Electronic Structure and Transport in Semiconductor Nanostructures: Experiments and Theoretical Challenges

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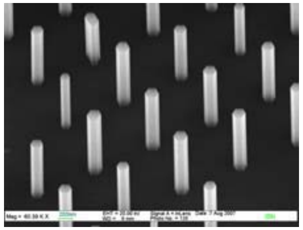
JARA-FIT (Fundamentals of Future Information Technology)

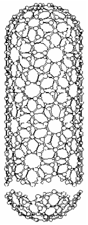
KITP Conference, Santa Barbara, Nov.2-6, 2009

Promising Semiconductor Nanostructures: Nano-Devices

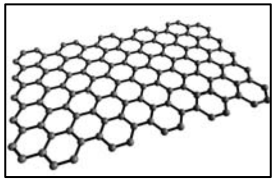
– **Semicond. Nanocolumns**



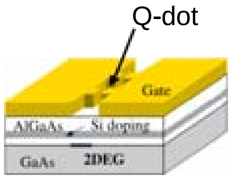
Carbon Nanotubes



– **Graphene Ribbons**



– **Quantum Dots**



OUTLINE

Semiconductor Nanowires

- Growth and Doping, Band Gap
- Electronic Transport
  - -Effect of Space Charge Layers
  - -Quantum Transport in Narrow Gap SC Wires

Theoretical Challenges

Graphene Ribbons

- General Properties, Doping
- Multilayer Stacks with Dirac Cone
- Dead Edge Region: Gap and Transport

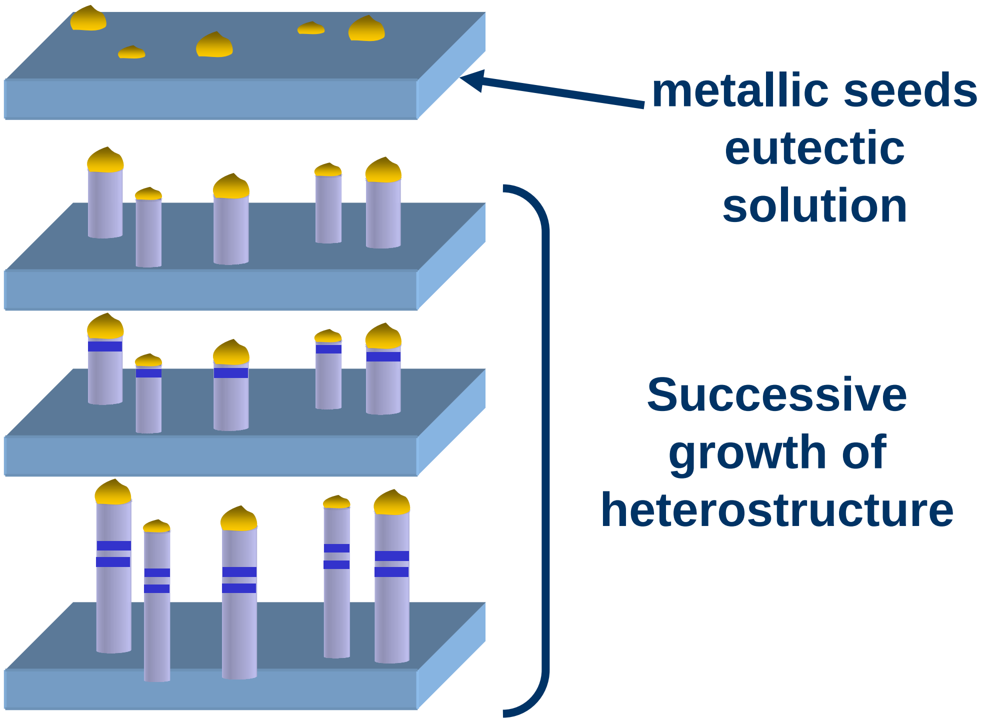
Theoretical Challenges

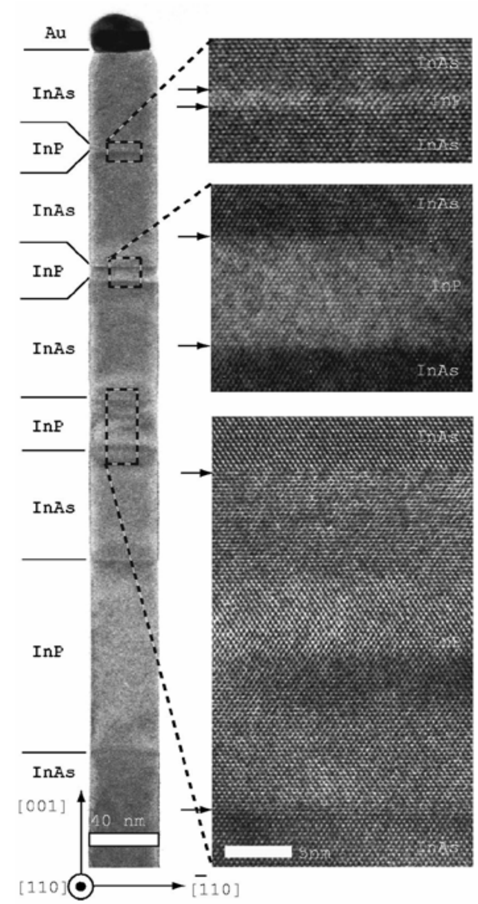
Coupled Quantum Dots as Q-bit

Theoretical Challenges

III-V Semiconductor Whisker Growth (bottom-up)

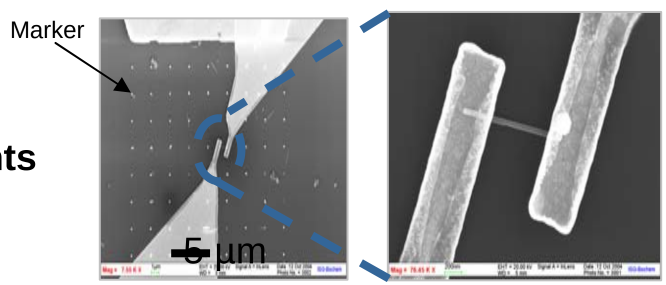
(Vapour-Liquid-Solid Growth)





M. T. Björk, B. J. Ohlsson, T. Sass, A. I. Persson, C. Thelander, M. H. Magnusson, K. Deppert, L. R. Wallenberg, and L. Samuelson, Appl.Phys.Lett.,80, (2002) 1058

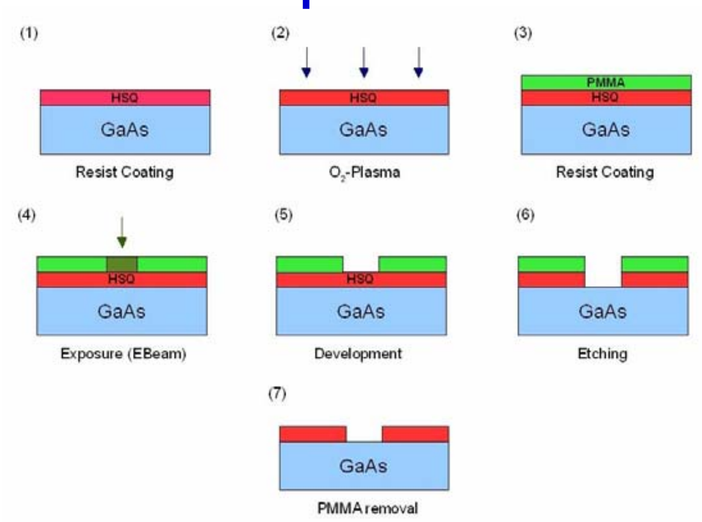
Preparation for Transport Measurements

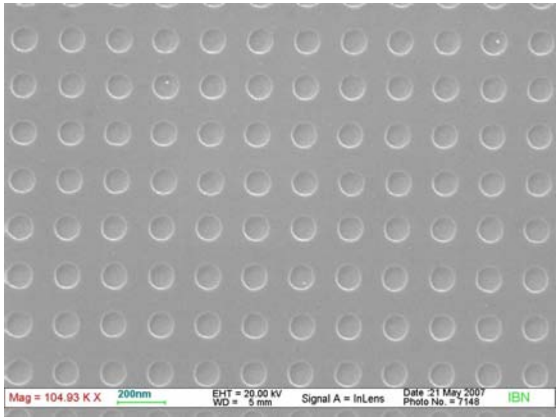


Ordered Selective Growth by means of Masks

Selected area Growth

Mask Preparation



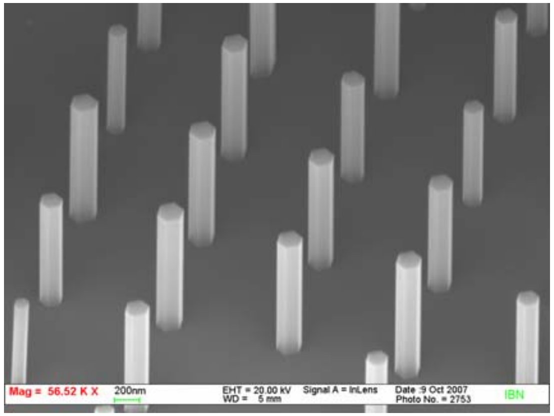


HSQ Mask on GaAs (111)

MOVPE Growth

Precursors: AsH_3, TMGa

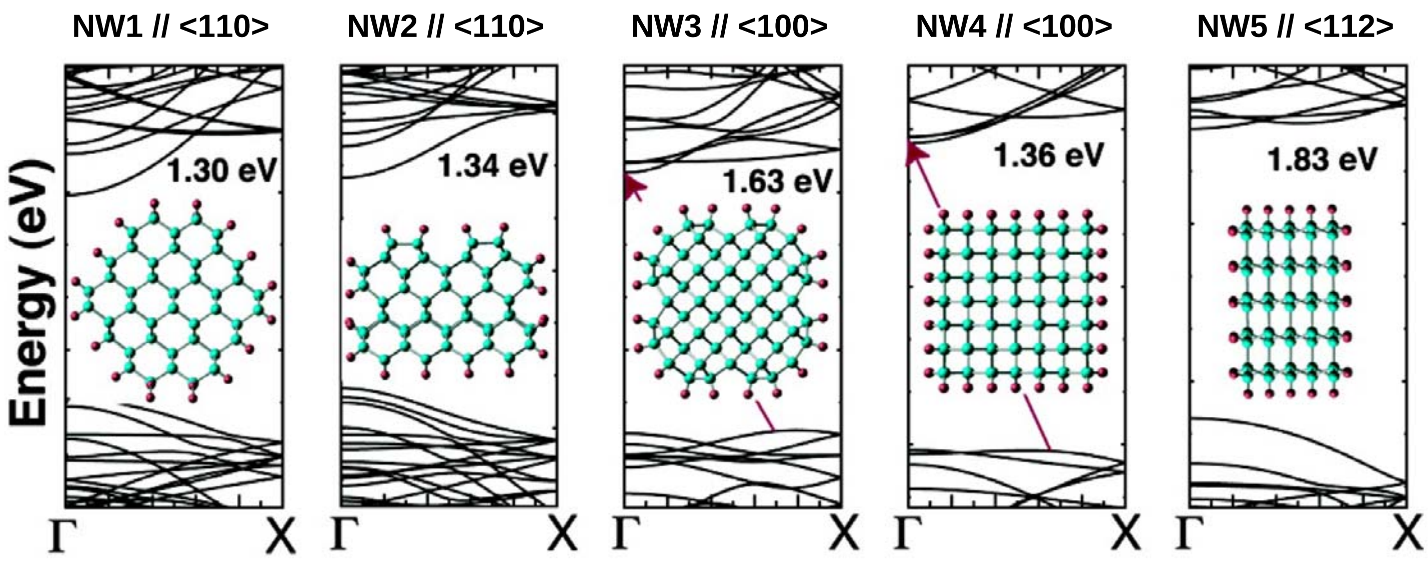
Growth Temp.: 750^0C

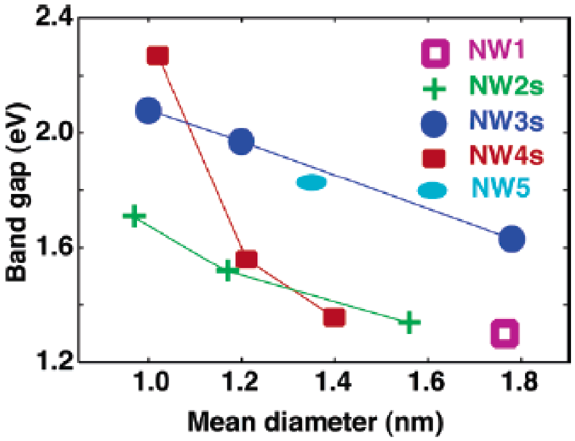


GaAs pillars on GaAs (111)

Vera Klinger, J. Wensorra et al. (2008)

Si Nanowires in the Quantum Confinement Regime:
Electronic Band Structure Calculations (DFT)





A.K. Singh, V. Kumar, R. Note,Y.Kawazoe :
Nano Lett. **6**, 920 (2006)

CdSe Nanowires in the Quantum Confinement Regime

Preparation by Solution-Liquid-Solid Synthesis (SLS)

1.Step: Bi nanoparticles as catalysts:

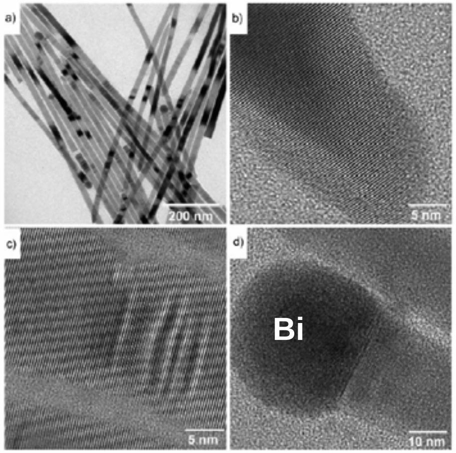
$BiCl_3$ and tri-n-octylphosphine (TOP) as reducing agent

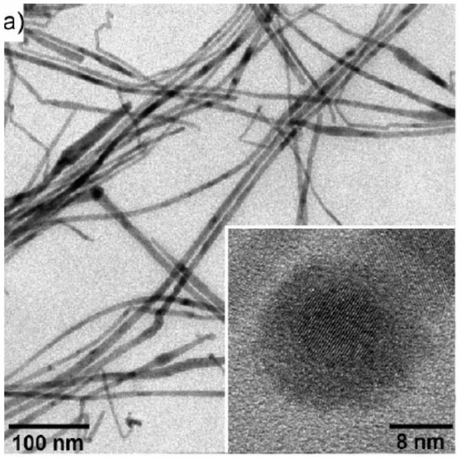
2.Step: CdSe wires by addition of:

CdO or $Cd(Me)_2$ and TOPSe, Reaction Temperature 330^{0}C

3.Step: Termination by Toluene

Precursor: CdO, Cd/Se=7/1

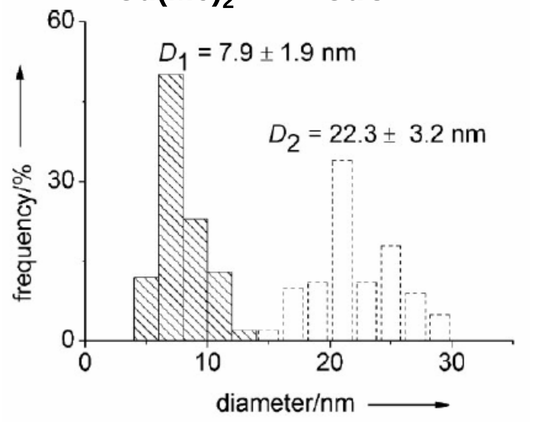




Precursor: $Cd(Me)_2$

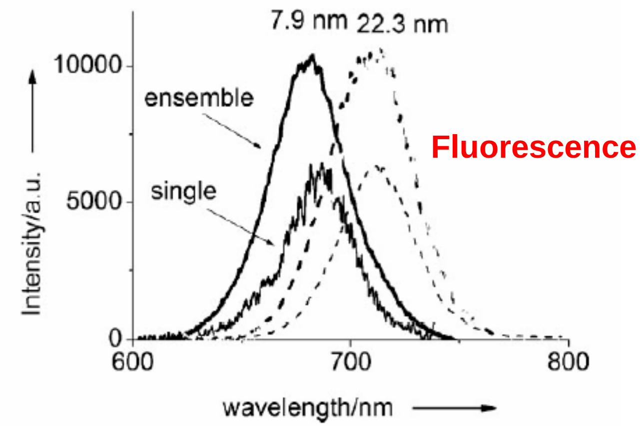
Precursors:

$Cd(Me)_2$ **CdO**



Bulk gap: 1.7 eV

1.82 eV **1.72 eV**



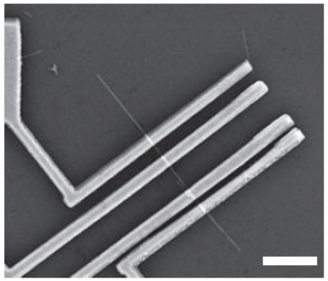
Fluorescence

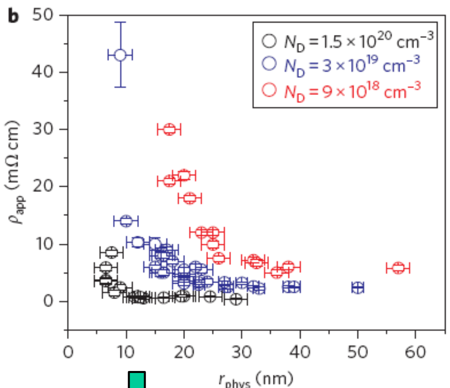
Zhen Li, A. Kornowski, A. Myalitsin, A. Mews: Small 4, 1698 (2008)

Doping Deactivation in Si Nanowires: Dielectric Mismatch

Preparation: Vapour-Liquid-Solid Growth (CVD)

Doping: PH_3, P built in as in Bulk Material



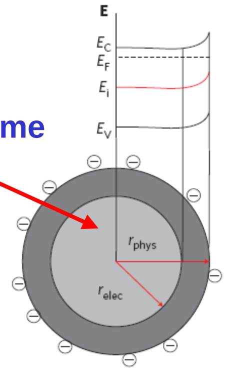


N_D determined from thick wires (resistivity)

$$r_{elec} = \sqrt{r_{phys}^2 + \frac{2r_{phys}Q_f - 2r_{phys}e^2 D_{it}\psi_o}{e(N_D - N_A)(1 + \frac{r_{phys}e^2}{2\varepsilon_0\varepsilon_s}D_{it})}}$$

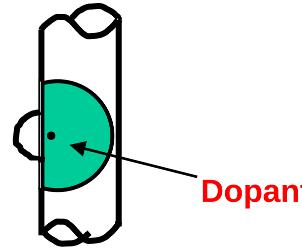
Effect of space charge layer

electrically active volume



From analysis of exp. data:
***D_{it}*=6x10^{12}cm^{-2}eV^{-1}**

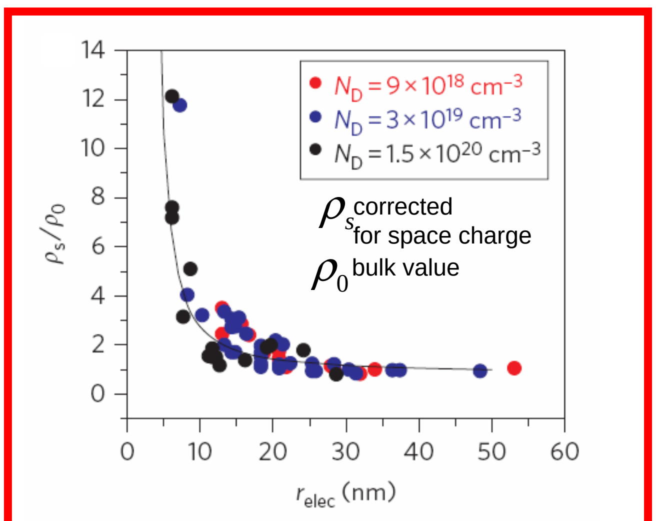
***Q_f=0* fixed oxide charge**

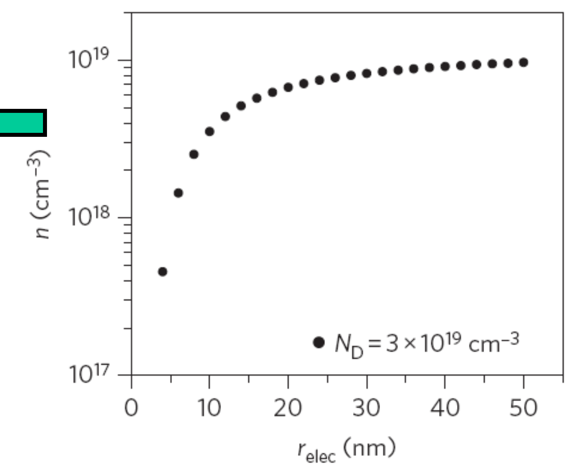


Change of Dopant Ionisation Energy:

$$E_I - E_I^0 \approx \frac{2e^2}{\varepsilon_0\varepsilon_s r_{elec}} \frac{\varepsilon_s - \varepsilon_{air}}{\varepsilon_s + \varepsilon_{air}} F\left(\frac{\varepsilon_s}{\varepsilon_{air}}\right)$$

$$\propto 1/r_{elec}$$





M.T. Björk, H. Schmid, J. Knoch, H. Riel, W. Riess: Nature Nanotechnology **4**, 103 (2009)

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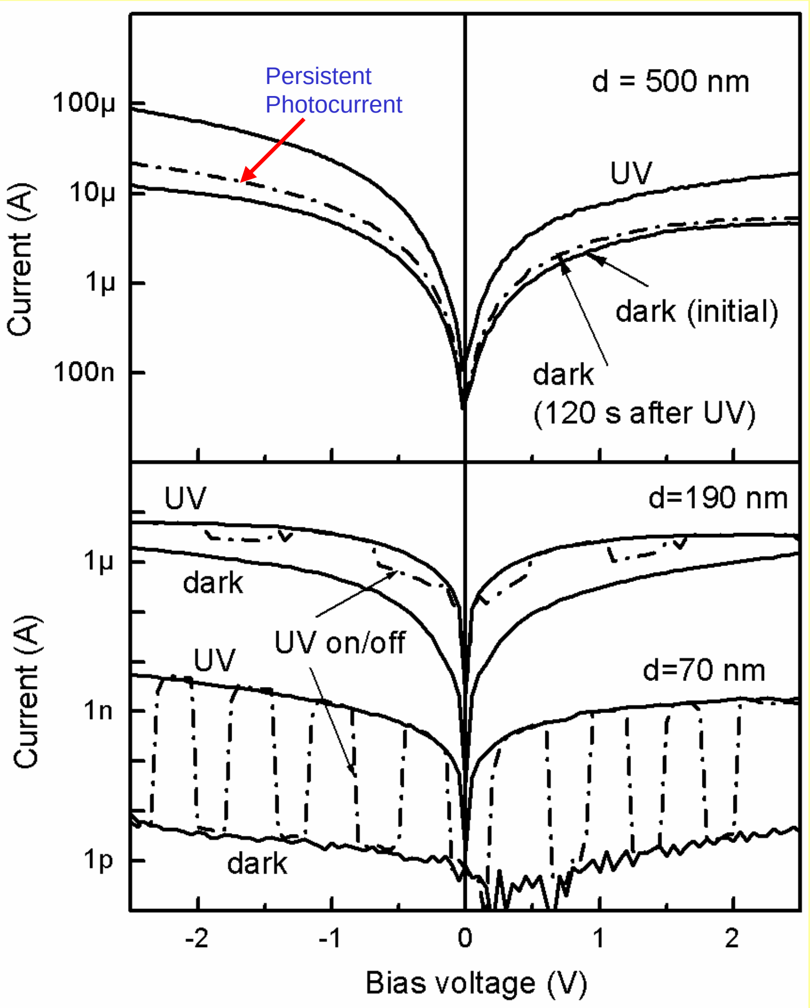
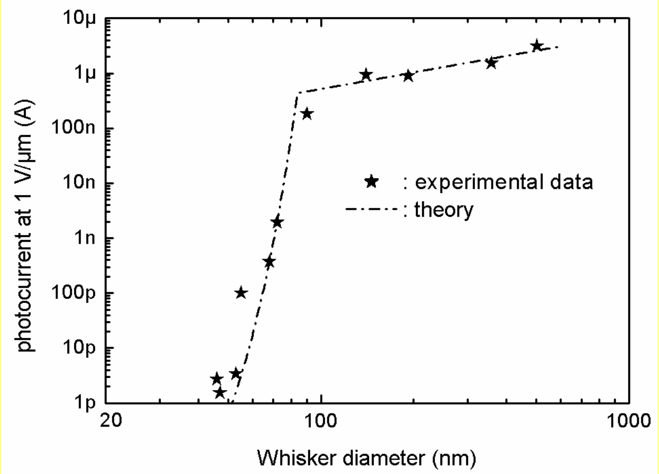
Coupled Quantum Dots as Q-bit

Theoretical Challenges

GaN Whiskers: Thickness dependent Photocurrent



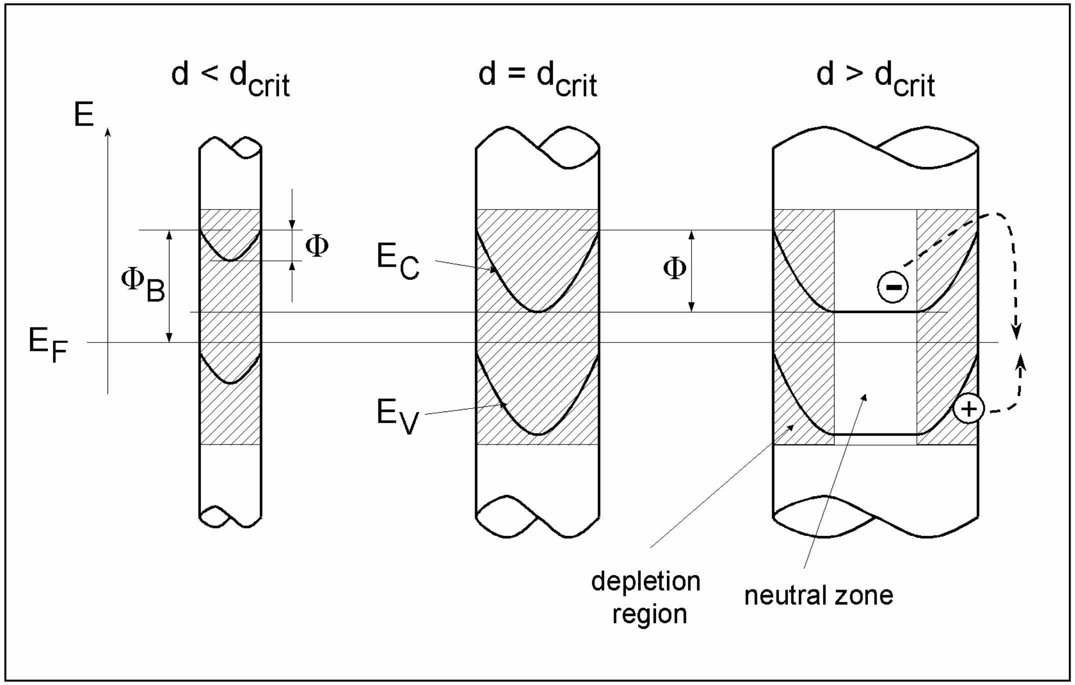


d>80nm: persistent photocurrents after UV illumination,

d<80nm: photocurrents exponentially decaying with decreas. thickness; fast response

R. Calarco, M. Marso, R. Meijers, T. Richter, A.I. Aykanat, N. Thillosen, T. Stoica, H.L.: NanoLetters 5, 981 (2005)

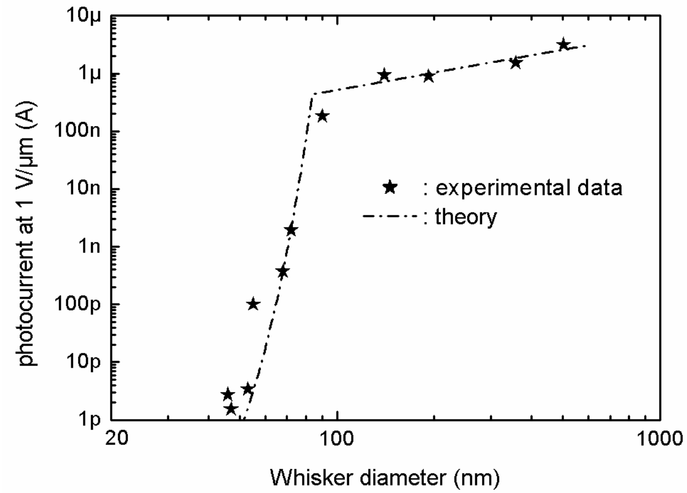
Model for Thickness dependent Surface Recombination



$$I_{Photo} \propto \exp(\Phi / kT)$$

$$with\ \ \Phi = \frac{qN_D}{16\varepsilon} d_{crit}^2 = const. \quad for\ d > d_{crit}$$

$$\Phi = \frac{qN_D}{16\varepsilon} d^2 \quad for\ d < d_{crit}$$



$$Photocurrent\ \ I_{Photo} \propto \frac{1}{recombination\ rate}$$

$$recombination\ rate \propto \exp(-\Phi / kT)$$

Fit param.: N_D=6.25x10^{17}cm^{-3}

Φ_B=0.555eV

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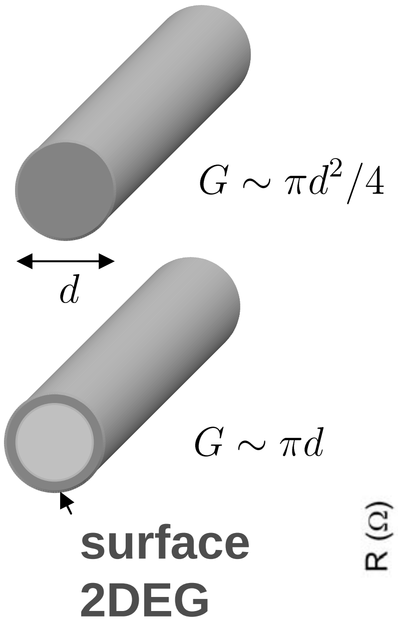
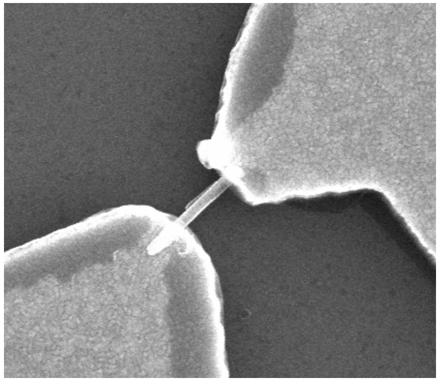
Coupled Quantum Dots as Q-bit

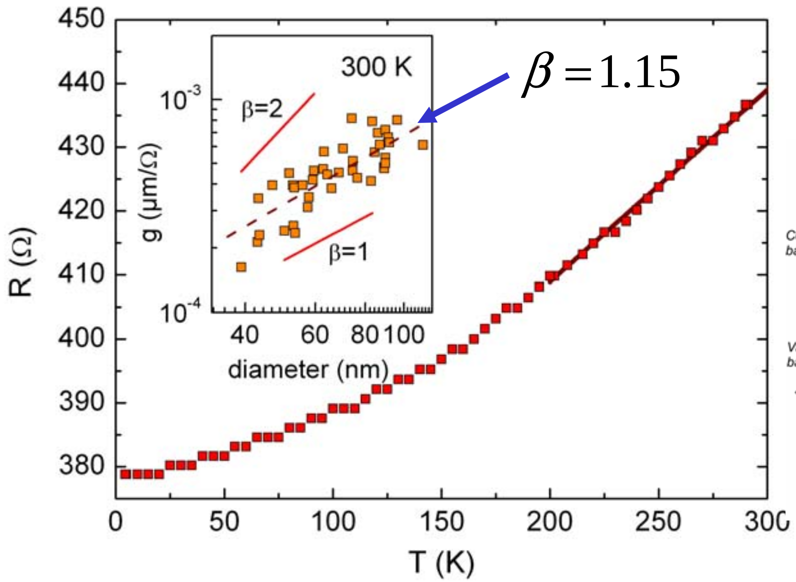
Theoretical Challenges

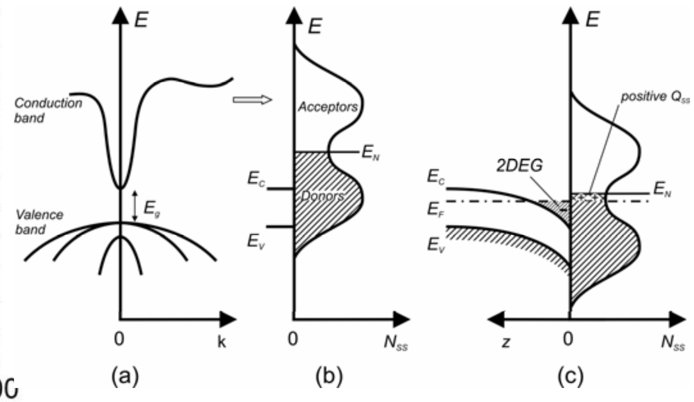
Resistance of InN Wires

grown as Whiskers on Si(111)









normalized conductance:

$$g = G \times L \propto d^{\beta}$$

$\beta = 2$ bulk

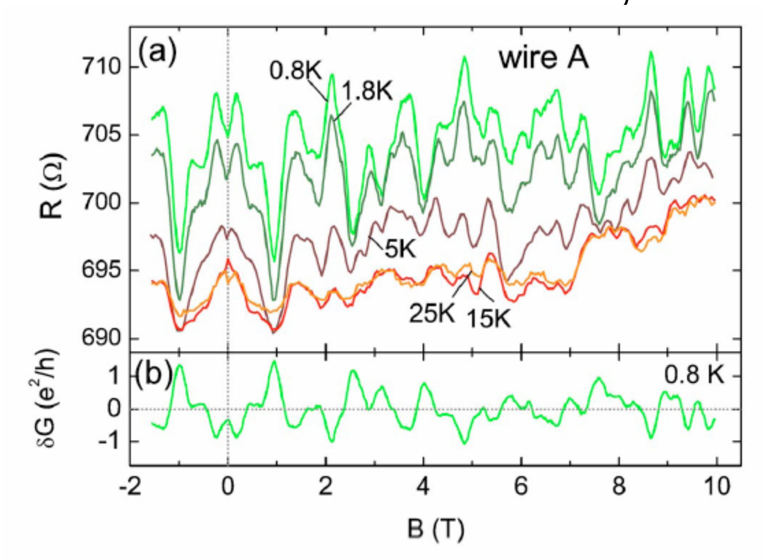
$\beta = 1$ surface

Metallic Surface 2DEG

Th. Richter, Ch. Blömers , H. Lüth, R. Calarco, M. Indlekofer, M. Marso, Th. Schäpers: NanoLetters (2008)

Phase Coherence from Univ. Cond. Fluct.: InN Wires

Dimensions: L=410nm , d=67nm

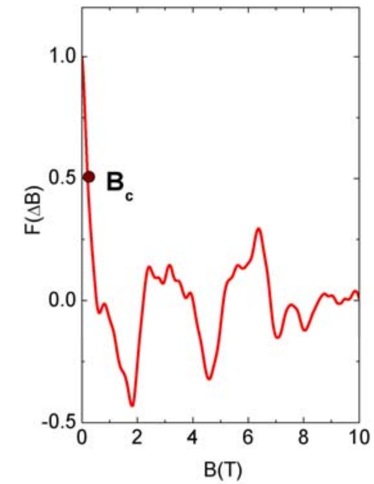


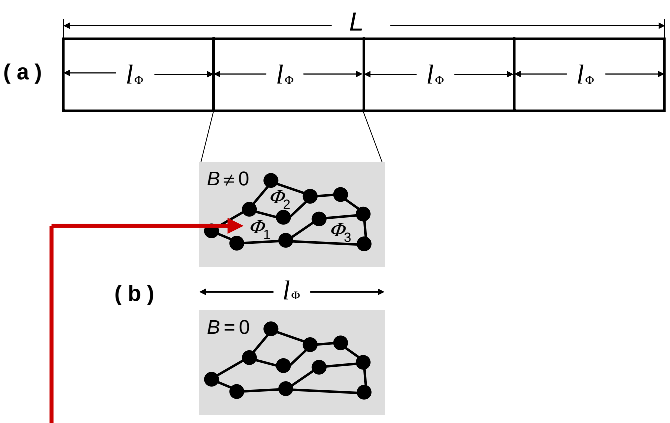
Correlation function

$$F(\Delta B) = \langle \delta G(B+\Delta B)\delta G(B)\rangle$$

***B_c*= Critical Correlation Field**

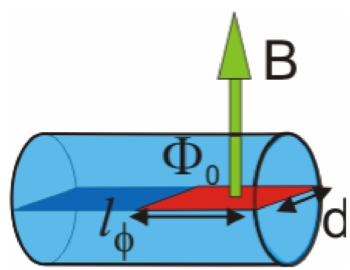
$$F(B_c) = \frac{1}{2}F(0)$$



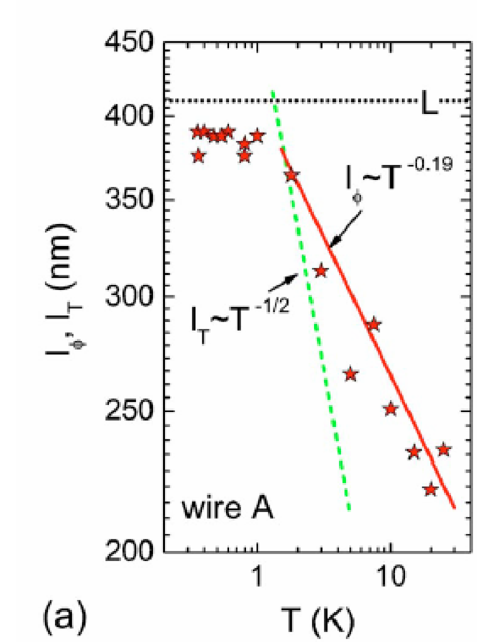


Closed Loops: Aharonov Bohm Interferencies

Phase Coherence Length:



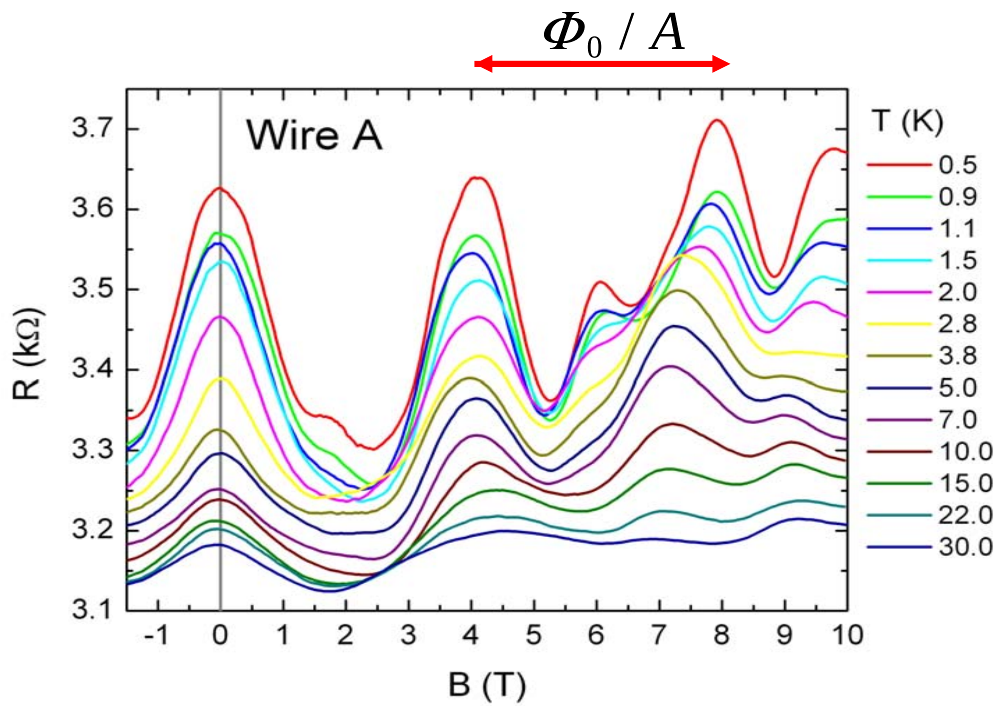
$$l_\phi \approx \frac{\Phi_0}{B_c d}$$

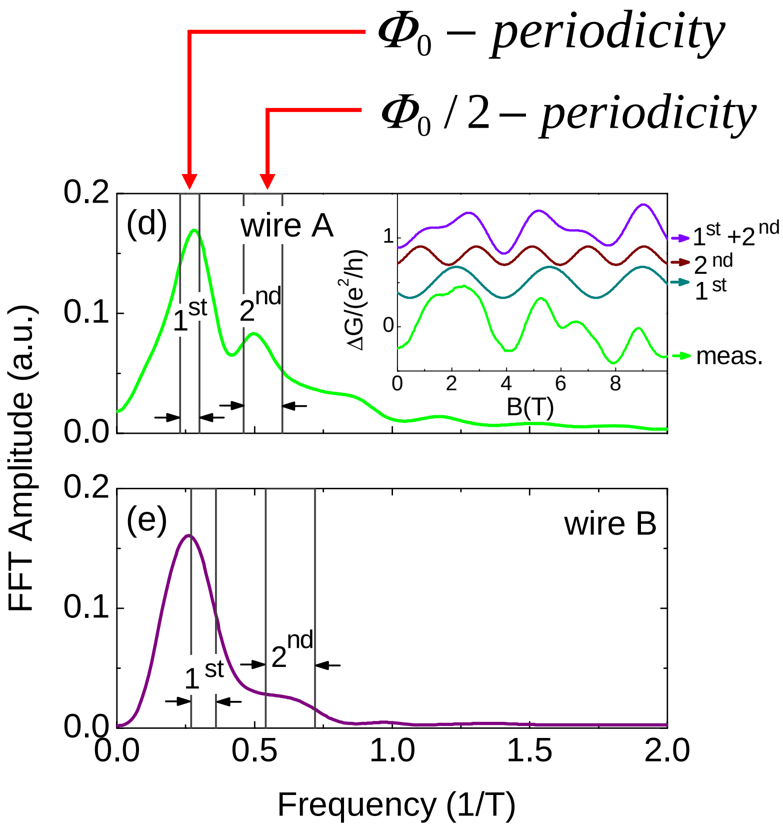


Ch. Blömers, Th. Schäpers, T. Richter, R. Calarco, H. Lüth, and M. Marso: Appl. Phys. Lett. 92, 132101 (2008)

InN Whisker (Nanowire): Magnetotransport (B // c-axis)

wire dimensions: length 420nm
diameter 37nm





$$\Phi_0 = \frac{h}{e}$$ **flux quantum:**

Th. Richter, Ch. Blömers , H. Lüth, R. Calarco, M. Indlekofer, M. Marso, Th. Schäpers: NanoLetters (2008)

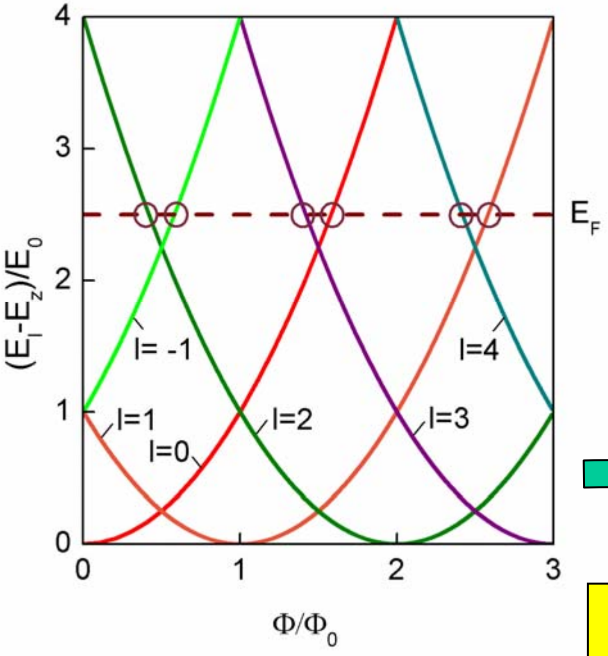
Flux Quantisation: Transport through Angular Momentum States

$$\hat{H}\,\psi(r,\varphi)\chi(z) = E_l\psi(r,\varphi)\chi(z)$$

$$E_l = \frac{\hbar^2 k_z^2}{2m^*} + \frac{\hbar^2}{2m^* r^2}\left(l - \frac{\Phi}{\Phi_0}\right)^2$$

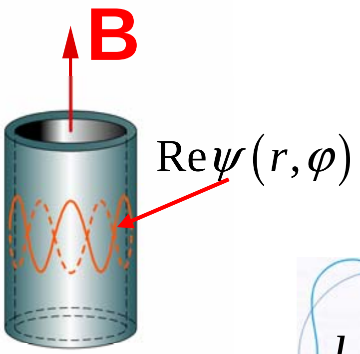
$$\hat{H} = \overbrace{\frac{1}{2m^* r^2}\left(\hat{L}_z - \frac{1}{2}eB_z r^2\right)^2}^{(\mathbf{p}-e\mathbf{A})^2/2m^*} - \frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}$$

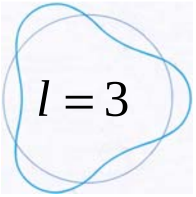
$$\Phi = \pi r^2 B_z \qquad \Phi_0 = \frac{e}{h}$$



Typical values:

$$(E_F - E_c)_{surf} \approx 0.9eV$$
$$\lambda_F \approx 5nm$$
$$l \approx 26 \ @ \ \Phi = 0$$

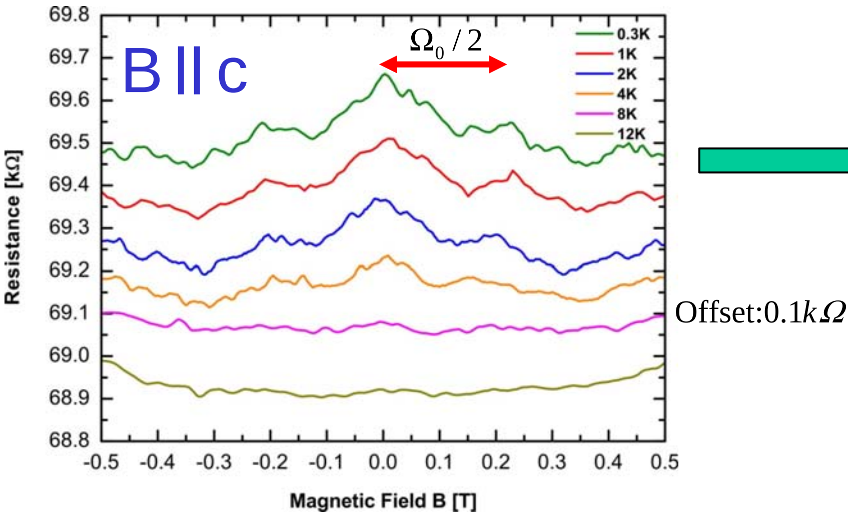


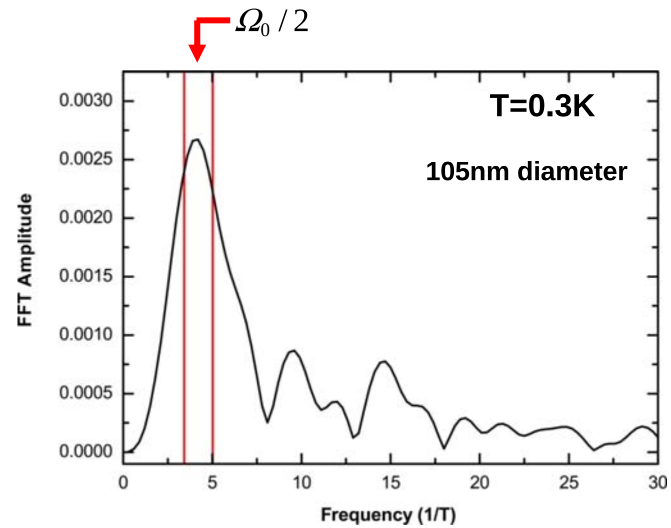


Period Φ_0

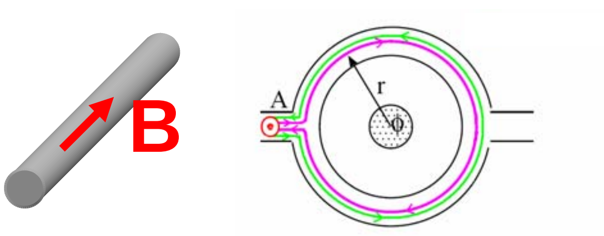
InAs Columns: Magnetoresistance Oscillations

Columns lithographically shaped from MBE grown Layers in [111] Direction (Top-down)





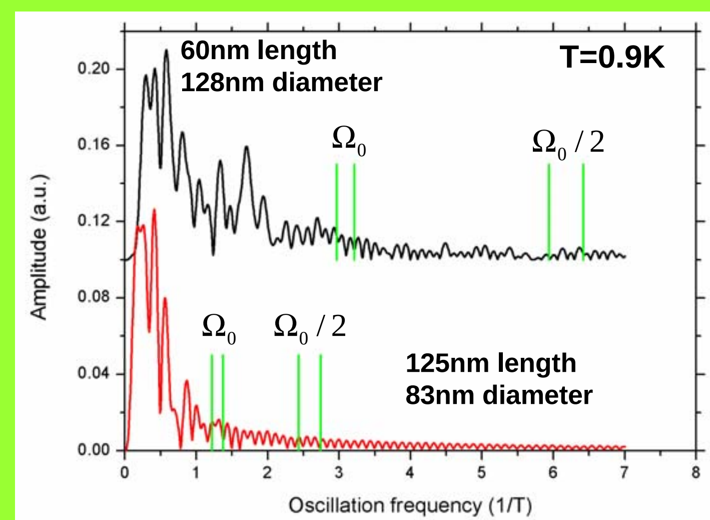
Alt`shuler-Aronov-Spivak Interferences



$$\Psi(\mathbf{r}) = \Psi_1 \exp\left(\frac{ie}{\hbar}\int_1 d\mathbf{s}\cdot\mathbf{A}\right) + \Psi_2 \exp\left(\frac{ie}{\hbar}\int_2 d\mathbf{s}\cdot\mathbf{A}\right)$$

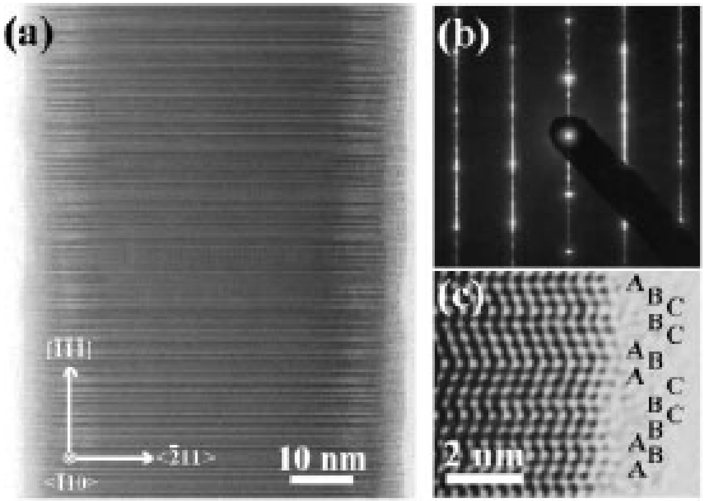
$$G(\Phi) = C + D\cos\left(2\pi\frac{2\Phi}{\Phi_0}\right) \qquad \Phi_0 = \frac{h}{e}$$

MBE grown Columns (Bottom-up)

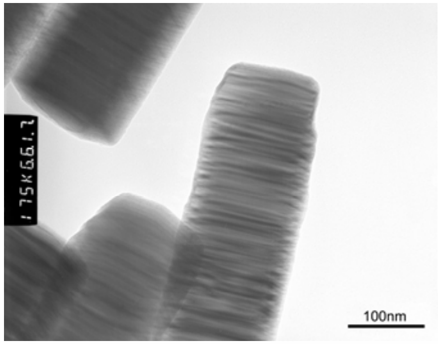


J. Wensorra et al., to be published (IBN, Res. Centre Jülich 2009)

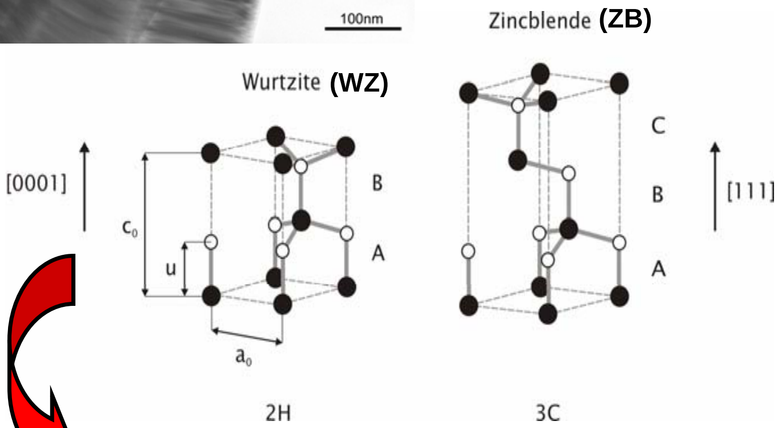
InAs Nanowires from MOCVD selected area Growth:
Stacking Faults



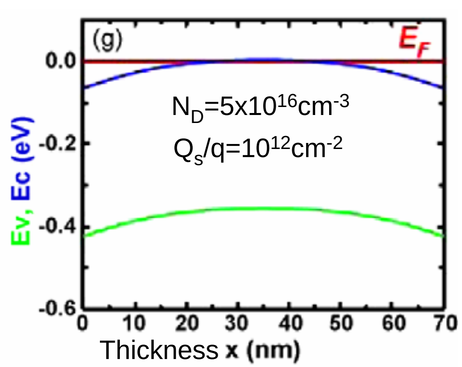
K. Tomioka, J. Motohisa, S. Hara, T. Fukui:
Jap. J. Appl. Phys. **46**, L1102 (2007)

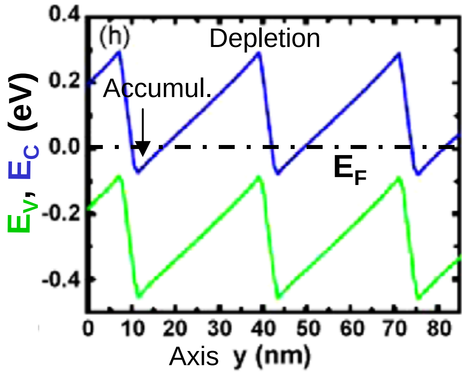


H. Hardtdegen et al.
IBN, Res.Centre Jülich (2009)



Spontaneous (pyroelectric) Polarisation along [0001]





Effect of Surface States masked by Polarisation Charges at Surface

No Surface Accumulation !?

S.A. Dayeh, D. Susac, K.L. Kavanagh, E.T. Yu, D. Wang: Adv.Funct. Mater.,in press
and S.A. Dayeh et al.: Nano Today **4**, 347 (2009)

Theoretical Challenges

– Growth and Doping

- **Tailoring of Stacking Faults in III-V Nanowires ?**

  Substrate, Growth Conditions........
- **Built-in of Dopants, Dopant Deactivation ?**

– Electronic Band Structure and Band Gap

– Surface States and Space Charge Layers ?

- **Nano Surface Science**
- **Space Charge Layers in the Presence of Defects ?**

– Electronic Transport

- **Scattering Mechanisms ?**

  Surface, Stacking Faults......
- **Phase Coherence Length, Coherent Transport ?**
- **Spin related Transport and Interferences (Weak Antilocalisation) ?**

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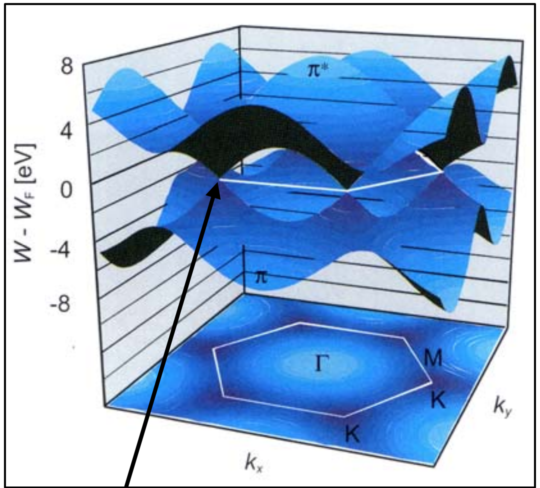
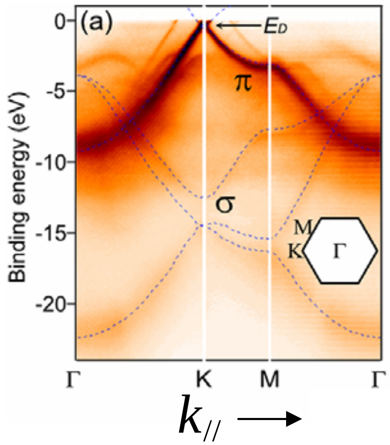
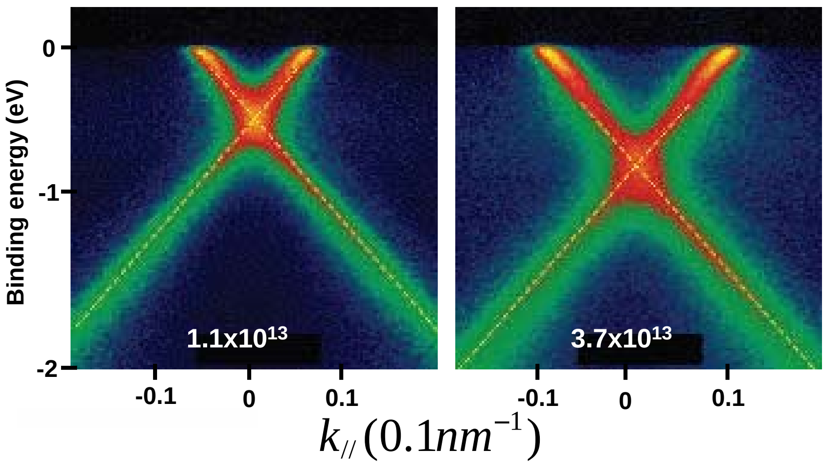
Graphene: Electronic Structure



ARPES: Photon energy 94eV
T=30K



K- Doping



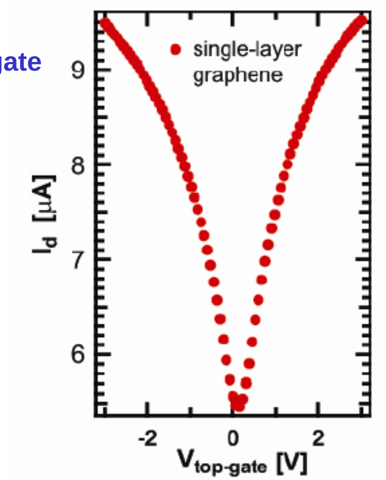
Dirac point

Removed by atomic H treatment:

Graphane

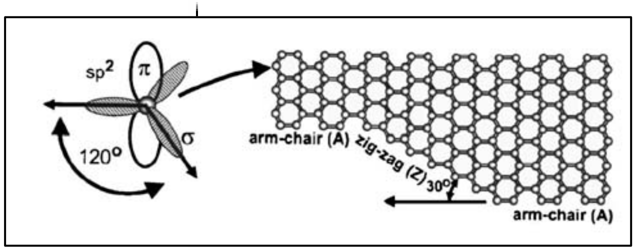
A. Bostwick, T. Ohta, Th. Seyller, K. Horn, E. Rotenberg: Nature Physics, **3**, 36 (2007)

Top Ti/Au-gate
10nm Al_2O_3



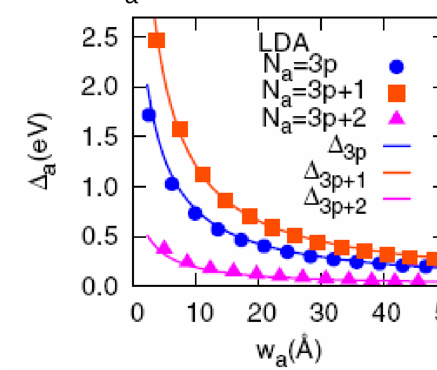
Zhihong Chen, J. Appenzeller
(IBM, Perdue Univ.)

Ribbons



Calcul. Band Gap of Ribbons

N_a=No. of arm chair dimers



DFT
(LSDA)

Edge
passivated
by H Atoms

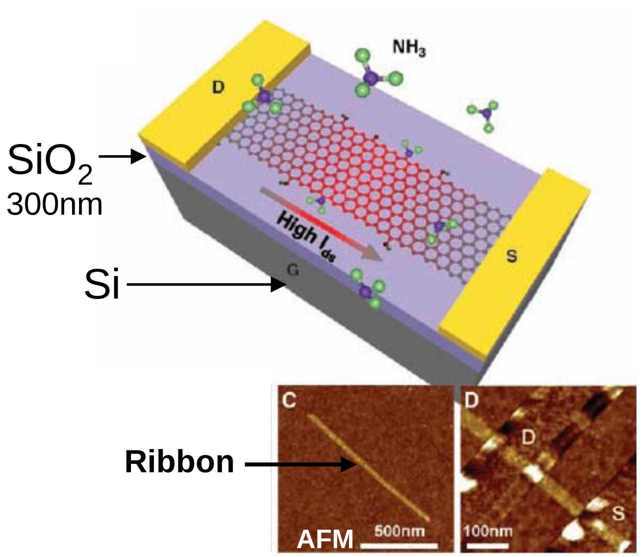
Young-Woo Son, M.L. Cohen, S.G Louie: Phys. Rev. Lett. **97,** 216803 (2006)

Graphene Ribbons: n-Doping with Ammonia

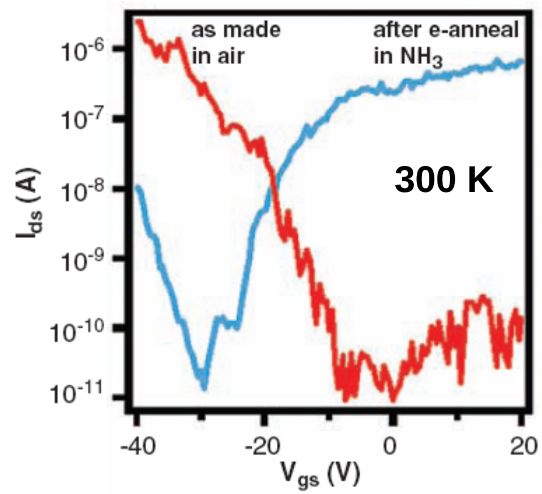
Peel-off Graphene (Monolayer)

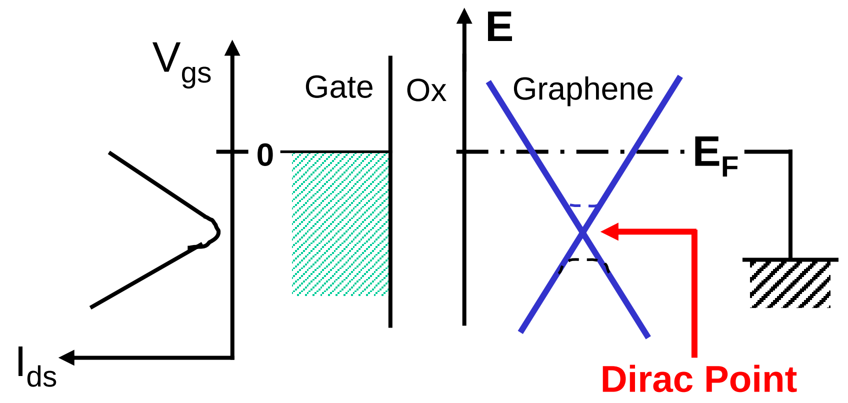
Ribbons by e-beam Lithography

Doping: Joule Heating to 300^{0}C in NH_3/Ar, 1Torr



Stable Doping Conditions,
in contrast to physisorbed NH_x Species





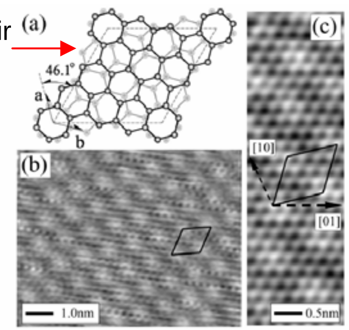
Unchanged Electron Mobility after Doping:
Edge Doping rather than Surface Doping

Xinran Wang et al.: Science **324**, 768 (2009) (Stanford, Gainsville, Livermore)

Multilayer Graphene on 4H-SiC $(000\bar{1})$, C-face :
a Dirac Cone like in a Single Sheet

fault pair unit cell

STM



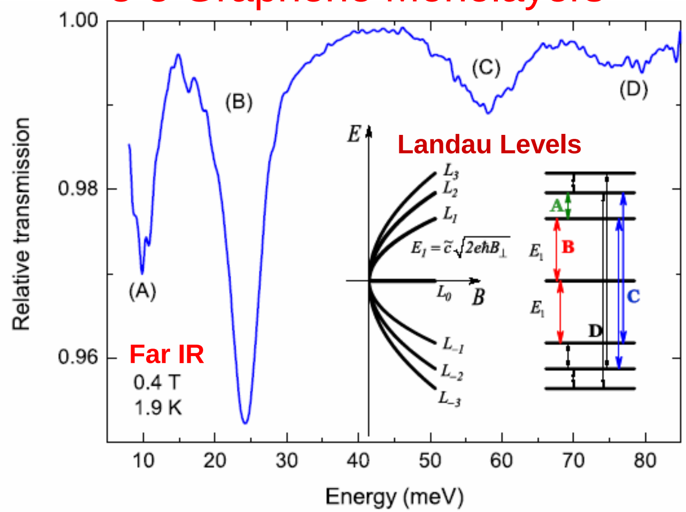
By Annealing to 1400 ^{0}C:

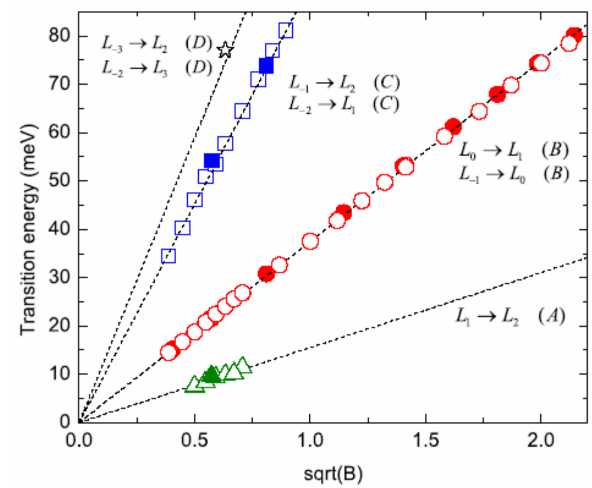
Interleaved Growth with:

30^0 rotated or
+/- 2.2^0 rotated } **vs. SiC** $[10\bar{1}0]$
(commensurate)

Stacking Faults: **Layer Decoupling**

3-5 Graphene Monolayers





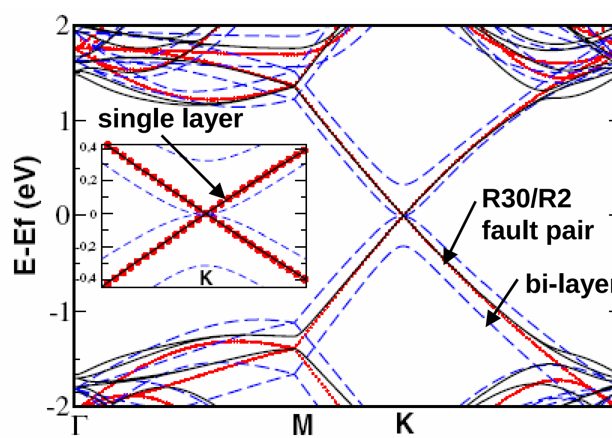
Landau levels for a Dirac cone:

$$E_n = \mathrm{sgn}(n)c^*\sqrt{2e\hbar B|n|} = \mathrm{sgn}(n)E_1\sqrt{|n|}$$

(for standard 2DEG: $E_n = (n + \frac{1}{2})\hbar eB/m^*$)

Electron velocity: c*~10^8cm/s

Dirac mass: m_D=E/c*~0.0012 m_0



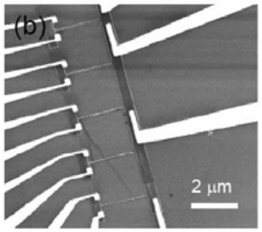
DFT (VASP code)

M.L. Sadowski, G. Martinez, M. Potemski, C. Berger, W.A. de Heer: Phys. Rev. Lett.. 97, 266405 (2006)

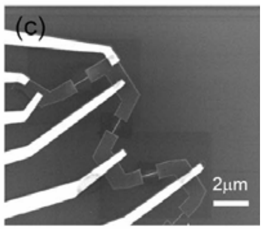
J. Hass, F. Varchon, J.E. Millan-Otoya, M. Sprinkle, N. Sharma, W.A. de Heer, C. Berger, P.N. First, L. Magaud, E.H. Conrad: Phys. Rev. Lett. 100, 125504 (2008)

Graphene Nanoribbons: Transport and Gap (lateral confinement)

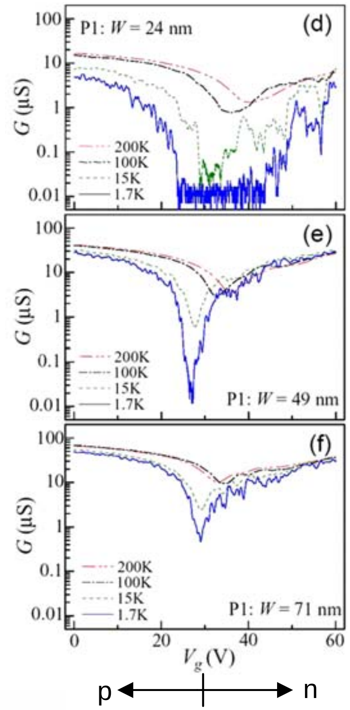
Graphene Single Sheets on SiO_2/Si (gate)

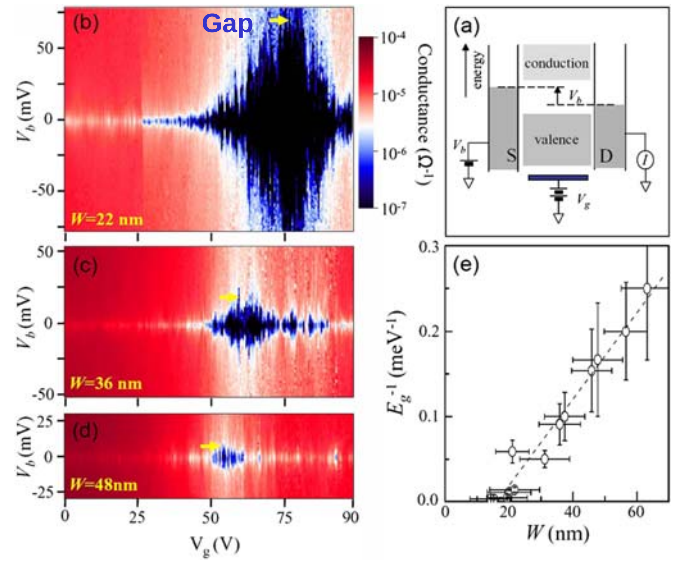


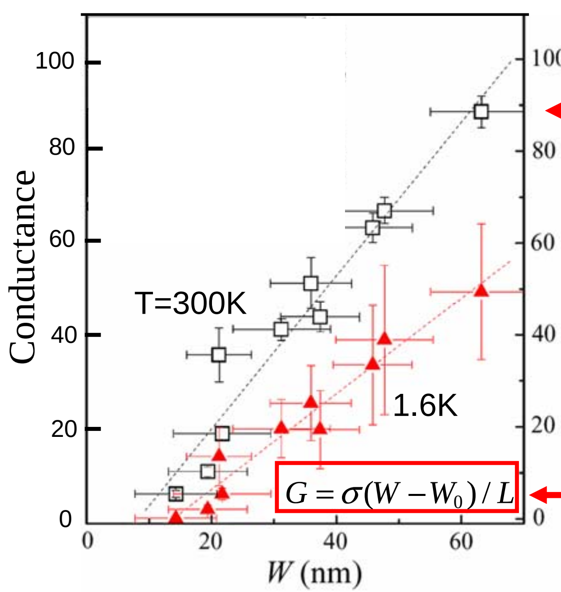
Different Widths



Different Orientations





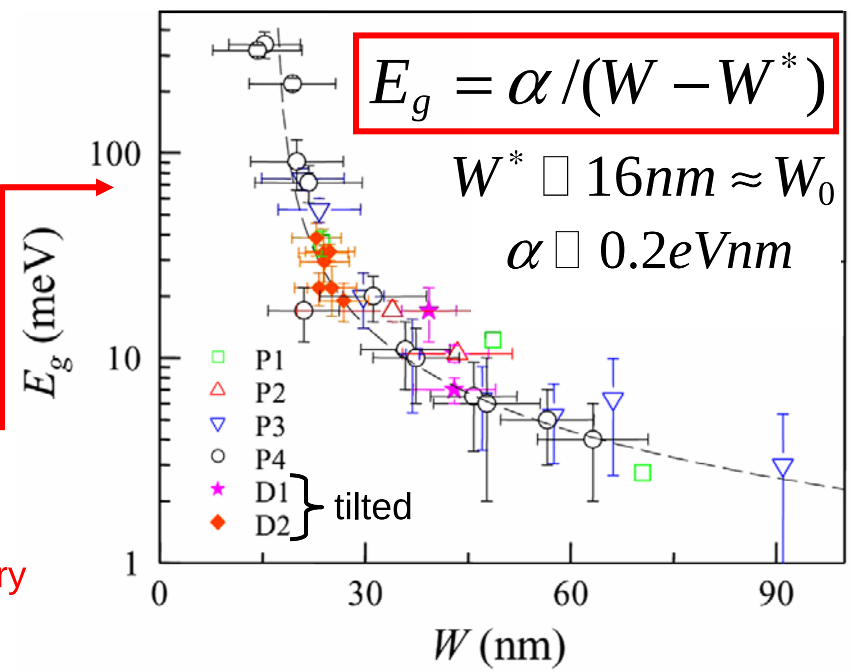


Inactive Widths:

$$W_0 \approx W^*$$

~16 nm

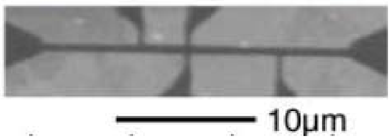
$G \sim \frac{e^2}{h}\frac{W}{L}$ from Theory



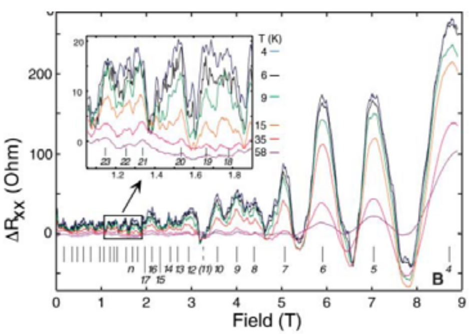
M.Y. Han, B. Özyilmaz, Y. Zhang, Ph.Kim: Phys. Rev. Lett. 98, 206805 (2007)

Graphene Nanoribbons: Electronic Confinement and Coherence from Magnetotransport

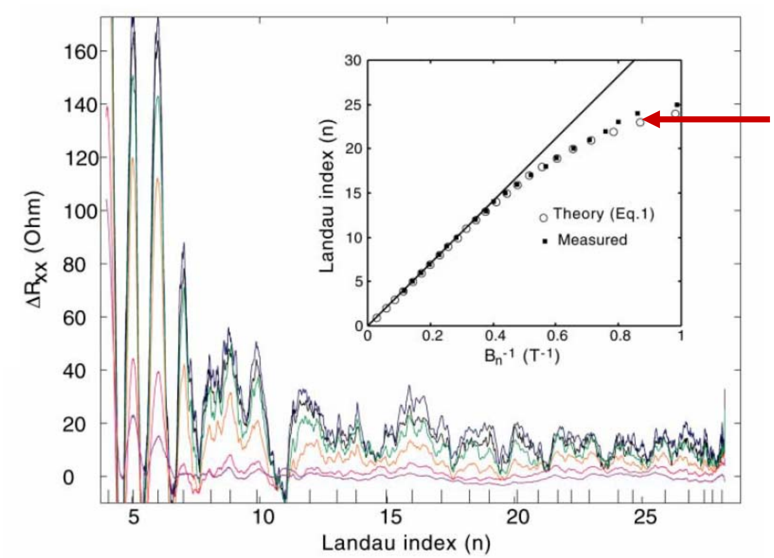
3 ML graphene on SiC(000-1)



Ribbon Width W=500nm



SdH Peaks



Landau Levels
in confining Ribbon:

$$E_n \approx \left[(n\pi\hbar v_0 / W)^4 + (2neBv_0^2\hbar)^2 \right]^{1/4}$$

Fit with $v_0 = 1\times10^8 \, cm/s$

$$W^* = 270nm \neq W$$

Dead Edge Region

From Analysis of
Universal Conduct. Fluctuations :

@ 2K: $l_\Phi \approx 1.1\mu m$

@ 58K: $l_\Phi \approx 430nm$

Claire Berger et al. : Science **312**, 1191 (2006)

Theoretical Challenges

– Multilayer Graphene with Dirac Cone (Dispersion)

- **Why growth of R30/R+/-2 decoupled layers on Si(000-1) ?**
  Graphene/SiC Interaction or Growth Kinetics
- **General Conditions for R30/R+/-2 Stacking Fault Growth ?**

– Surface and Edge Doping of Ribbons, Surface Chemistry in General

- **Chemistry and Doping Activity ?**
- **2D-doping and Dopant Deactivation ?**

– Edge Structure of Ribbons

- **Atomistic Structure and States of Disorder ?**
- **Electronic Edge States and 2D-Space Charge Zones ?**

– Coherent Transport In Ribbons

- **Type of Scattering ?**
- **Effect of Substrate ?**

OUTLINE

Semiconductor Nanowires

- Growth and Doping, Band Gap
- Electronic Transport
  - -Effect of Space Charge Layers
  - -Quantum Transport in Narrow Gap SC Wires

Theoretical Challenges

Graphene Ribbons

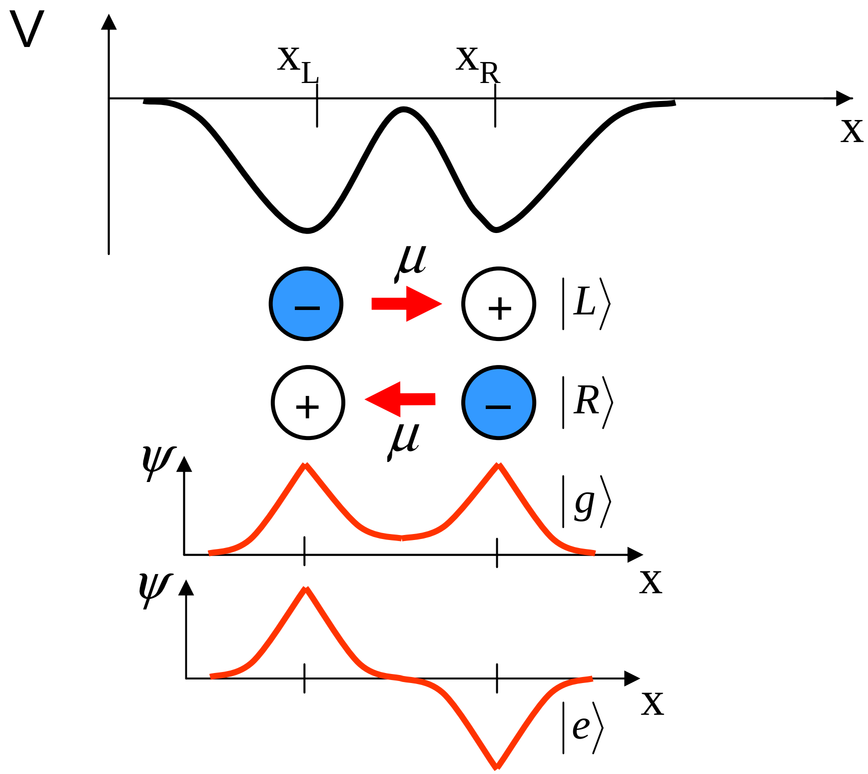
- General Properties, Doping
- Multilayer Stacks with Dirac Cone
- Dead Edge Region: Gap and Transport

Theoretical Challenges

Coupled Quantum Dots as Q-bit

Theoretical Challenges

Realisation of a Q-bit by 2 coupled Q-Dots



Q-bit = 2-level System:

$$\alpha |g\rangle + \beta |e\rangle$$

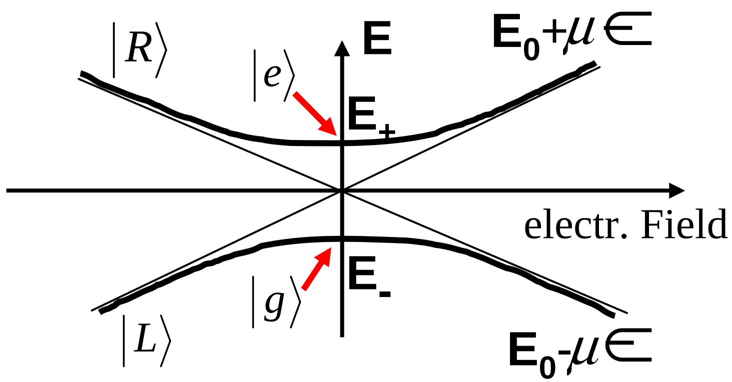
Superposition State
for $\in$ ~0

$$E_{\mp} = E_0 \pm \sqrt{t_{LR}^2 + \mu^2 \in^2}$$

t_{LR} is Tunnelling Amplitude between $|L\rangle$ and $|R\rangle$

Probability for Electron in $|R\rangle$:

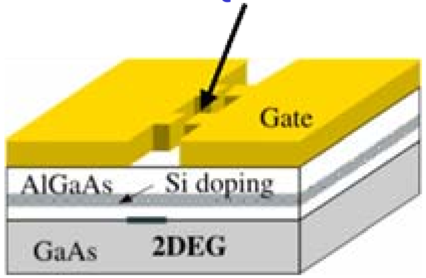
$$|c_R(t)|^2 = \sin^2(t_{LR} t / \hbar)$$

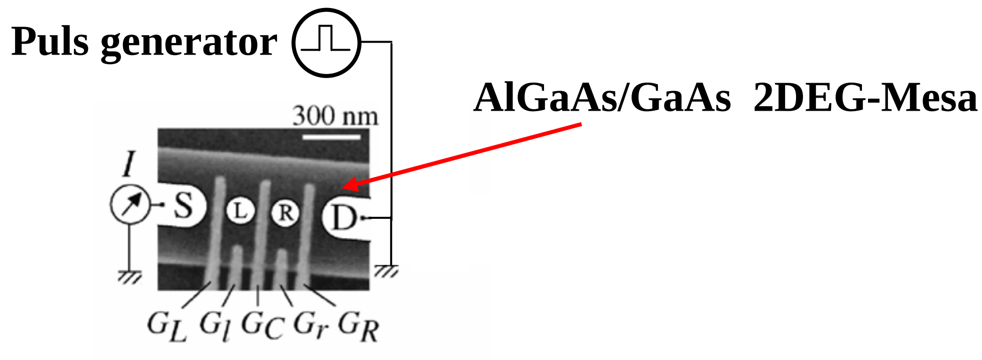


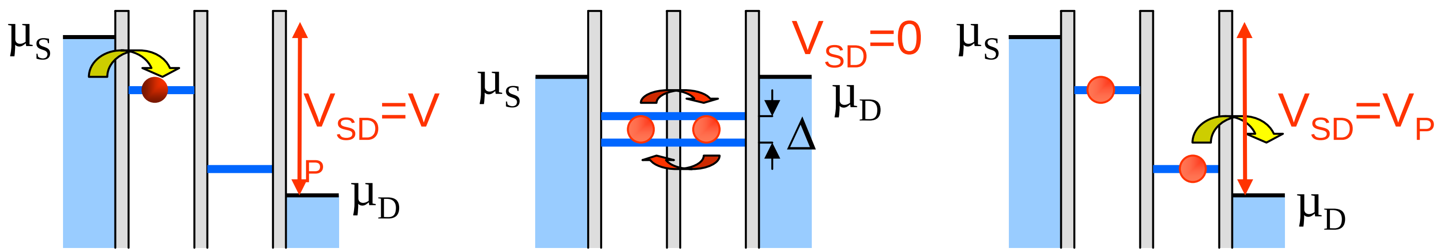
With increasing electric Field
$|\in|>0$
Preparation of
$|R\rangle$ or $|L\rangle$

Q-bit Realization: 2 coupled GaAs Qantum Dots

Split-gate Technique: Q-dot within 2DEG



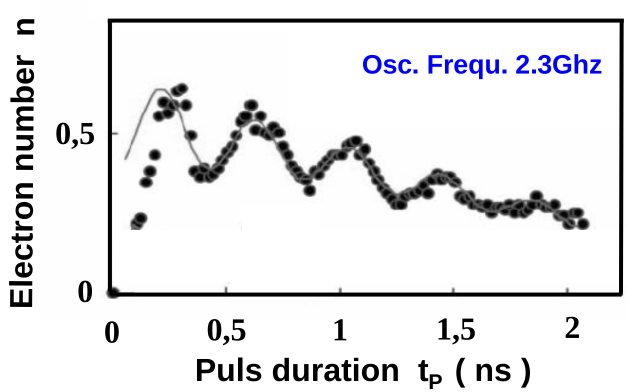




Preparation of $|L\rangle$

Q-bit Realisation (by puls t_p=80....2000ps)

Recording (after pulses t_p of variable duration time)



Dephasing time:
1 ns

Measurement contacts coupled electrically

T. Hayshi, T. Fujisawa, H.D. Cheong, Y.H. Yeong, Y. Hirayama: Phys. Rev. Lett. **95**, 090502-1 (2005)

Q-bit Realization: 2 coupled Si Quantum Dots in SOI

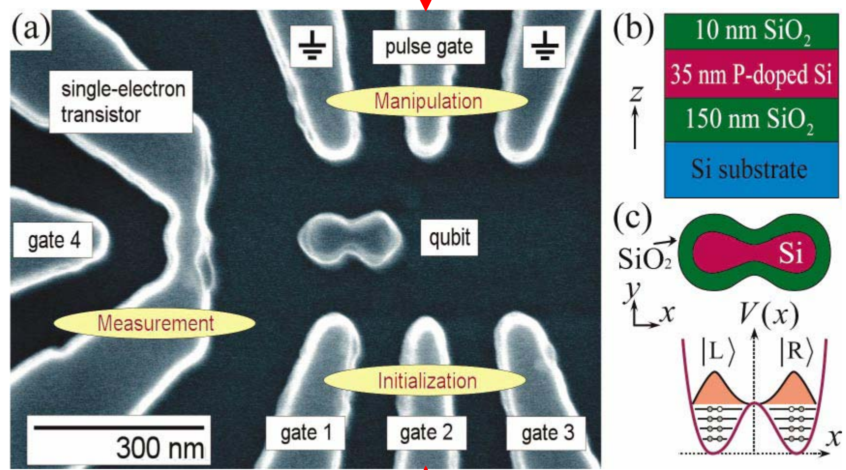
Pulse sequence:

1) Preparation of $|R\rangle$

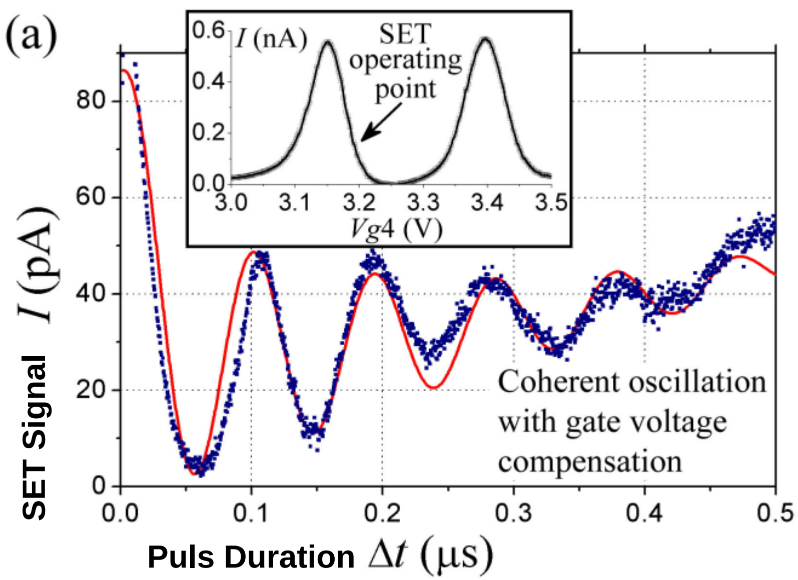
2) Q-bit Realization:
$$|R\rangle \pm |L\rangle$$

3) Measurement of $|L\rangle$

Manipulation in time domain



For preparation of $|L\rangle$ **or** $|R\rangle$



Dephasing time:
200 ns

SET coupled only via electric field!

J. Gorman, D.G. Hasko, and D.A. Williams : Phys. Rev. Lett. **95**, 090502-1 (2005)

Theoretical Challenges

– Decay of Superposition State (Q-bit)

- **Coupling of 2-state System to Environment (E) ?**
- **Dephasing time τ ?**

– General Description by Density Matrix $\hat{\rho}$

Q-bit: Superposition State $\left(\alpha|g\rangle + \beta|e\rangle\right)$

Time Development ($\hat{U}$ unitary) of Q-bit imbedded in Environment $|E\rangle$ leads to Entangled State:

$$\left(\alpha|g\rangle + \beta|e\rangle\right)|E\rangle \xrightarrow{\hat{U}} \underbrace{\alpha|g\rangle|E_0\rangle + \beta|e\rangle|E_1\rangle}$$

$$\hat{\rho} = |\alpha|^2 |g\rangle\langle g||E_0\rangle\langle E_0| + |\beta|^2 |e\rangle\langle e||E_1\rangle\langle E_1| + \alpha\beta^* |g\rangle\langle e||E_0\rangle\langle E_1| + \beta\alpha^* |e\rangle\langle g||E_1\rangle\langle E_0|$$

Only Q-bit is interesting: $\hat{\rho}_{red} = Tr_E\,\hat{\rho} = \begin{pmatrix} |\alpha|^2 & \alpha\beta^*\langle E_1|E_0\rangle \\ \beta\alpha^*\langle E_0|E_1\rangle & |\beta|^2 \end{pmatrix}$

Environment develops according to: $\langle E|E\rangle = 1 \xrightarrow{\hat{U}} \langle E_0|E_1\rangle = 0$

– Q-bit decays according to $\langle E_0|E_1\rangle \propto e^{-t/\tau}$

CONCLUSIONS

The great theoretical Challenges:

- Preparation, Doping and Electronic Bands
- Nano-Surface(Edge) Science
- Electronic (Qantum) Transport incl. Spin
- Dephasing of Superposition States