Surface State Dynamics Dictating Transport in InAs Nanowires

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Motivation

- Surface states induce scattering centers
  - Limit electron mobility
  - Prevent ballistic, phase coherence transport

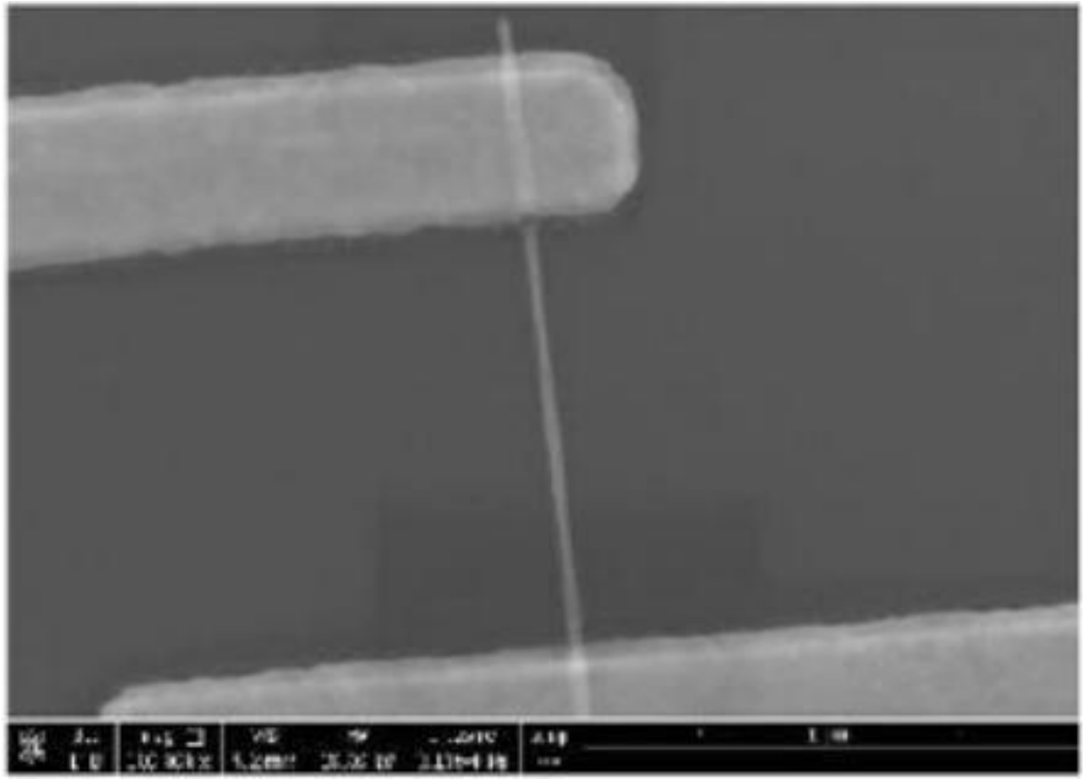
- Sidenote: Strong coupling to surface states can be used for catalysis and biochemical sensing

- Understand the interplay between microscopic interactions at the surface and macroscopic properties (e.g. electrical conductivity)

- Invesigation of the nonequilibrium carrier population dynamics
  - Hysteretic and dynamic behaviour in response to an electric potential

Device

- MBE grown InAs nanowires (20 – 50 nm diameter)
- Substrate: p-doped Si with 100 nm SiO2 serving as a global backgate
- Ti/Au source and drain contacts (1.6 µm apart)
  - Nanowire Field Effect Transistor (NW FET)
- Measurements performed in a cryostat (10 – 300 K)



$G - V_g$ Hysteresis I

- All measured NW FETs showed similar hysteresis behaviour at RT
    - Higher conductance for positive scan direction
    - Lower conductance for negative scan direction

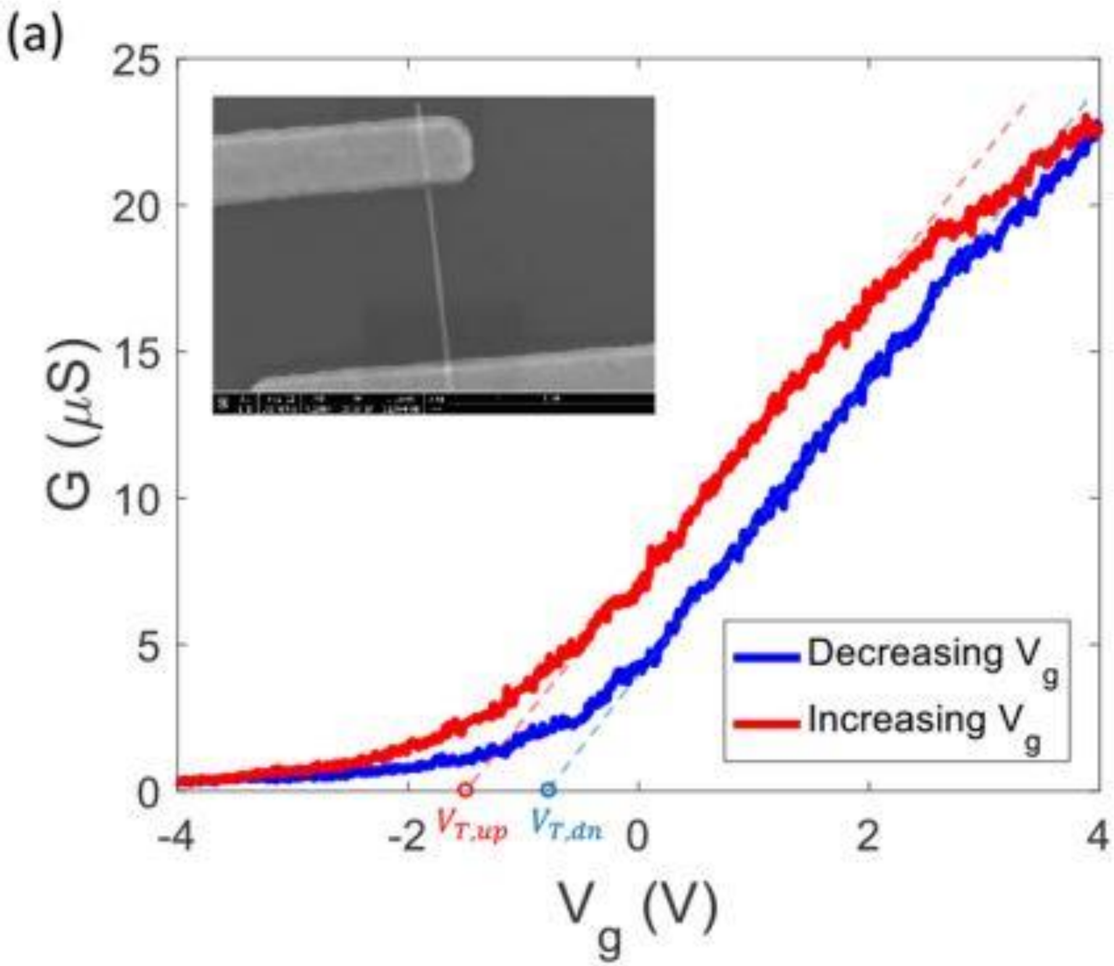
➢ Occurs due to trap states with similar capture and emission rates as the sweep rate

- Emission of electrons from traps causes faster depletion of free electrons by V_g -> lower free carrier density compared to equilibrium $n_{dn}(V_g) < n_0(V_g)$

- Free carrier density can be estimated via V_T by

$$n = \frac{(V_g - V_T)\,C_{ox}}{e}$$

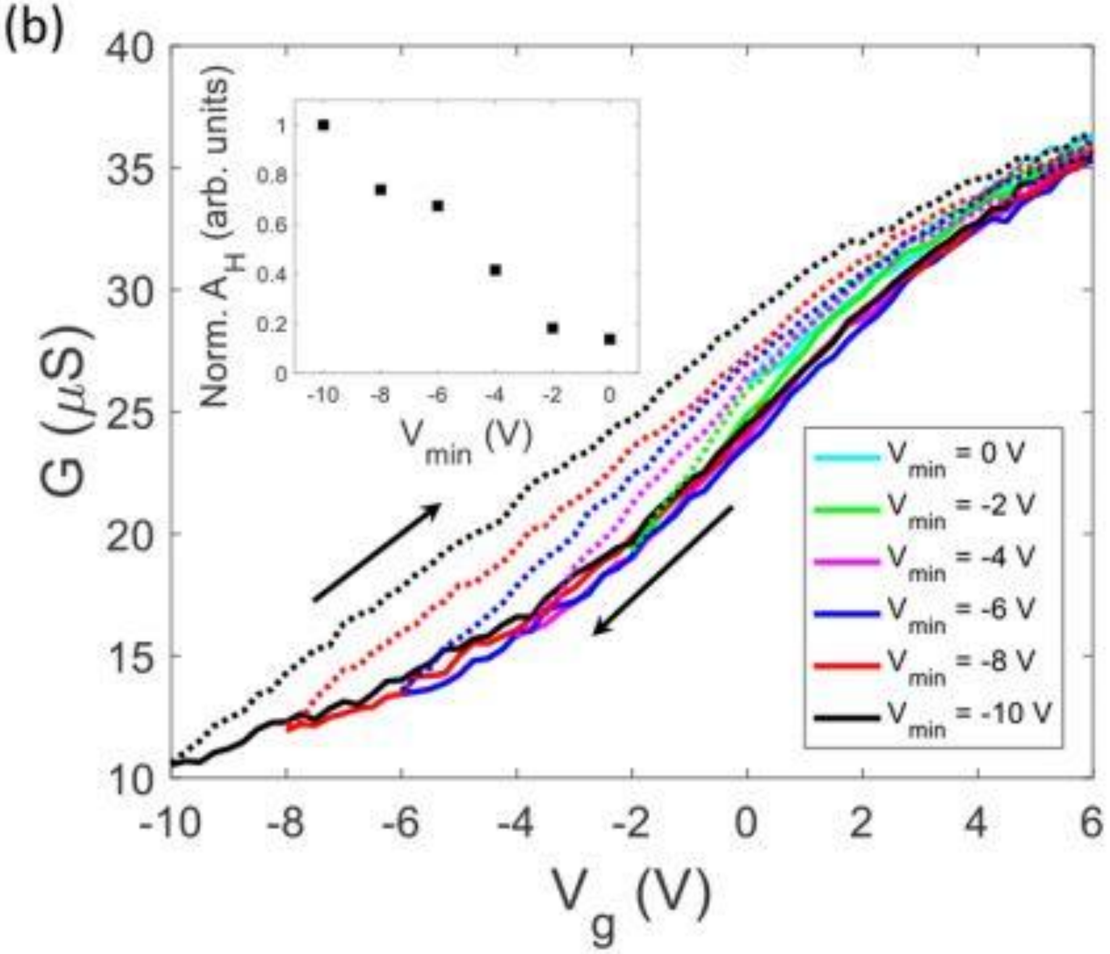
- Because $V_{T,up} < V_{T,dn} \Rightarrow n_{up}(V_g) > n_{dn}(V_g)$



$G \; - V_g$ Hysteresis II

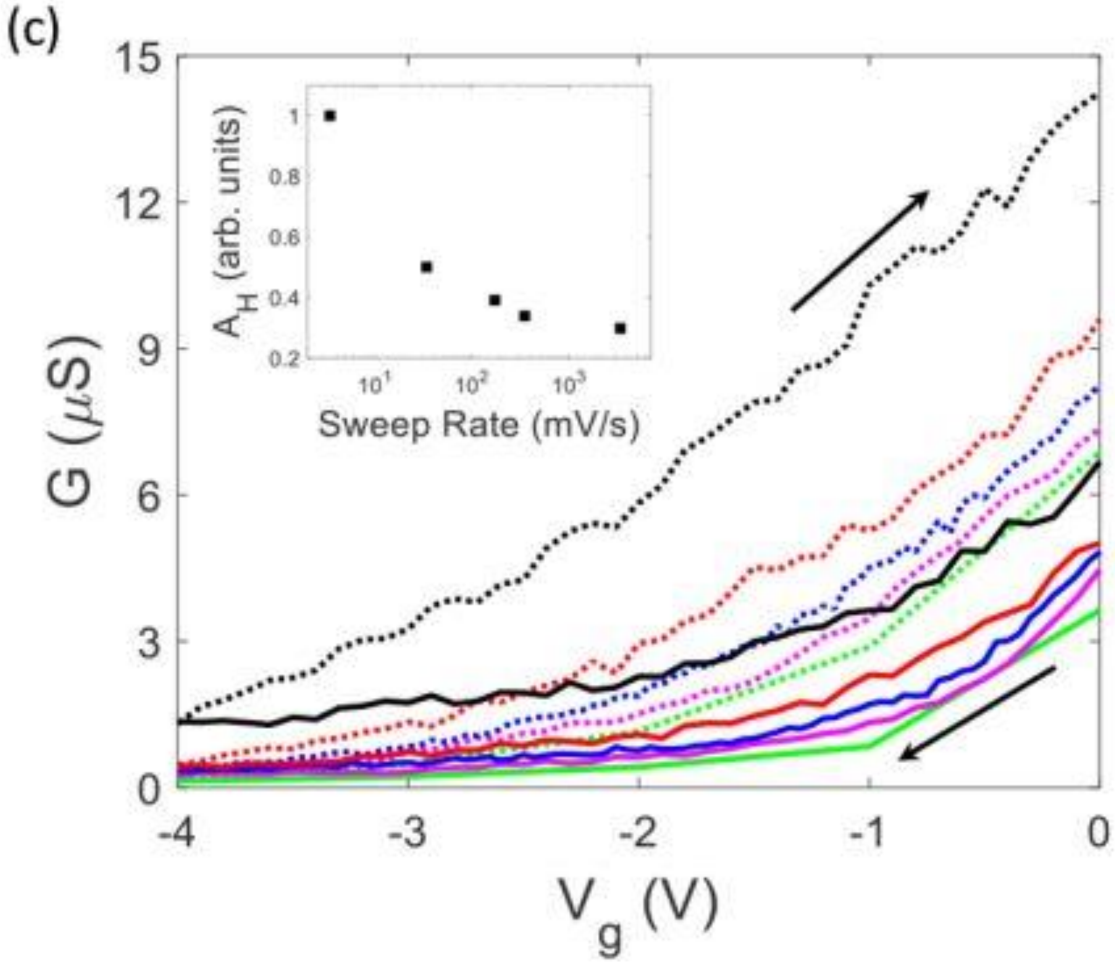
- Definition: $A_H = \int (G_{up} - G_{dn})\, dV_g$
- Results in reproducible trends independent of channel length or wire diameter
- Here: V_g was swept from 6 V to V_{min}, then back to 6 V at a constant sweep rate
- Inset: Normalized hysteresis $A_H/(6 - V_{min})$ increases with decreasing V_g

➢ Attributed to activation of lower lying trap states (deep states) due to the relatively low Fermi level



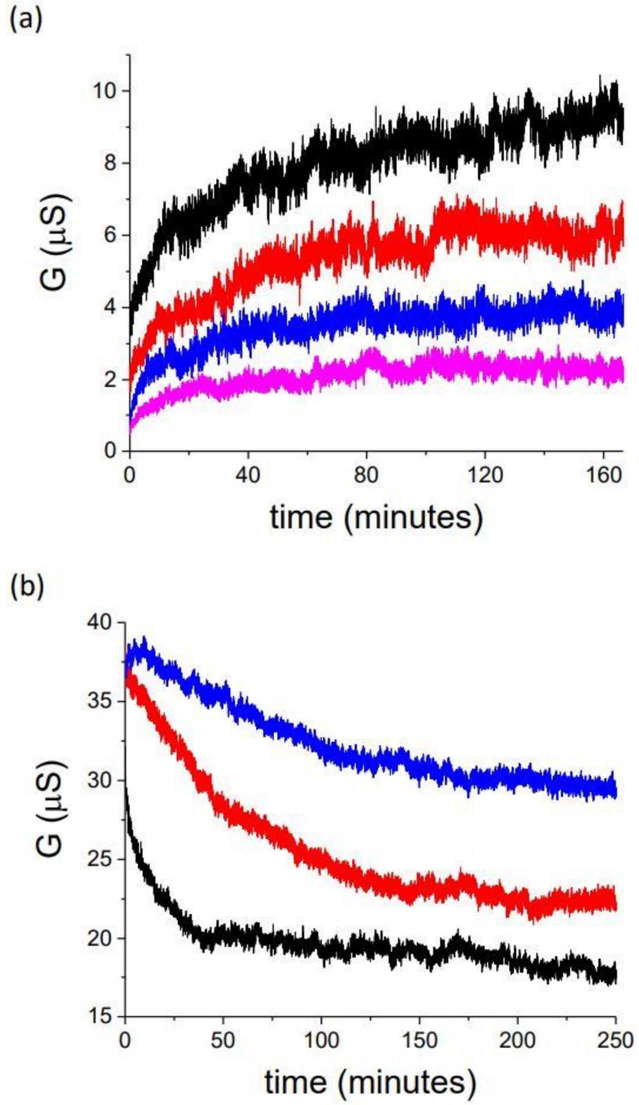
$G - V_g$ Hysteresis III

- Room temperature V_g sweeps in the subthreshold regime with several different sweep rates
- Hysteresis increases with decreasing sweep rate
- ➢ Indicates existence of deep trap states with long time constants (minutes to hours)
- In contrast to previous measurements (slow sweep rates supress hysteresis [1,2])
  - Difference is in the use of ZrO2/Y2O3 as a local gate dielectric and as a passivating layer
  - Modifies the native oxide and eliminates these surface traps
- Further: SiO2 gate oxide also provides slow trap states [3]



[1] Dayeh *et al.*, Appl. Phys. Lett. **90** (2007)
[2] Chobpattana *et al.*, Appl. Phys. Lett. **104** (2014)
[3] Shen *et al.*, Sci. Rep. **5** (2015)

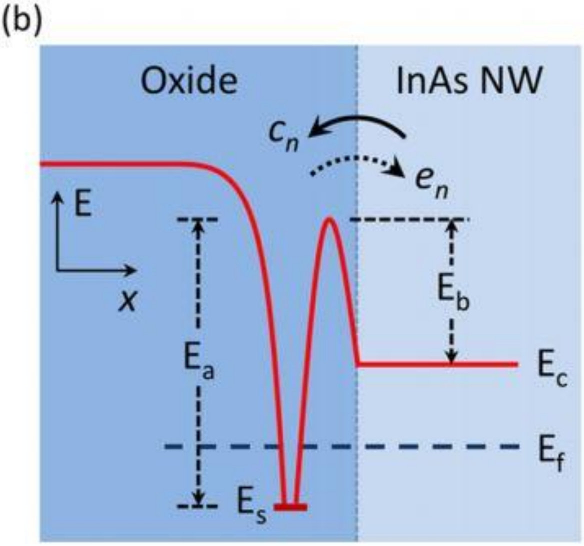
Long Term Shifts in Conductance



- Note the shift in conductance at $V_g = 0$
- Investigation of the gate voltage pulse transient response (both negative (a) and positive pulses (b))
- Initialize at V_0 for 24 h, then pulse to V_i at $t = 0$
- Results are time constants on the order of hours and nonexponential time dependence
  - Probably due to a mixing of different traps with multiple time constants
- Consistent with previous measurements [4]

[4] Astromskas *et al*., Appl. Phys. Lett. **98** (2011)

Spectral Distribution of InAs NW Trap States I



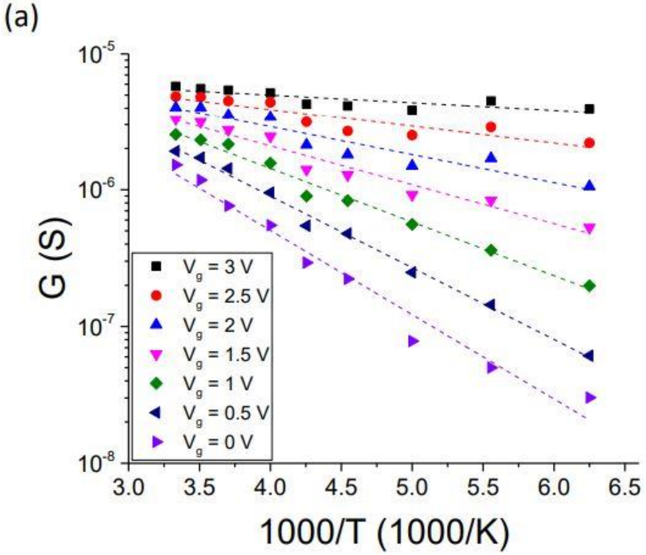
- Extract the spectral distribution of InAs NW trap states active in a given time intervall from gate voltage dependence of the conductance activation energy

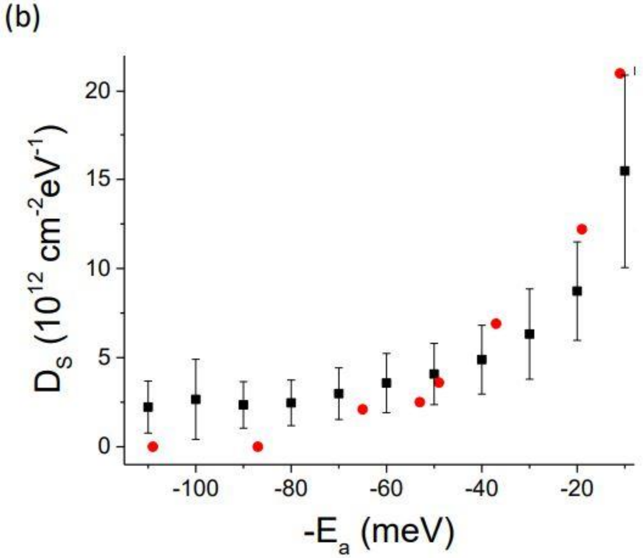
$$E_a \approx E_c + E_b - E_s$$

$$D_s(E_a) = \frac{C_{ox}}{2e^2\pi R}\left[\left(-\frac{dE_a}{e\ dV_g}\right)^{-1} - 1\right]$$

- Shows agreement with previous studies (red dots) [5]

➢ Direct interpretation not strictly feasable, not all traps have the same capture barrier E_b due to their nonequilibrium dynamics





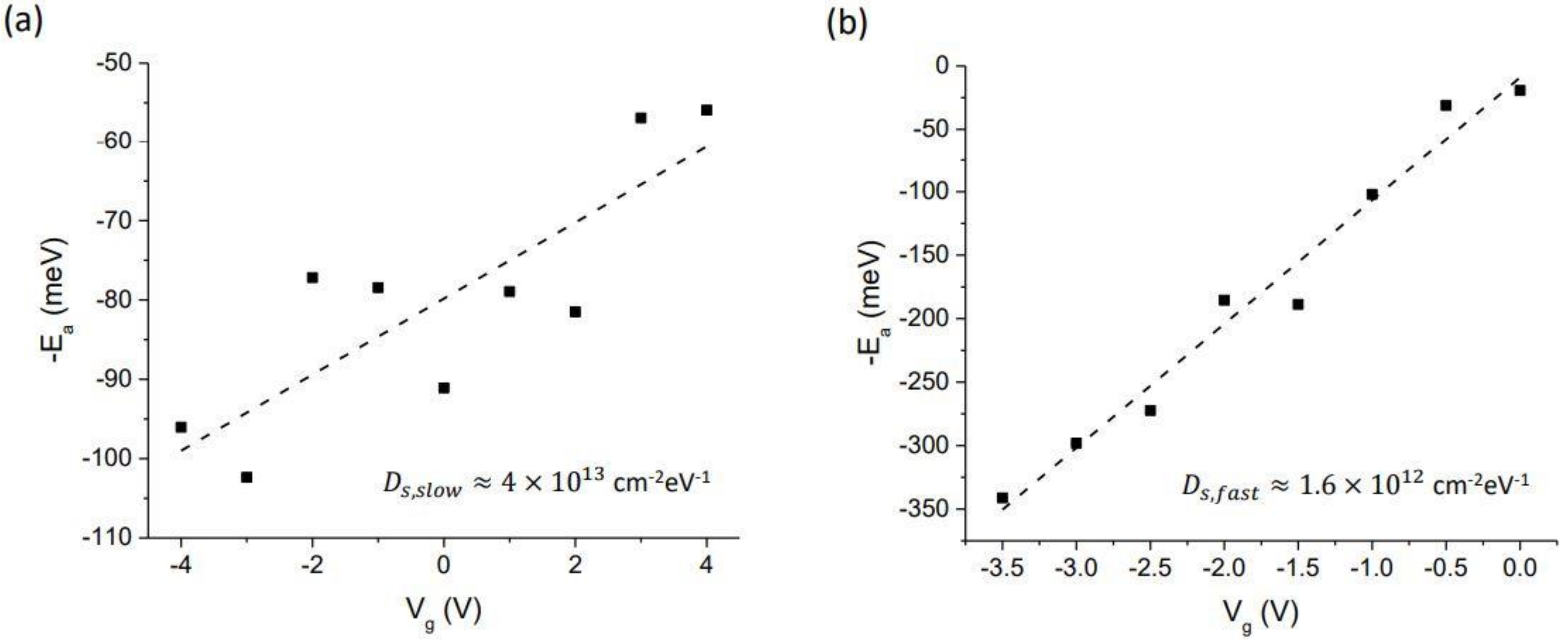
[5] Halpern *et al.*, Appl. Phys. Lett. **100** (2012)

Spectral Distribution of InAs NW Trap States II

- It is possible to extract the average trap density from the linear regime of $E_a - V_g$ curves
- Here $D_{s,slow}$ (2 h) is **25 times greater** than $D_{s,fast}$ (5 min)

➢ Indicates a significantly higher trap density with slower time constants

➢ Electrical properties vary strongly depending on the dynamic conditions of the measurement

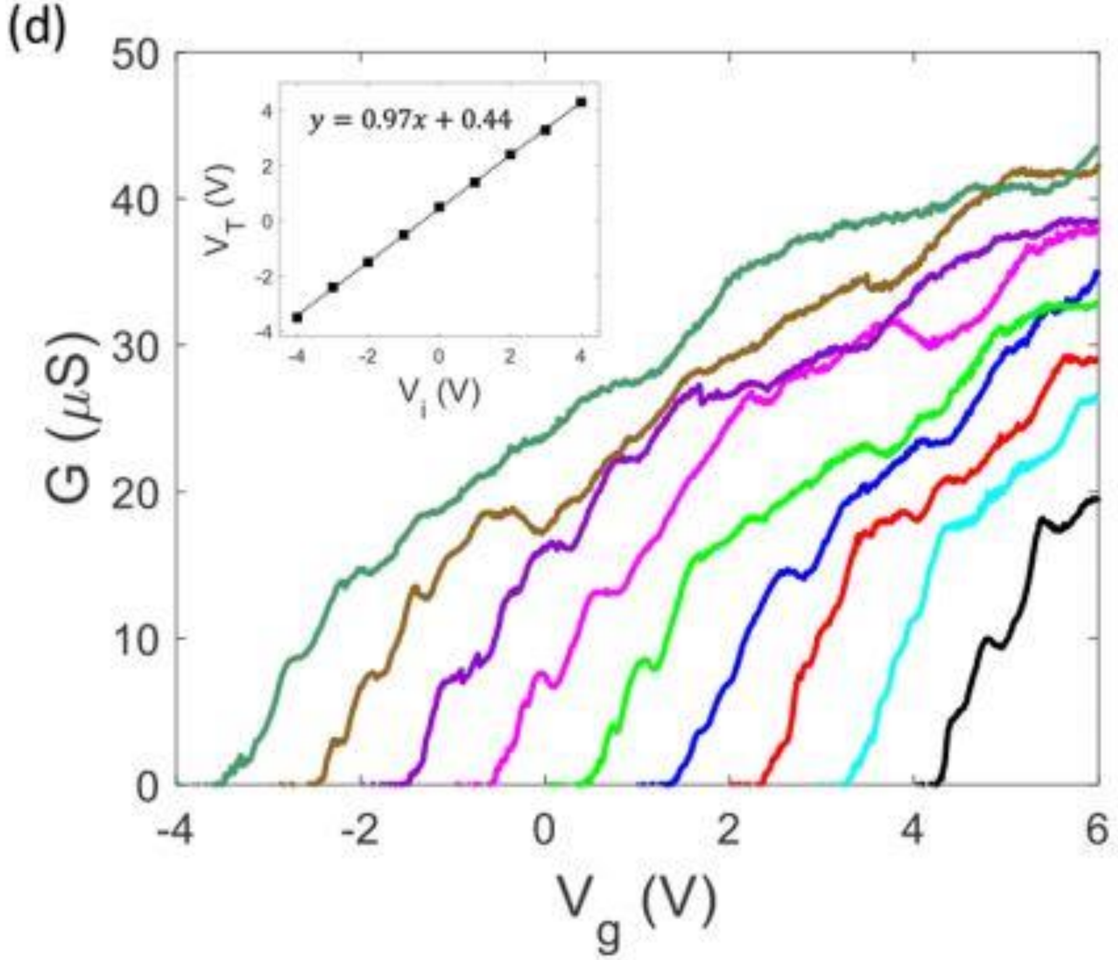


Thermal Dependence

- Initialize $V_i = V_g$ at RT, then cool down to 10 K and measure $G - V_g$ characteristics
    - negligible amount of hysteresis observed

- V_T directly proportional to V_i and the charge fixed in the NW

➢ Most surface traps are deactivated
    - emission and capture barrier height $\gg kT$
    - V_T is determined by electrostatic history of the NW



$$n = \frac{(V_g - V_T)\, C_{ox}}{e}$$

Time-Dependent Transport Model I

- In gated NW devices $Q_{tot} = Q_{free} + Q_{fixed} + Q_{gate} = 0$

$$n - p - N_D^+ + N_A^- - \frac{C_{ox} V_g}{e} + C_{ox}\left(\frac{E_f - E_{f0}}{e^2}\right) = 0$$

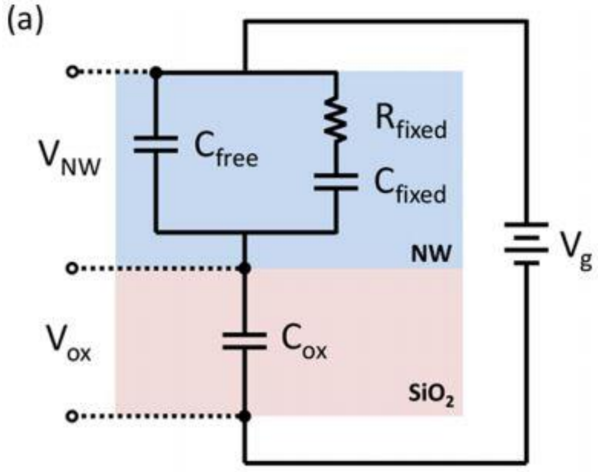
- In order to determine E_f, insert known distribution for $N_s^{\pm} = 2\pi R \int D_s(E) f_s(E) dE$
  - ➢ Result is a solution for the equilibrium case

- Have to use a rate equation describing the time evolution of the probability of occupancy of an individual trap state $f_s(E)$

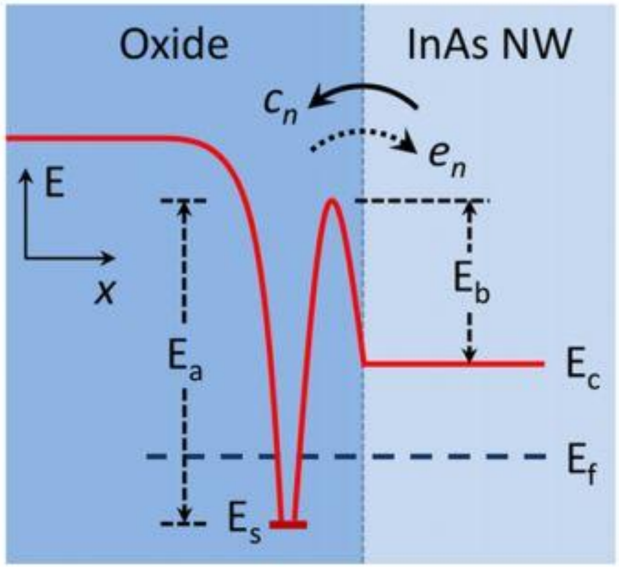
$$\frac{\mathrm{d}f_s(E)}{\mathrm{d}t} = \underbrace{2\gamma[1 - f_s(E)]\exp\left[\frac{-(E_c + E_b - E_f)}{kT}\right]}_{\text{capture}} - \underbrace{\gamma f_s(E)\exp\left[\frac{-(E_c + E_b - E_s)}{kT}\right]}_{\text{emission}}$$

➢ Include many trap states ($D_s(E)$) and numerically solve for E_f and nonequillibrium $f_s(E)$

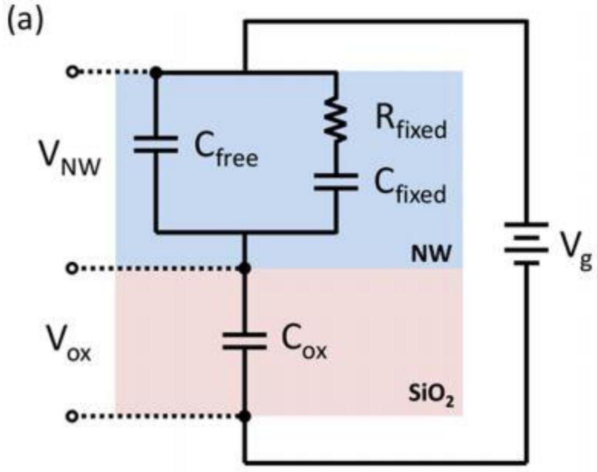
(a)



(b)



Time-Dependent Transport Model II

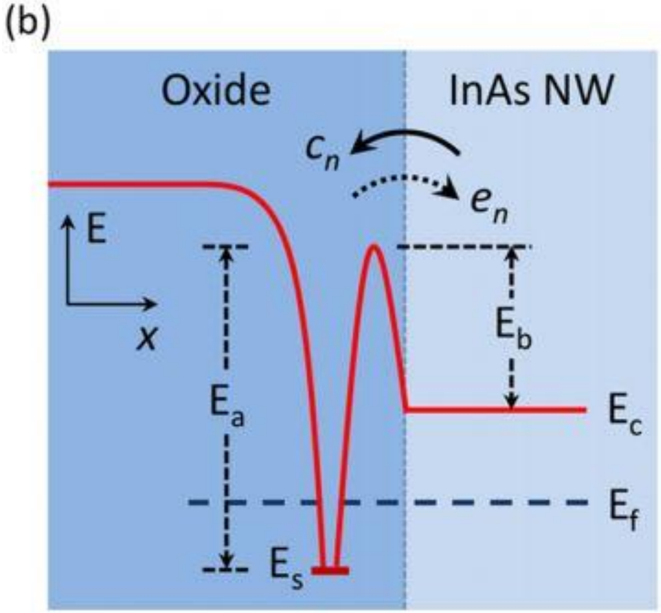


- Electron mobility μ scales inverse to the number of scattering centres

$$G \sim n\mu \sim \frac{n}{N_D^+ + \alpha N_A^-}$$

➢ This model now allows for fast simulations of trends in $G - V_g$ characteristics

- Investigation of
  - Surface trap dynamics
  - Surface trap properties



$G - V_g$ Characteristics I

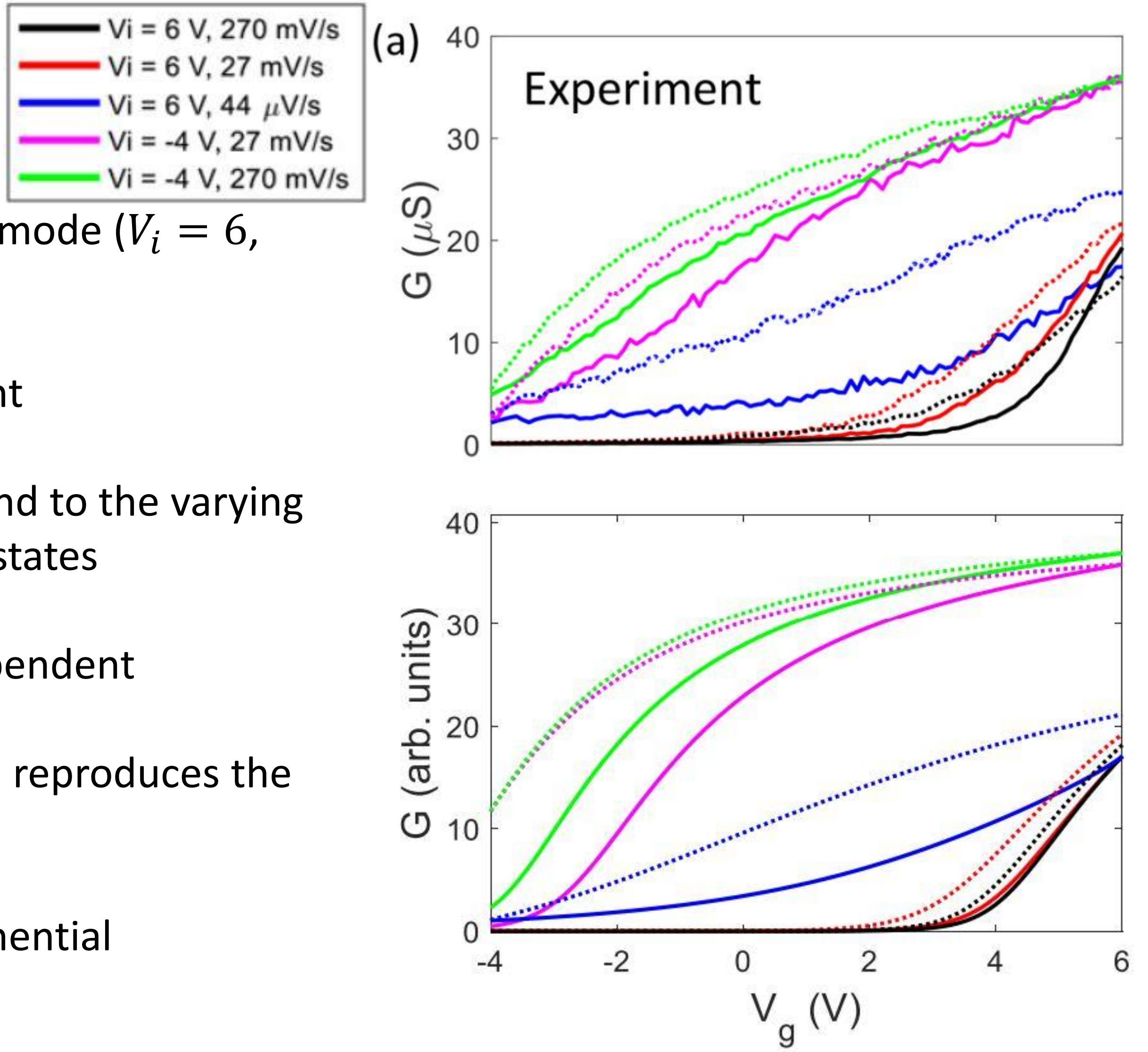
- Initialize V_i and sweep with different speeds
- Depending on the electrostatic history, the NW FET changes from depletion ($V_i = -4$, $V_T < 0$) to enhanced mode ($V_i = 6$, $V_T > 0$)

➢ Slow trap states are inactive during the fast measurement

- At slow sweep rates, slow trap states have time to respond to the varying gate potential, leading to a higher density of active trap states

➢ Shows the system is far from equilibrium and is time dependent

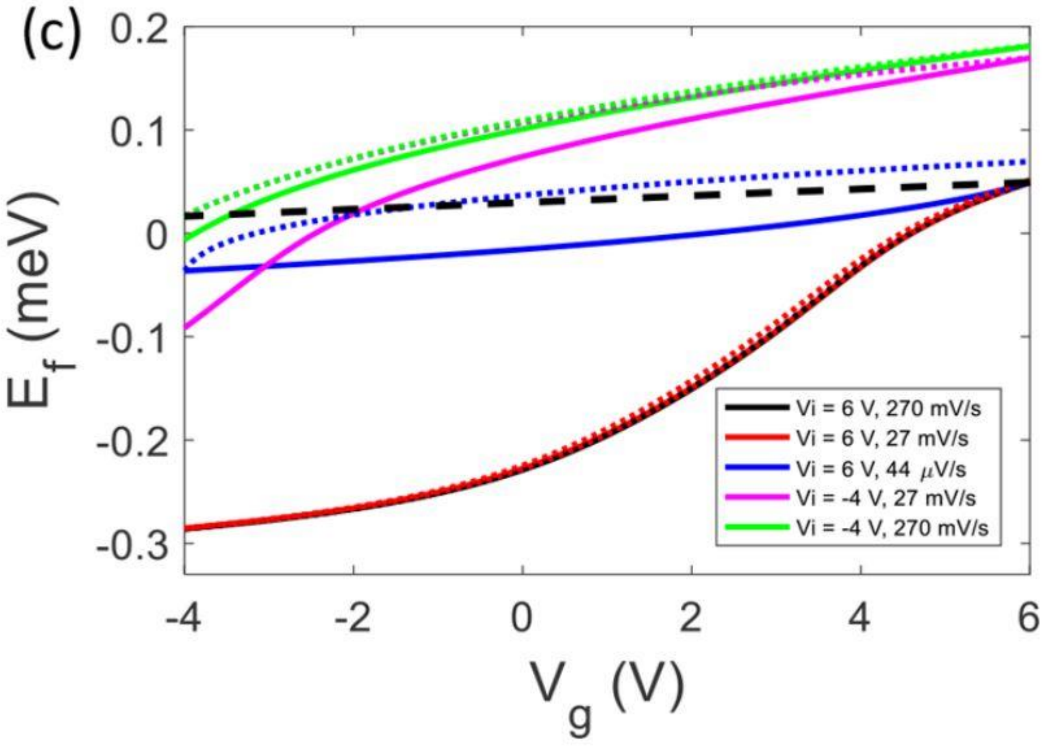
- Model assumes both acceptor and donor trap states and reproduces the experiments with two activation energies E_a
- Some histeresis effects can be reproduced with an exponential distribution of E_a, but others are then exaggerated

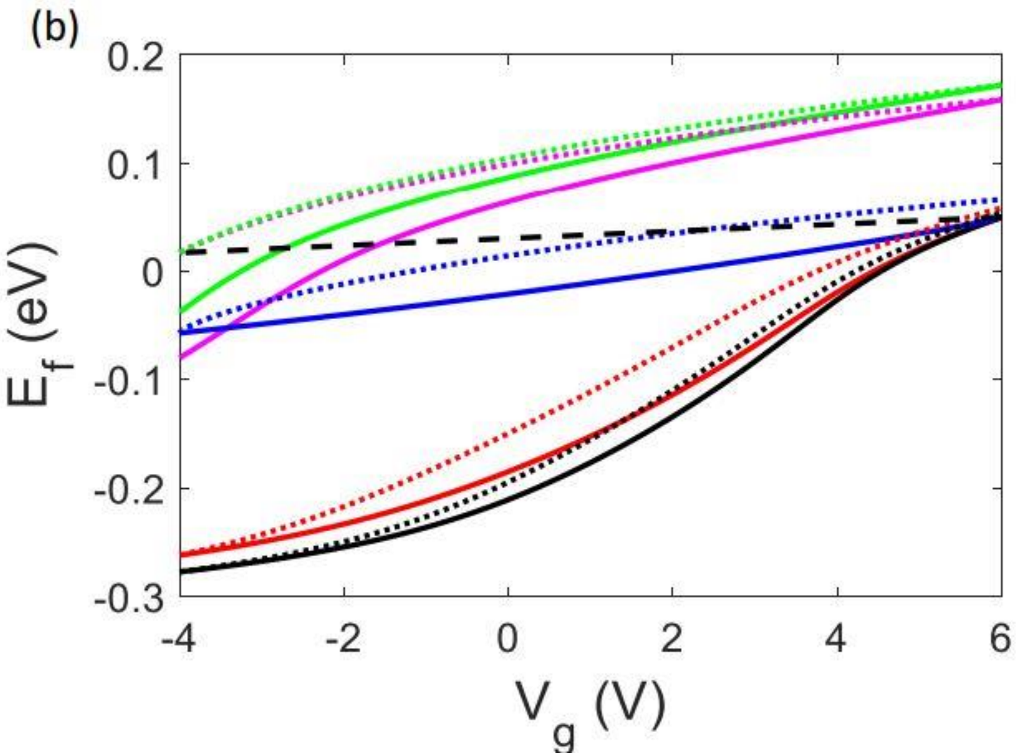


$G - V_g$ Characteristics II

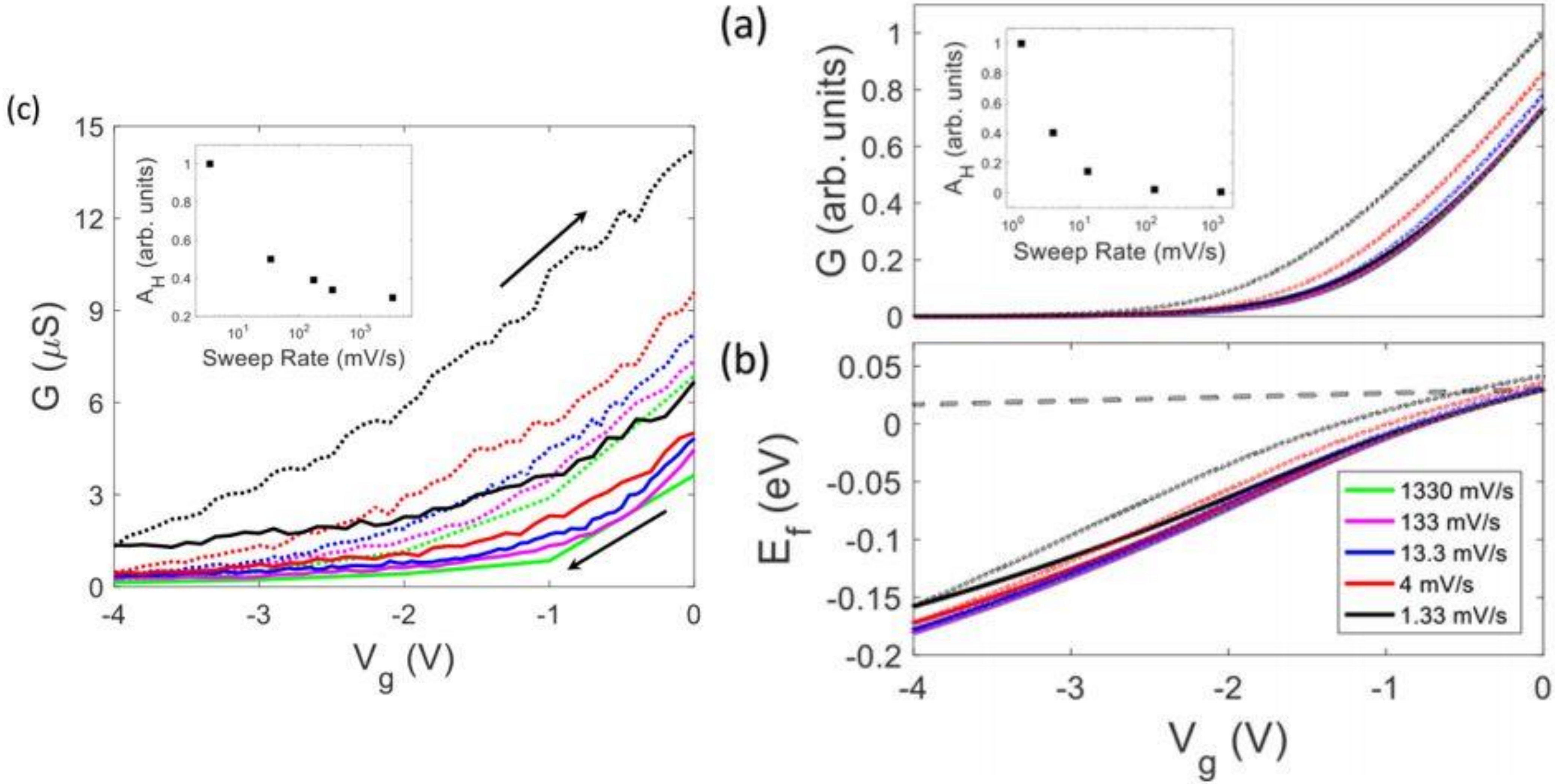
- Calculated Fermi levels show large discrepancy from equilibrium

➢ Characteristics cannot be reproduced with an equilibrium model

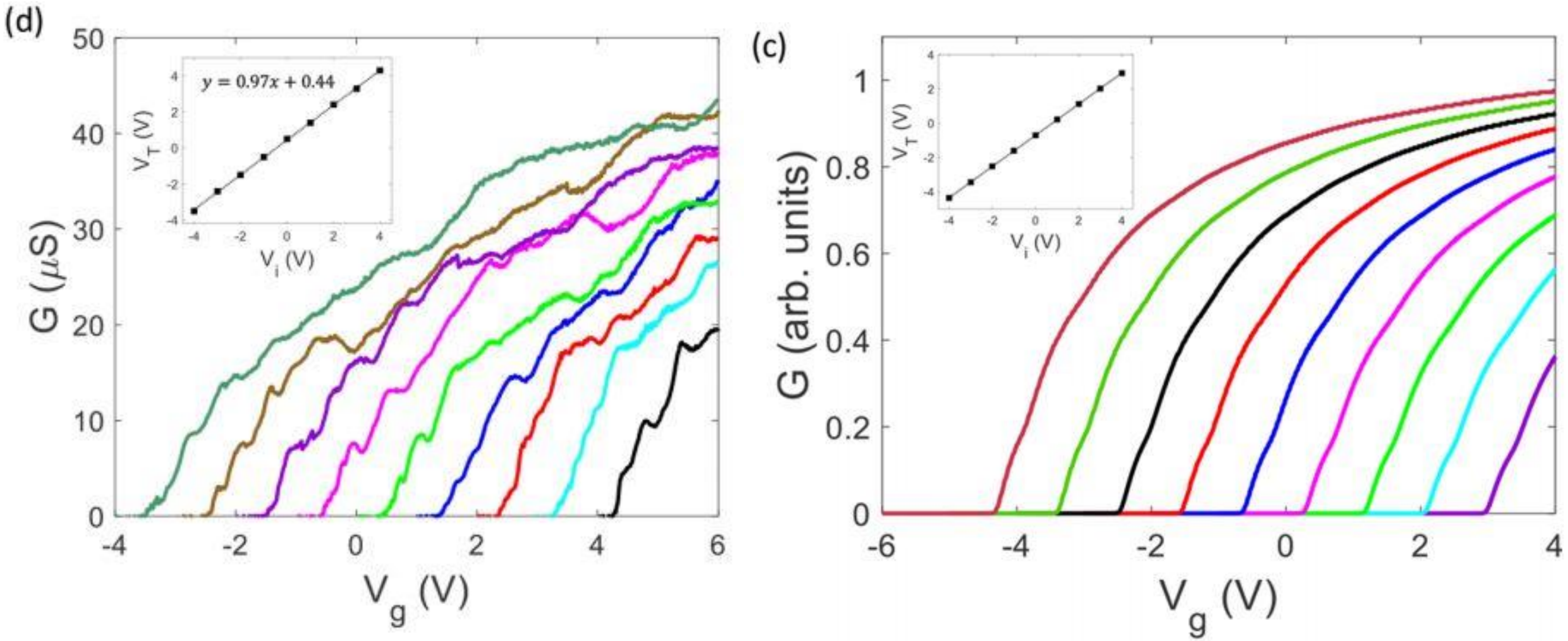




$G - V_g$ Characteristics III



$G - V_g$ Characteristics IV



Conclusion and Outlook

- Demonstration of the significance of nonequilibrium surface trapping dynamics in InAs NW
- Key characteristics are dependent on the V_g sweep rate and history
- Reason are surface trapping states with multiple capture and emission time constants
- Traps show thermally activated character with effects on the NW $G - V_g$ characteristics
- Development of a time dependent model with good agreement with the experimental data
- Clear and direct link between microscopic processes at the surface and macroscopic electrical conductivity
- Possible future use
    - Biological sensors
    - quenching of quantum interference effects and phase decohering scattering events