, Yu He, Tillmann Kubis,
Michael Povolotskyi, Xiaoyan Liu, Gerhard Klimeck

Objective:

- Investigate NEGF calculation towards drift-diffusion limit in long device.

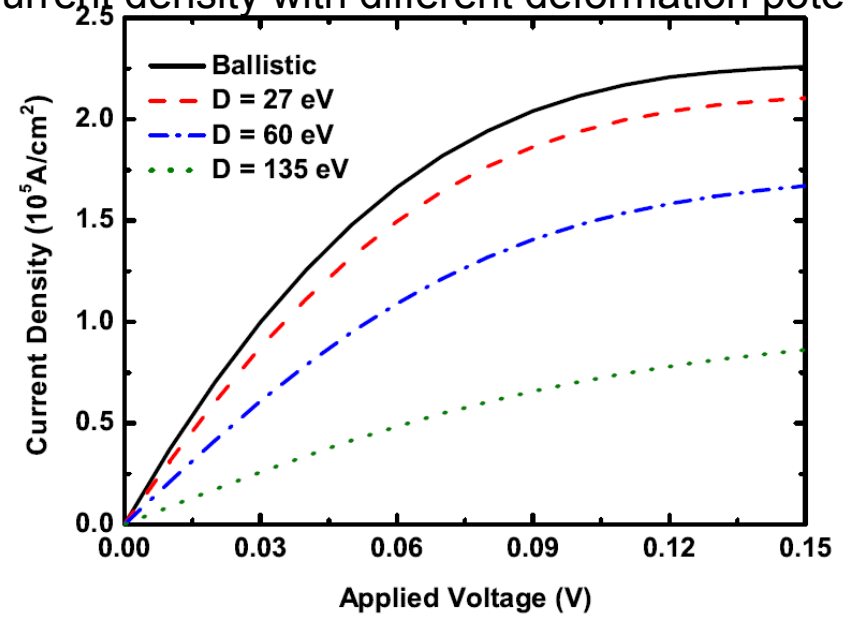
Method:

- LRA+NEGF with phonon scattering.
- Investigate different scattering rate (phonon deformation potential D).

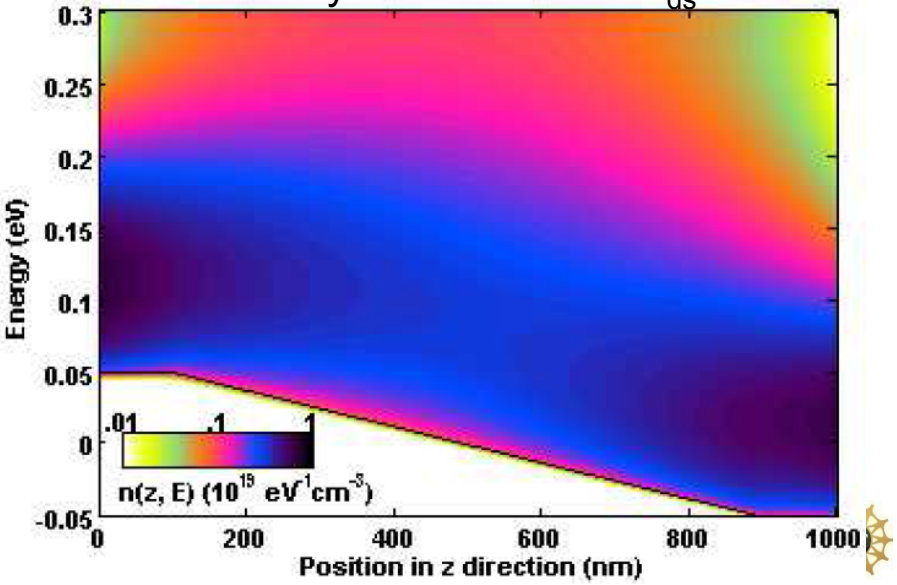
Impact:

- With 20% of original matrix rank the I-V characteristic is achieved, while exact solution is not feasible.
- With D=135eV energy dissipation is observed in the charge density.
- Transition from effective ballistic transport into drift-diffusion is observed in the device channel.

Current density with different deformation potential



Electron density with D=135eV V_{ds}=0.1V



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Low Rank Approximation in self-energy

Yu He, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck

Objective:

- Solving contact self-energy is expensive in tight binding model, especially for big cross-section device.

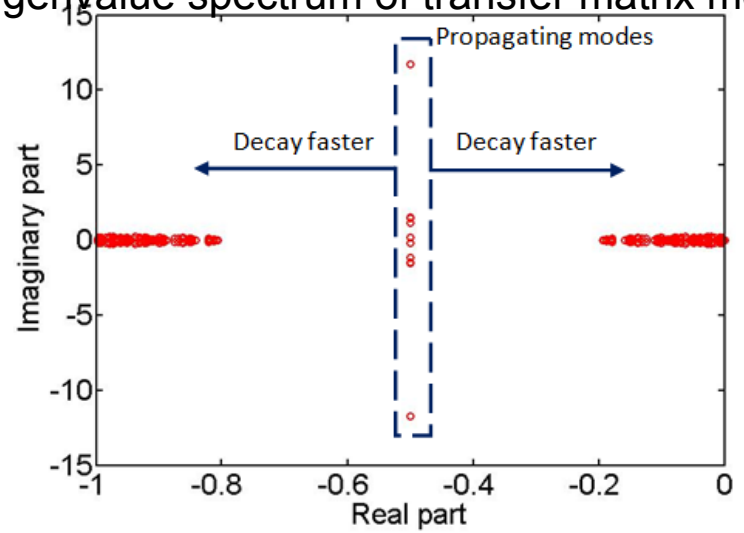
Method:

- Transfer matrix method is adopted.
- Solve the eigenvalue spectrum such that keep only the propagating modes and slowly decaying modes in the solution.
  → propagating modes with Real part of eigvalues =-0.5eV

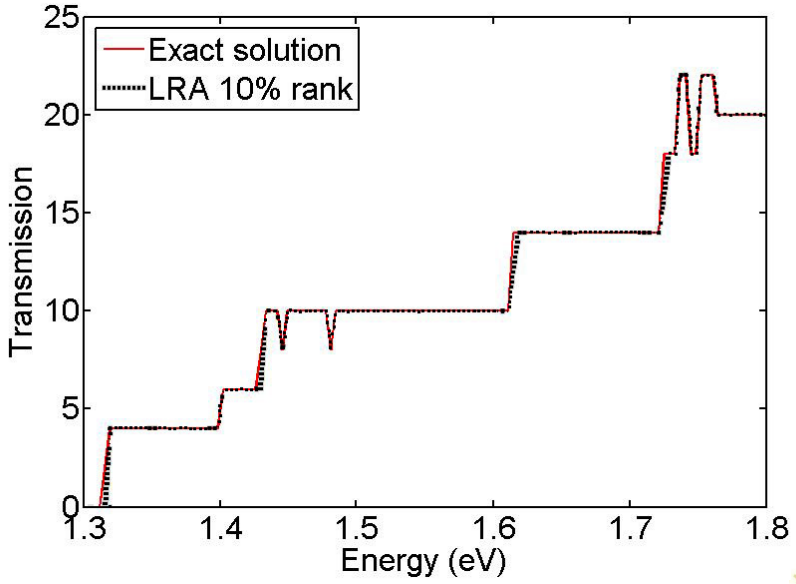
Impact:

- Significantly reduce the numerical load and speed up ~3x in self-energy calculation.
- Results are well reproduced with 10% of original matrix rank.

Eigenvalue spectrum of transfer matrix method



Transmission w/wo LRA in contact self-energy



General lead method in NEGF

Yu He, Yu Wang, Gerhard Klimeck and Tillmann Kubis

Objective:

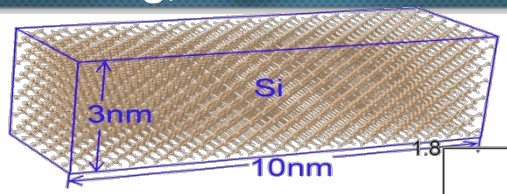
- Common lead methods can only deal with semi-infinite periodic leads
- Realistic leads are non-periodic

Method:

- Assume some lead self-energy far from the lead/device interface
- Add artificial dephasing to the lead Hamiltonian that decays fast towards device
- Solve lead surface Green's function via RGF until convergence

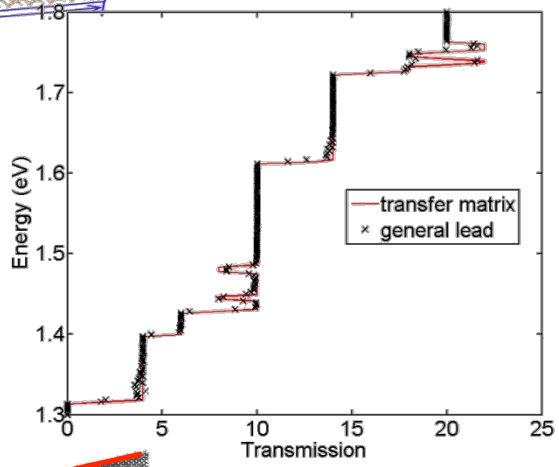
Impact:

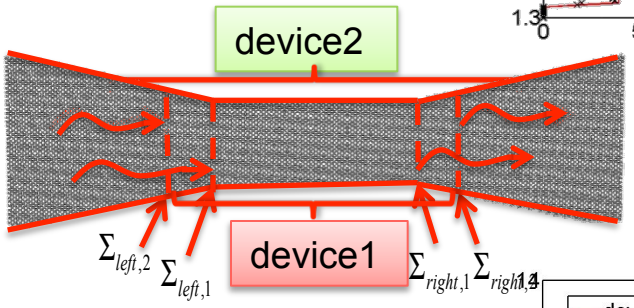
- General lead algorithm agrees with common method for regular leads, deviations observed only very close to van Hove singularities
- General lead method can represent irregular lead geometry



3x3nm Si nanowire in $sp^3d^5s^*$ tight binding

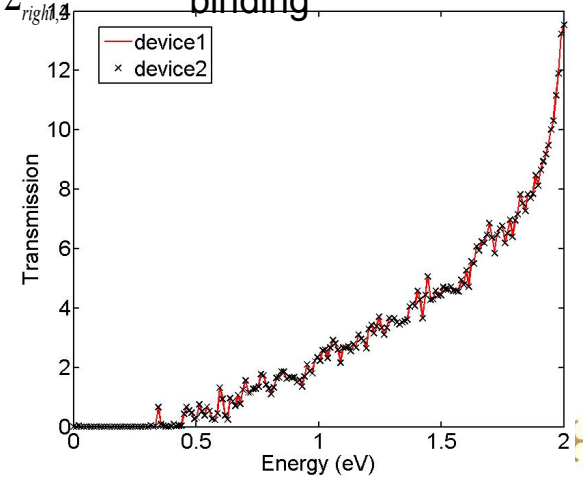
Transmission comparison common method vs. general leads





20x10nm graphene nanoribbon with trumpet shaped leads, Electrons in P/D tight binding

- Device1 and device2 are physically equivalent
- Transmission identical for device1 and device2



Random alloy in the lead

Yu He, Yu Wang, Gerhard Klimeck and Tillmann Kubis

Objective:

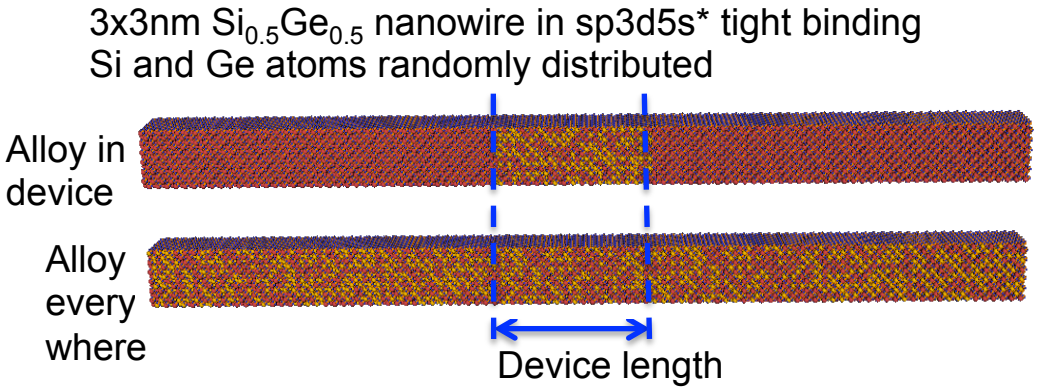
- Device lengths approach ballistic limit, contact resistances dominate;
- Random alloy in the leads influence overall performance

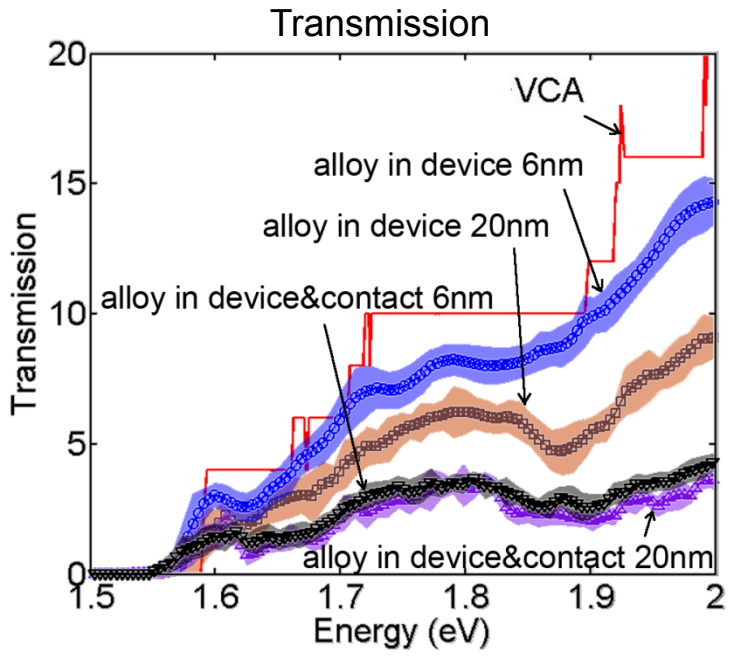
Method:

- Include random alloy in the leads
- Apply general lead algorithm to solve the leads with alloy

Impact:

- 50 samples are simulated.
- Alloy disorder in leads yields length independent transmission.
- DOS of alloy leads matches with alloy device better.
- General lead algorithm can represent randomness in leads.





Surface passivation model

Yu He, Zhengping Jiang, Yaohua Tan,
Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck

Objective:

- Dangling bonds at surfaces introduce undesired eigenstates within band gap → need to be passivated;
- Existing model works for zincblende and diamond structure only → general and flexible model required;

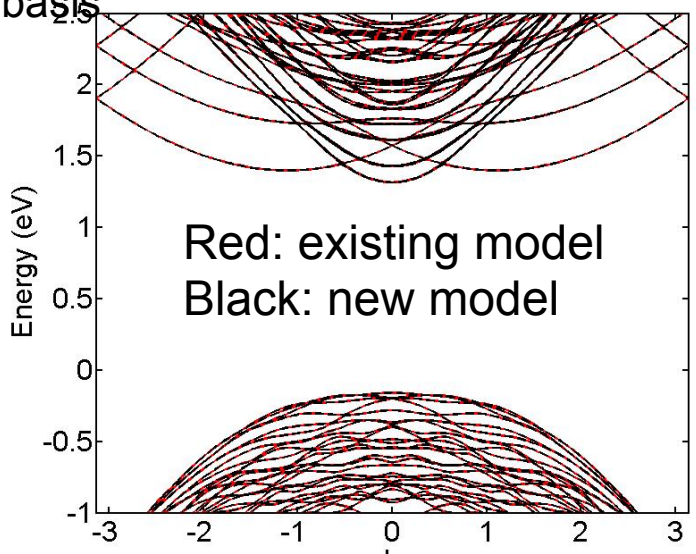
Method:

- Explicitly add passivation materials (H, O, SiO_2, etc) to the structure;
- The surface atoms are passivated by a self-energy of the passivation materials;
- Parameters are optimized by fitting TB results to DFT results.

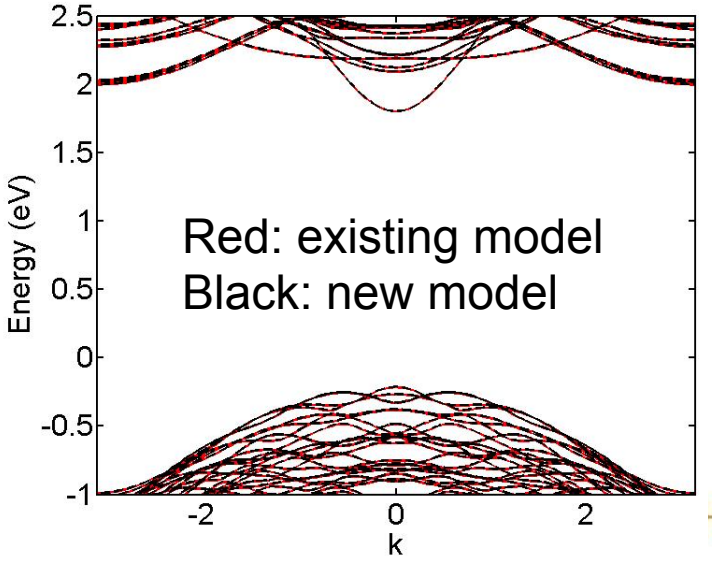
Impact:

- Bandstructure matches well with the existing model on zincblende and diamond structure with proper parameters.

Bandstructure for 3nmx3nm Si nanowire, sp3d5s* basis



Bandstructure for 3nmx3nm GaAs nanowire, sp3d5s* basis



Passivation applied to Si/SiO_2 interface

Yu He, Zhengping Jiang, Yaohua Tan,
Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck

Objective:

- Investigate the Si UTB/SiO_2 interface and evaluate the normally used hydrogen atom passivation treatment.

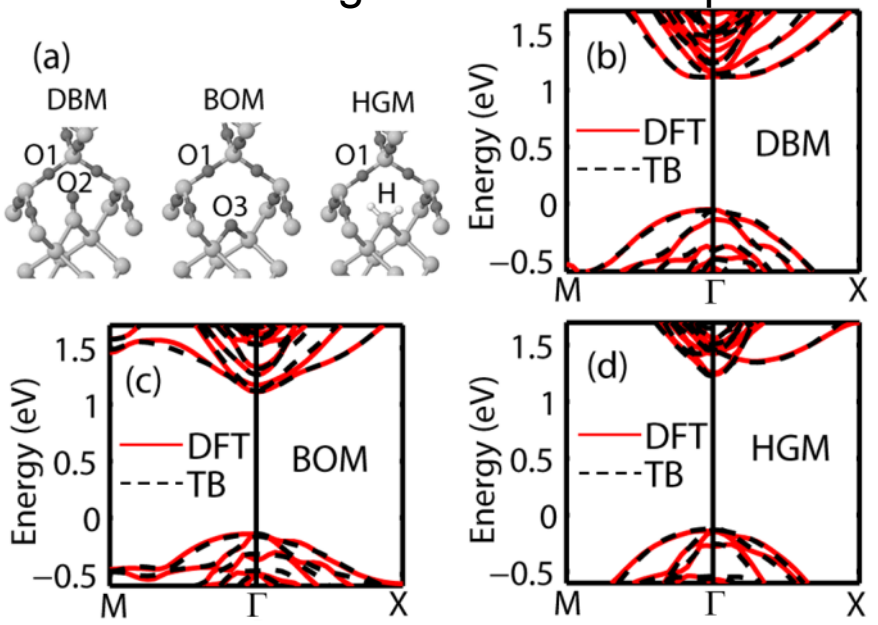
Method:

- Passivation for three relevant oxidation configurations are parameterized.
- Parameters are optimized by fitting TB dispersions to DFT-HSE06 calculations.

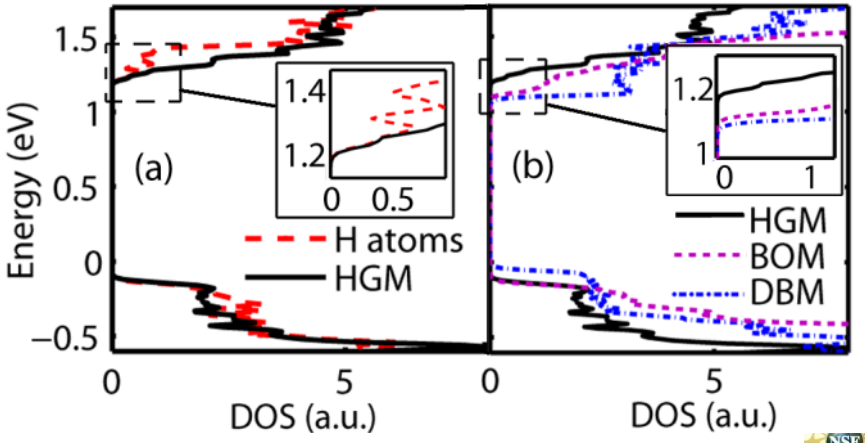
Impact:

- UTB band structures of TB match well with DFT calculations.
- HGM gives higher DOS compared to hydrogen atom passivation.
- Oxidation configurations involved more oxygen atoms contribute higher DOS.
- DBM and BOM configurations are not well confined, which are suggested to be avoided in experiment.

oxidation configurations and dispersions



DOS for the oxidation configurations



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Passivation applied to Si/SiO_2 interface

Yu He, Zhengping Jiang, Yaohua Tan,
Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck

Objective:

- Investigate the Si UTB/SiO_2 interface and evaluate the normally used hydrogen atom passivation treatment.

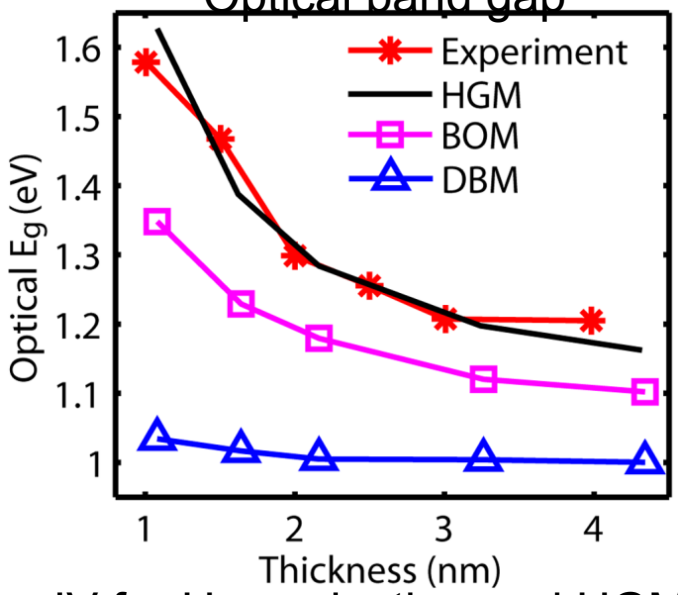
Method:

- Optical band gaps are calculated by considering the exciton energies, and compared to measurements.
- ITRS2020 target UTB transistors are simulated with H atom passivation and HGM configuration.

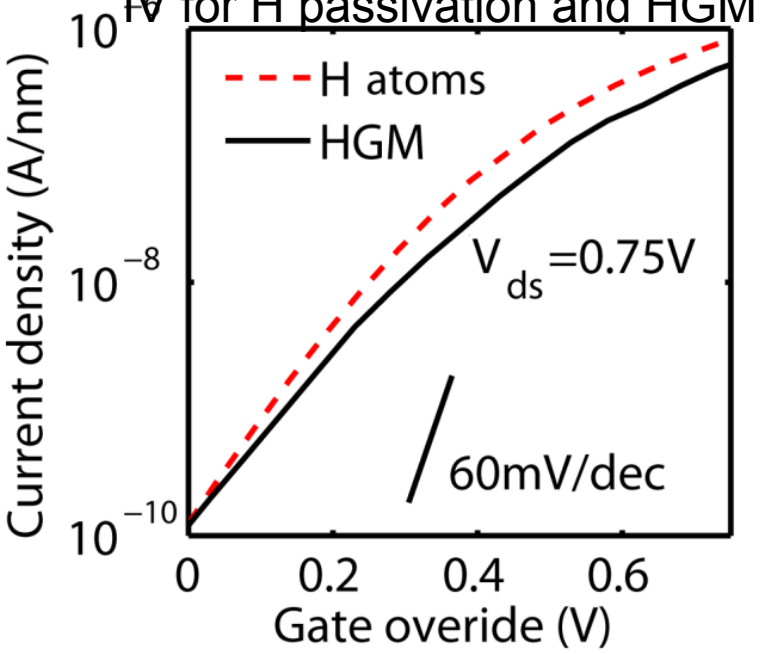
Impact:

- HGM shows nice agreement to measurement in band gaps for various UTB thickness.
- H atom passivation overestimates the transistor performance compared to proper oxidation.

Optical band gap



I-V for H passivation and HGM



Tight binding model for black phosphorus

Yu He, Yaohua Tan, James Charles, Gerhard Klimeck, Tillmann Kubis

Objective:

- Existing four-band tight binding model underestimates band splitting → might affect charge distribution especially if scattering exists.

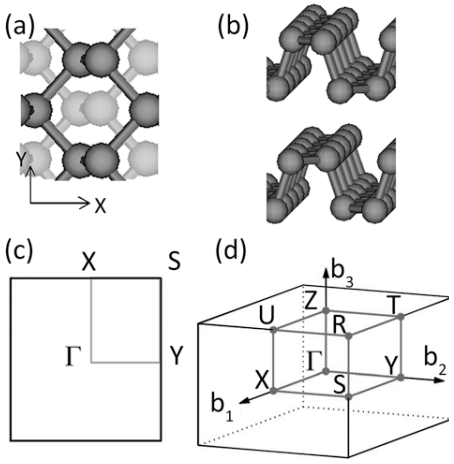
Method:

- Ten-band TB model considering 2NN interactions.
- Harrison's scaling law for bond length dependence of parameters.
- One parameter set for in-plane, one parameter set for inter-layer.
- Optimize parameters by fitting to DFT, for monolayer, bilayer, and bulk.

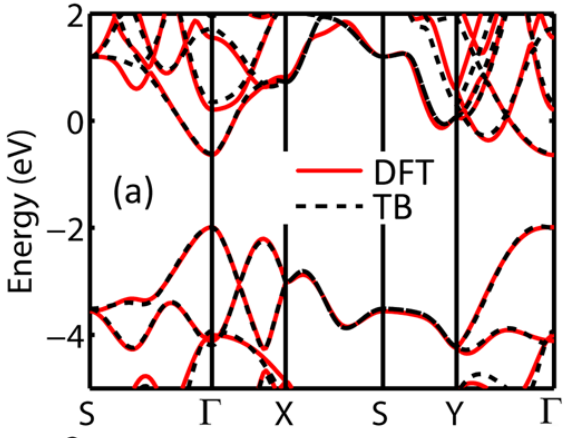
Impact:

- TB bandstructure well reproduce DFT results.
- Band splitting is well captured.

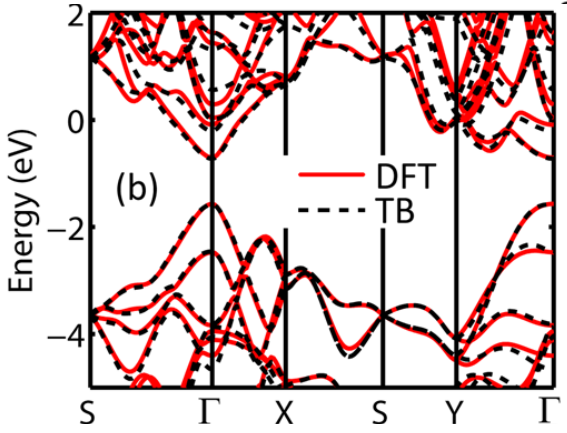
Structure and BZ



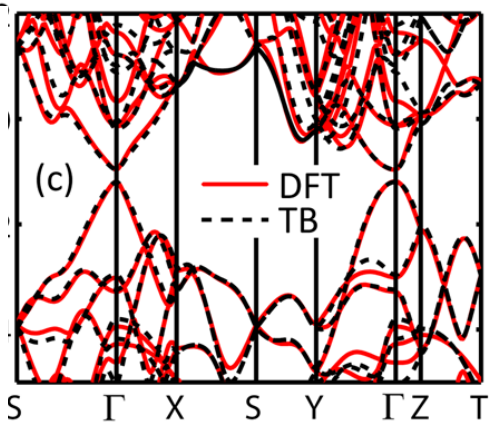
monolayer



bilayer



bulk



Transport for black phosphorus

Yu He, Yaohua Tan, James Charles, Gerhard Klimeck, Tillmann Kubis

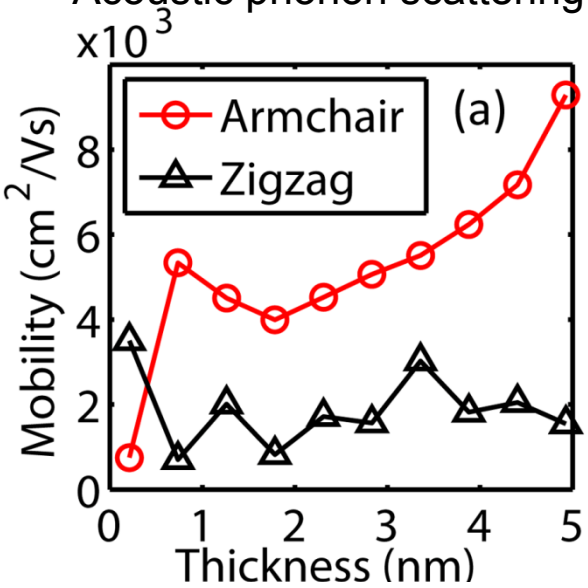
Objective:

- Measured mobility 300cm^2/Vs << expected value of 10^{4}cm^2/Vs.
- Surface roughness experimentally observed while its impact not fully understood.

Method:

- NEGF+TB with scattering.
- Acoustic phonon and surface roughness scattering are considered.
- ITRS2020 target transistor using black phosphorus is studied.

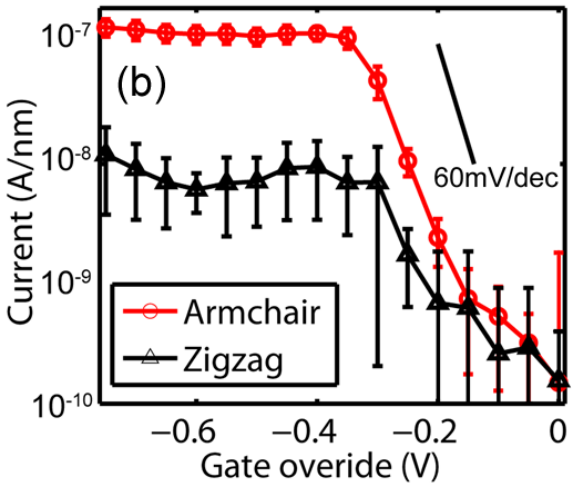
Acoustic phonon scattering



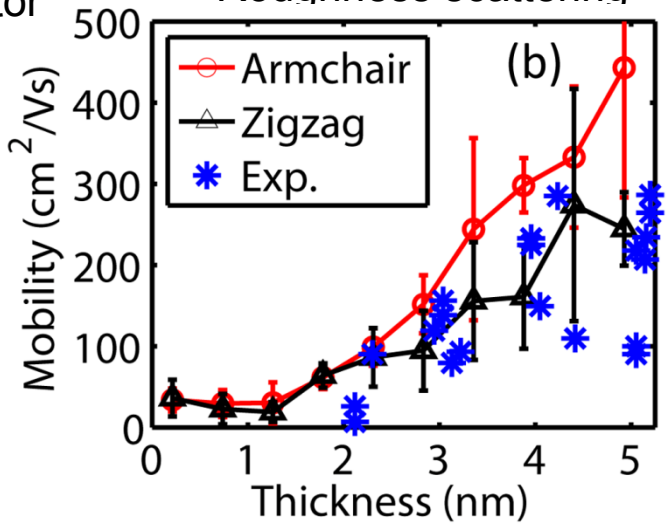
Impact:

- Acoustic phonon mobility >10^{3}cm^2/Vs suggests it is not dominant mechanism.
- Roughness scattering mobility matches well with measurement suggests it is the dominant mechanism.
- IV demonstrates the anisotropic properties.

I-V for ITR2020 target transistor



Roughness scattering



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Randomness in BTBT device

Yu He, Zhengping Jiang, Kai Miao, Tillmann Kubis, Gerhard Klimeck

Objective:

- Randomness such as interface roughness and alloy has significant effects on BTBT device performance.

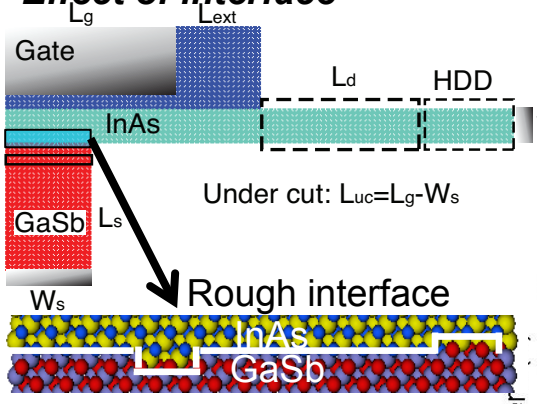
Method:

- Simulate I-V charasteristics for randomly generated alloy/roughness structures of BTBT device.

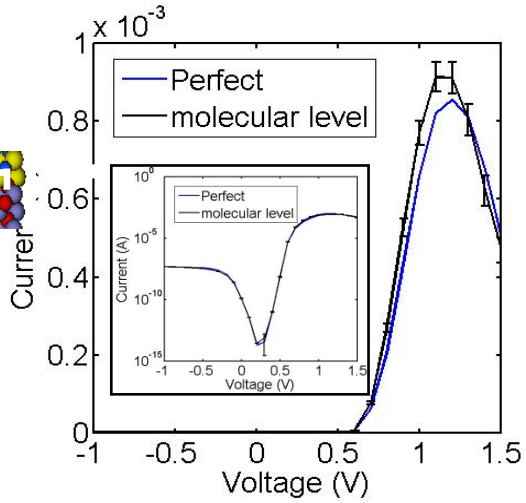
Impact:

- 500 samples for random alloy/ interface roughness in GaSb-InAs TFET are simulated.
- AlGaSb random alloy with different Al fractions, decreases on-state current by ~10 times
- GaSb/InAs interface roughness increases the on-state current by ~9%

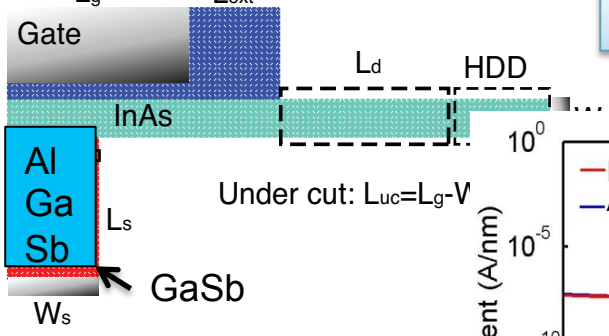
Effect of interface



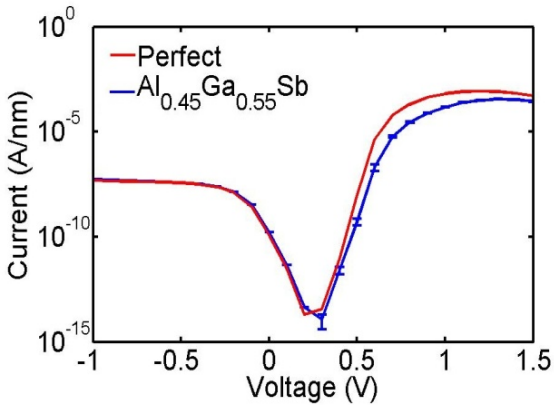
roughness at GaSb-InAs interface



Effect of random alloy



AlGaSb random alloy



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Thank you !

Back up

Method: tight binding parameterization

- TB model: sp3d5s*, different onsite energy for p_x and p_y.
- Consider 2nd NN, bond length dependence of parameters considered with Harrison's scaling law

$$U = U_0 (\frac{d_0}{d})^{\eta}$$

T Boykin et al, Phys. Rev. B 66, 125207 (2002).

- Interatomic interactions: generic model, different parameters for in-plane and interlayer couplings

- Ab-initio mapping method to obtain TB parameters
  → optimize TB parameters by fitting TB results to DFT calculations

Y Tan et al, J. Comput. Electron. 12, 56 (2013)

- Fitting target: monolayer, bilayer, bulk
  → transferable for arbitrary layers

Method: calculation of mobility

Low field resistance of channel length L written

$$R = R_0 + \frac{L}{\mu n q}$$

R_0 is contact resistance independent of L
With given scattering mechanism, mobility can be written

$$\mu = \frac{\Delta L}{\Delta n} \frac{1}{q \Delta R}$$

Y Niquet et al, J. Appl. Phys. 115, 054512 (2014)

Transport solved with NEGF and mobility extracted:

- Acoustic Phonon
- Surface roughness

Explicit surface roughness

- The roughness effects are generated by randomly distributing the atoms at the black phosphorus surfaces
- Distribution controlled by autocovariance function

$$ACVF_{ij} = \Delta^2 \exp(-\sqrt{2}\,|\,r_i - r_j\,|\,/\,L_c)$$

r_i, r_j the coordinates of surface atoms i, j
[?] root mean square of roughness
L_c correlation length

Kim et al, IEEE Trans. Elect. Dev. 58, 1371 (2011).

- Atomistic structure changes with surface roughness → device Hamiltonian changes
- Surface roughness exists in both device and contacts → **RGF+general lead** method
- [?]=0.2nm, L_c=1.1nm used; average over 50 samples
- Transverse k-direction for black phosphorus UTB → thicker structure used (6nm for 1L~3L; 3nm for 4L~7L; 2nm for 8L~10L)

Acoustic phonon scattering in NEGF

Linear phonon dispersion is assumed

$$|U_q|^2 = \frac{\hbar D_{ac}^2}{2\rho v_s} q$$

For black phosphorus
ρ material density 2.69 g/cm^3

H Liu et al, Chem. Soc. Rev. 44, 2732 (2015)

D_{ac} deformation potential is thickness dependent
Increase from 1L to 5L and saturate

J Qiao et al, Nature Comm. 5, 4475 (2014)

v_s sound velocity 3.8km/s armchair direction, 7.8km/s zigzag direction

Z Zhu et al, Phys. Rev. Lett. 112, 176802 (2014)

Self-energy due to acoustic phonon scattering (low energy, high temperature)

$$\Sigma(r_1, r_2, k, E) = \frac{D_{ac}^2 k_B T}{2\hbar\rho v_s^2} \delta(r_1, r_2) \int \frac{dk'}{2\pi} G(r_1, r_2, k', E)$$

$$(E - H - \Sigma - \Sigma_{S/D})G = 1$$

Self-consistent Born iteration

Lake et al, J. Appl. Phys. 81, 7845 (1997)