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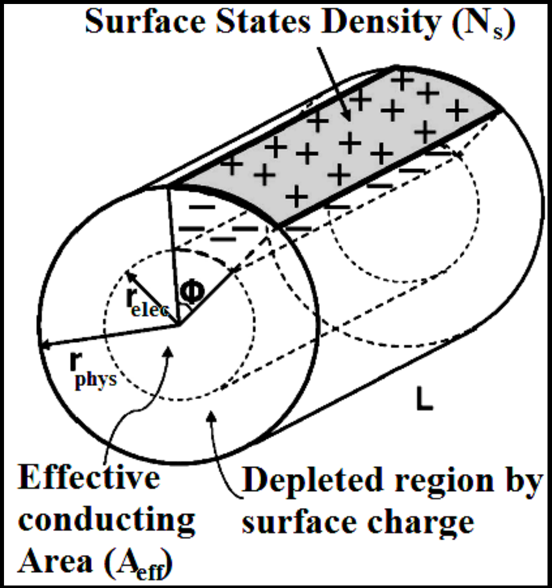
MODEL FOR CALCULATING THE DENSITY AND RESISTIVITY OF SURFACE STATES IN N-DOPED GAAS NANOPILLARS

Outline

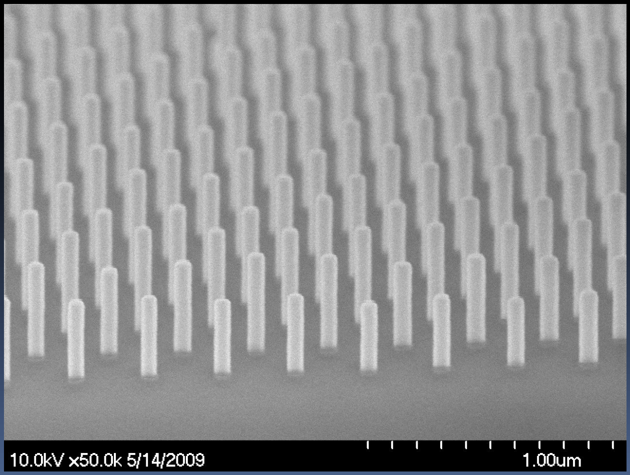
- Objective
- Motivation
- Background
- Approach
- MATLAB Model
- Device Fabrication
- Experimental Results
- Summary

Objective

- At the nanoscale, negligible effects on a semiconductor’s electrical properties such as surface states become significant
    - Large surface area-volume ratio
- The existence of surface states dramatically changes the overall doping profile of a nanopillar
- The effective radius of a pillar decreases and changes the conductive size
- By studying resistivity and taking into account the changes due to surface states, we can estimate the actual surface state density on a nanopillar



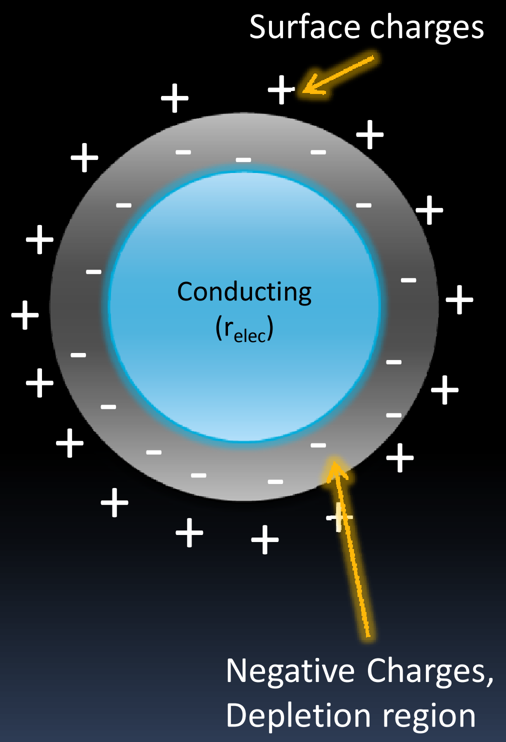
K. Seo *et al.* "Surface charge density of unpassivated and passivated metal-catalyzed silicon nanowires." Electrochemical and Solid-State Letters, 2006, Issue 3, Vol. 9.



Motivation

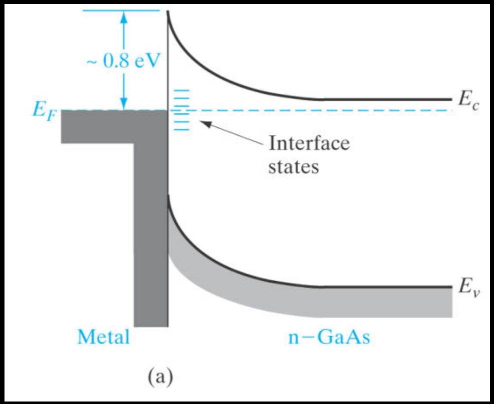
- Would like to ideally determine the surface state density N_S
- Surface state reduction techniques such as passivation need accurate measurements
- An effective, easy and simple way to determine N_S is desired
- Ability to determine density using easily taken or already existing IV measurements

Background – Surface States



- Surface states occur due to abrupt transition between solid material to outside
    - Periodicity of lattice is interrupted
    - Creates energies in the forbidden band gap of material
- Opposite charges are created within material to balance out surface charges
    - Creates a depletion region
- Transport is not available within the depletion region, effectively electronically “shrinking” the pillar

Background – Surface States



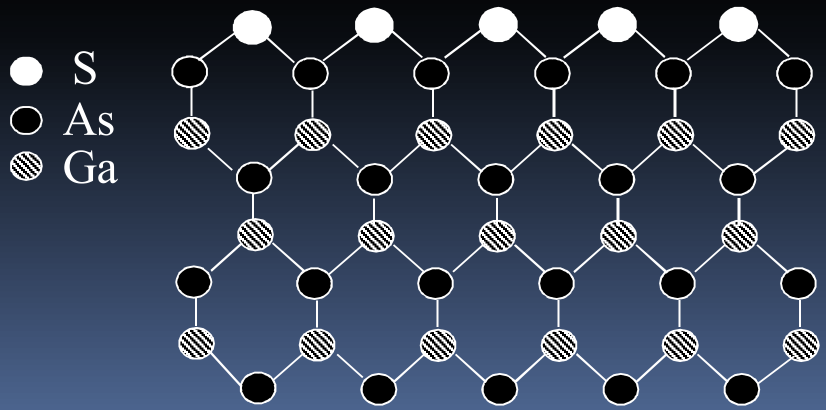
Pinned Fermi level at metal-GaAs contact

Banerjee, Sanjay and Streetman, Ben., "Solid State Electronic Devices." Upper Saddle River, NJ : Pearson Education, Inc, 2006.

- Detrimental effects of surface states
  - Energy bands within bandgap
  - Create carrier trapping centers
  - Lowers effective carrier concentration
    - Depletes the pillar - hinders carrier transport
  - Pins the Fermi level, bending conduction and valence bands
    - Creates a high Schottky barrier regardless of contact

Background - Passivation

- Passivation reduces the surface state density
- Uses replacement atoms to bind to vacancies created by the abrupt change in periodicity of lattice
- Dangling bonds are “capped” and thus charges are lessened, decreasing N_S
- Accomplished with a sulfuric solution
  - High chemical affinity between GaAs and sulfur



Approach

- Considering two radii, one physical r_{phys} and one decreased by the depletion region r_{elec}, we model the "effective" radius
- Begin with Poisson's equation

$$\nabla^2\psi(r) = -4\pi\rho$$

- Put into cylindrical coordinates

$$\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{\partial^2\psi}{\partial z^2} = -4\pi\rho, \quad \psi = \psi(r,z)$$

Approach

- Assuming abrupt transition in charge density ρ at radius, potential ψ within nanopillar becomes

$$\rho = \begin{cases} 0 & 0 \le r < r_{elec} \\ q(N_D - N_A), & r_{elec} \le r \le r_{phys} \end{cases}$$

$$\psi(r) = \begin{cases} \psi_0 & 0 \le r < r_{elec} \\ \psi_0 - \frac{\rho}{4\varepsilon_G}\left(r^2 - r_{elec}^2\right) & r_{elec} \le r \le r_{phys} \end{cases}$$

- And thus the surface potential becomes

$$\psi_s = \psi_0 - \frac{\rho}{4\varepsilon_G}\left({r_{phys}}^2 - r_{elec}^2\right)$$

Schmidt et al., Applied Physics A 86 187 (2007)

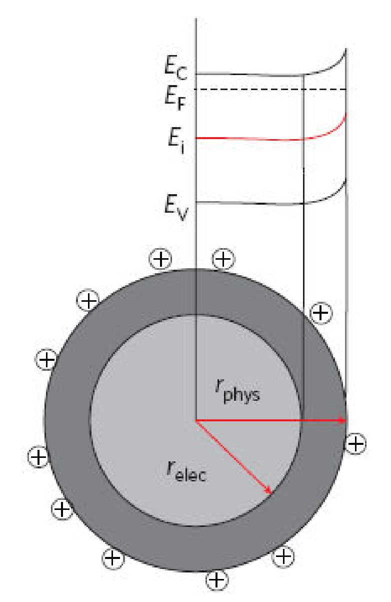
Approach

- Using charge neutrality, we find that the difference between the surface potential and the charge density below the surface must be zero

$$\pi\left(r_{phys}{}^{2} - r_{elec}^{2}\right)\rho + 2\pi r_{phys}\left(Q_f + Q_{it}\right) = 0 \qquad Q_{it} = -q^2 N_s \psi_s$$

- When solved for r_{elec} , we see that

$$r_{elec} = \sqrt{r_{phys}{}^{2} + \frac{2r_{phys}Q_f - 2r_{phys}N_s\psi_0}{q(N_D - N_A)\left(1 + \frac{r_{phys}q^2}{2\varepsilon_G}N_s\right)}}$$



M. T. Bjork, *et al.* "Donor deactivation in silicon nanostructures." Nature Nanotechnology, 2009, Vol. 4.

Approach

- Next, we must define a critical radius a_{crit} which determines if the pillar is depleted or not, when r_{elec} goes to zero

$$a_{crit} = \frac{\varepsilon_G}{q^2 N_S}\left\{-1+\left[1+\frac{4q^2N_S}{\rho\varepsilon_G}\left(q^2N_S\psi_0-Q_f\right)\right]^{\frac{1}{2}}\right\},$$

$$\approx \frac{2}{\rho}\left(q^2N_S\psi_0-Q_f\right)$$

Schmidt et al., Applied Physics A 86 187 (2007)

Approach

- Depending if our physical radius is below or above the critical radius, we find the effective carrier concentration to be

$$n_{eff} = n_0 \exp(\beta\psi_0)\left\{\frac{r_d^2}{a^2} + \frac{4\varepsilon_s}{\beta\rho r_{phys}^2}\left[1 - \exp\left(\beta\,\frac{\rho}{4\varepsilon_G}\left(r_{elec}^2 - r_{phys}^2\right)\right)\right]\right\}, \boldsymbol{r_{phys} > a_{crit}}$$

$$n_{eff} = n_0 \exp(\beta\psi_s)\,\frac{4\varepsilon_s}{\beta\rho r_{phys}^2}\left[\exp\left(\beta\,\frac{\rho r_{phys}^2}{4\varepsilon_G}\right) - 1\right], \boldsymbol{r_{phys} < a_{crit}}$$

Schmidt et al., Applied Physics A 86 187 (2007)

Approach

- Finally, we can relate this effective carrier concentration with resistivity via the mobility

$$\rho = \frac{1}{q\mu_k n_{eff}}, \quad \mu_k = \frac{\mu_0}{1 - \sqrt{\frac{n_{eff}}{10^{18}}}},$$

$$where\ \mu_0 = 8500\frac{cm^2}{Vs}\ (n - type)$$

- And given resistance from measured I-V curves

$$R = \frac{\rho L}{A_e}, \quad where\ A_e = \pi r_{elec}^2$$

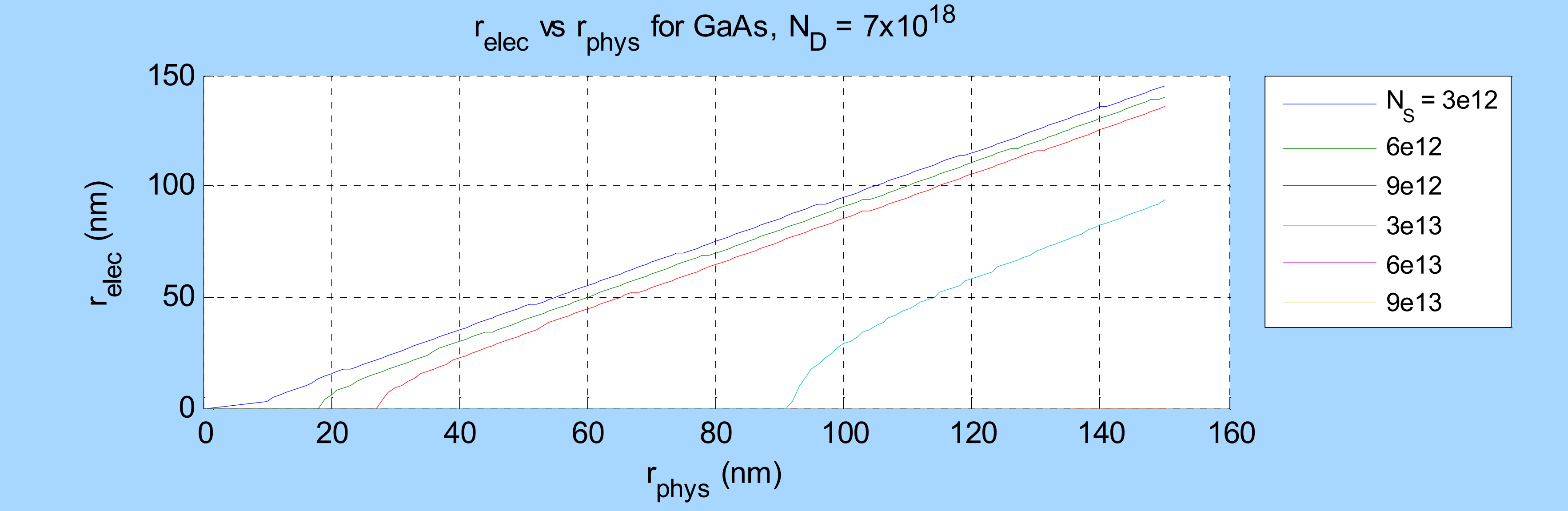
Stichtenoth et al., APL 92 163107 (2008)

MATLAB® Model

- We can now simulate the effect on the electrical radius, effective carrier concentration, and resistivity of a nanopillar due to the presence of surface states
- For simulation, we consider an *n*-doped GaAs nanopillar with different doping concentrations, surface state densities and radii
- For a physical device, we use an 82 nm radius , and for fixed doping, we use 7 x 10^{18} cm^{-3} .
- Simulate the changes on r_{elec}, n_{eff}, and ρ due to N_S
- The simulations are then repeated, sweeping over several surface states densities (from 3 x 10^{12} cm^{-2} to 1x 10^{14} cm^{-2})

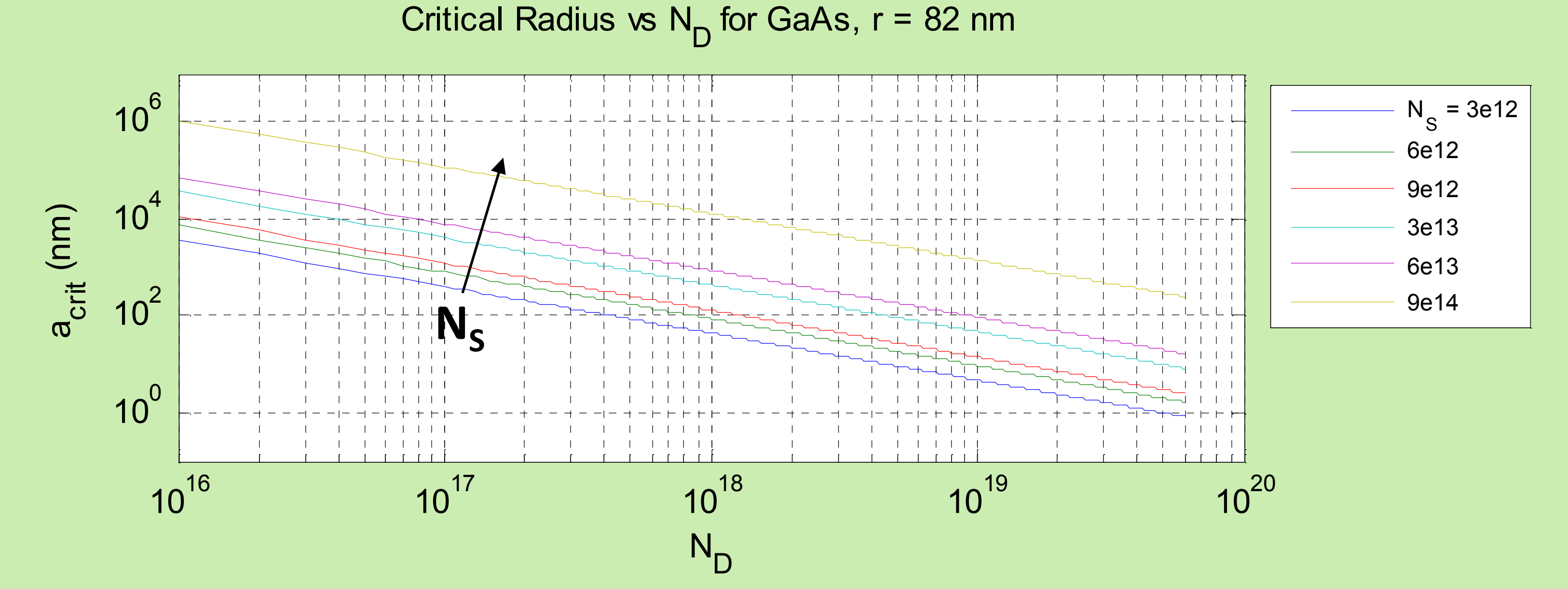
Model - Radius

- Electronic radius r_{elec} is the effective conducting radius
- For higher surface states density, the difference between physical radius and electrical radius is larger
  - Fully depleted region gets wider
- The point where r_{elec} begins is at the critical radius, determined by N_S
- Large effect of small changes in surface state density is shown



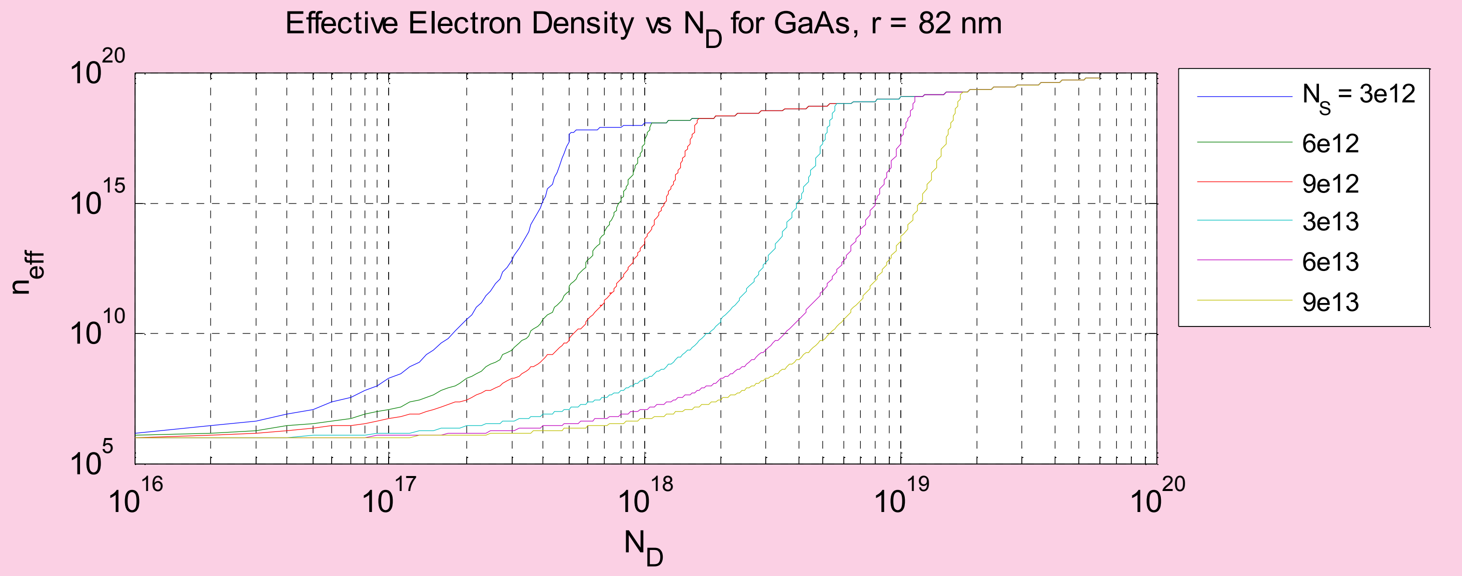
Model – Critical Radius

- Linear relationship between surface state density and depletion region
- a_{crit} decreases linearly with doping
- Value of a_{crit} corresponds to point where r_{elec} becomes non-zero



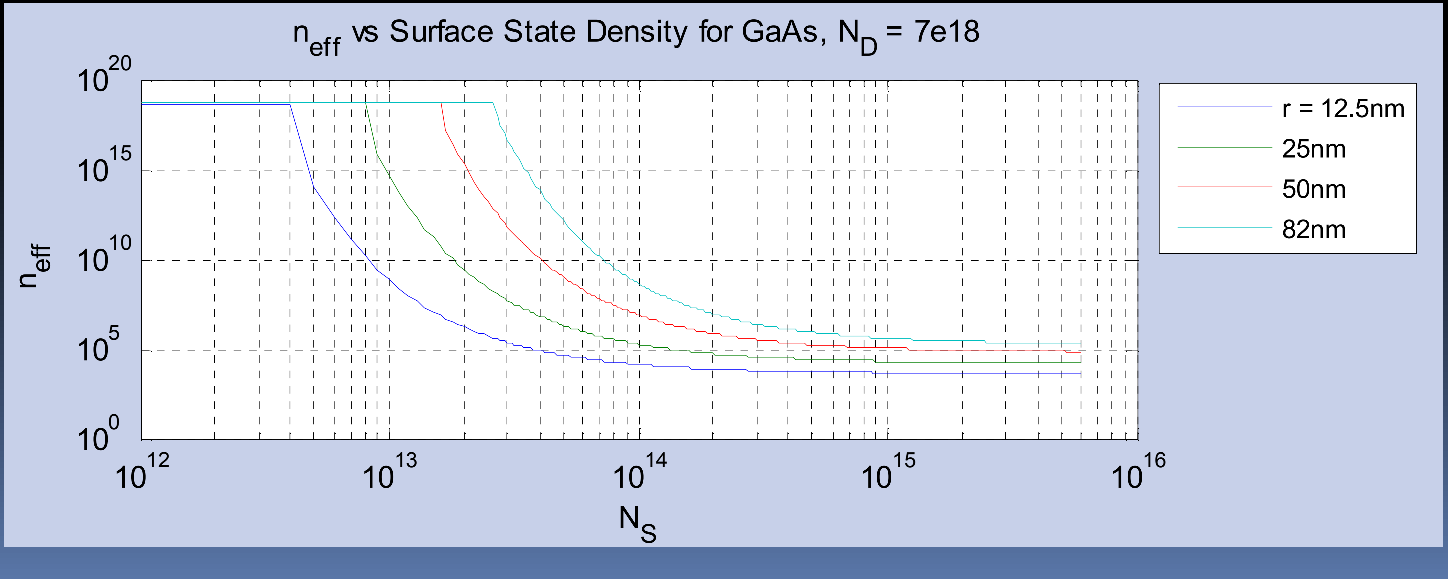
Model – Effective Carrier Concentration

- Based on the surface state density at a constant doping level, the effective carrier concentration changes
- A drastic difference (compared to actual doping) in orders of magnitude until N_S is reduced to a specific level based on N_D
    - At lowest doping, concentration reaches intrinsic value of 2.25 x 10^6 cm^{-3}
    - At high doping or low N_S the pillar is almost non-depleted
- Shows a dramatic change in carrier transport ability of the nanopillar



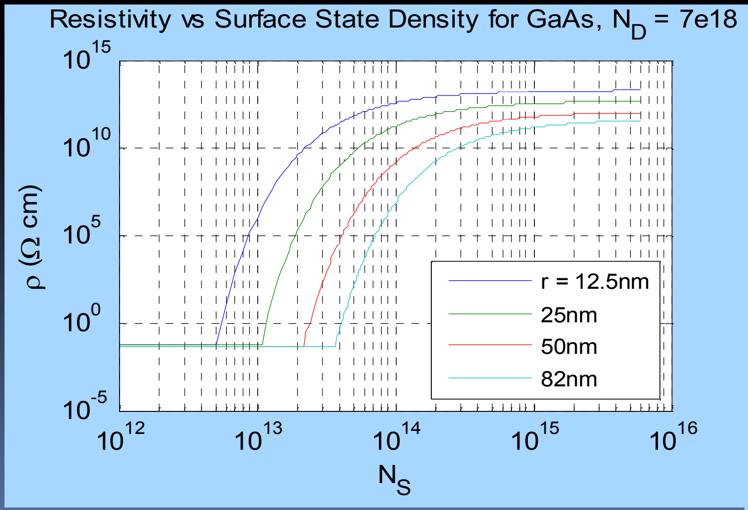
Model – Effective Carrier Concentration

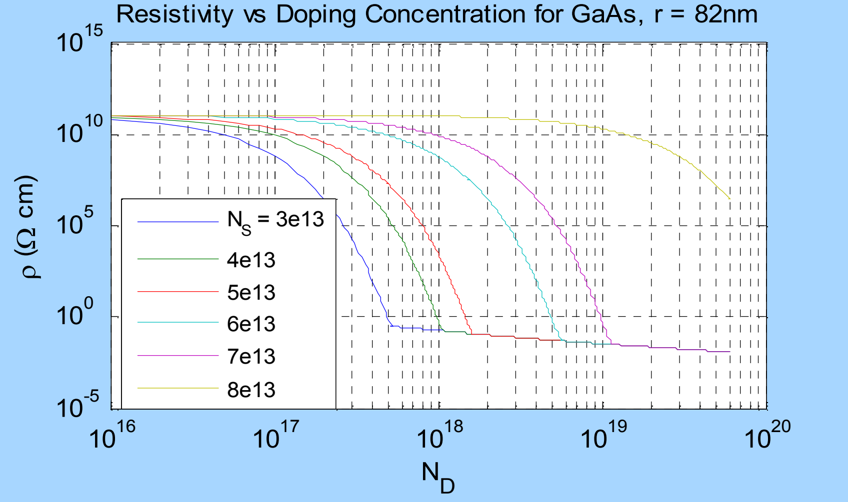
- The model can also account for another case of changing surface state density with different radii (constant N_D)
- Below a certain density for each size, the surface states no longer adversely affect the carrier concentration
- We see that the smaller the nanopillar, the more affected its transport is by surface state density
  - Depletion area remains the same size for specific N_S, leaving less area for transport as pillar radius decreases



Model - Resistivity

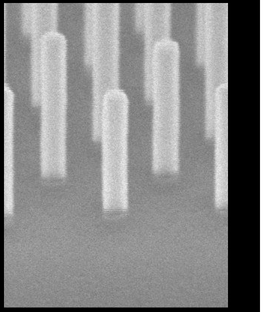
- Relating n_{eff} to resistivity, we can model the behavior of N_S or N_D
- As surface state density decreases, so does resistivity
  - Depletion region decreases, more carrier transport
- Can match these values to resistivity gained from I-V measurements on real pillars



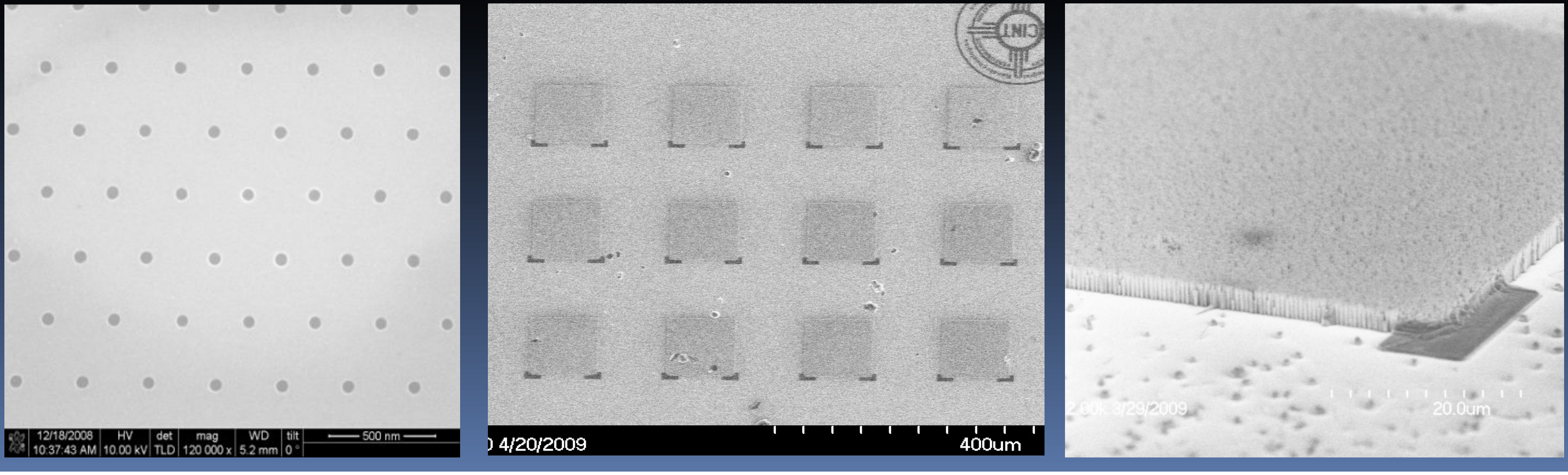


Device Fabrication

- *n*-doped GaAs nanopillars
    - Catalyst-free via selective-area epitaxy using MOCVD
    - 700° C, V-III ratio of 10:1, 20 minute planar growth at 1 A/s
- Hexagonal shaped, using a SiO_2 mask for patterning
- Grown in different arrays of constant height and width
    - Height range: 265 – 626 nm
    - Width range: 27-82 nm
- Pillars studied in an array with height 306 nm, radius 82 nm



10.0kV x50.0k 5/1



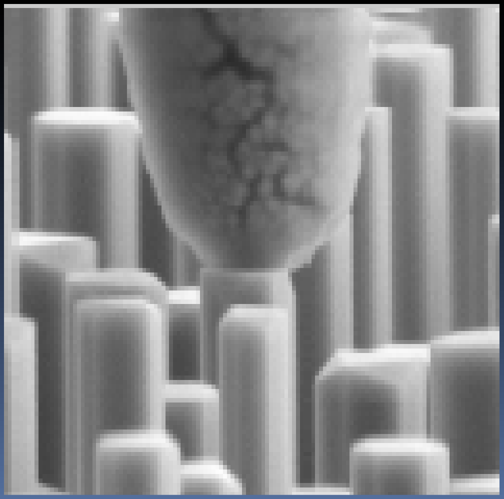
Doping & Passivation

- Device doped using Si for *n*-type
- Concentration determined using Hall measurements
  - Used different concentrations for calibration
  - Both passivated and unpassivated pillars used
- Doping level determined to be 7 x 10^{18} cm^{-3}

- Passivation done using ammonium sulfide solution $(NH_4)_2S$, at 22% concentration
- Process created one monolayer of sulfur on As-terminated surface
- Same sample measured, passivated, and re-measured twice

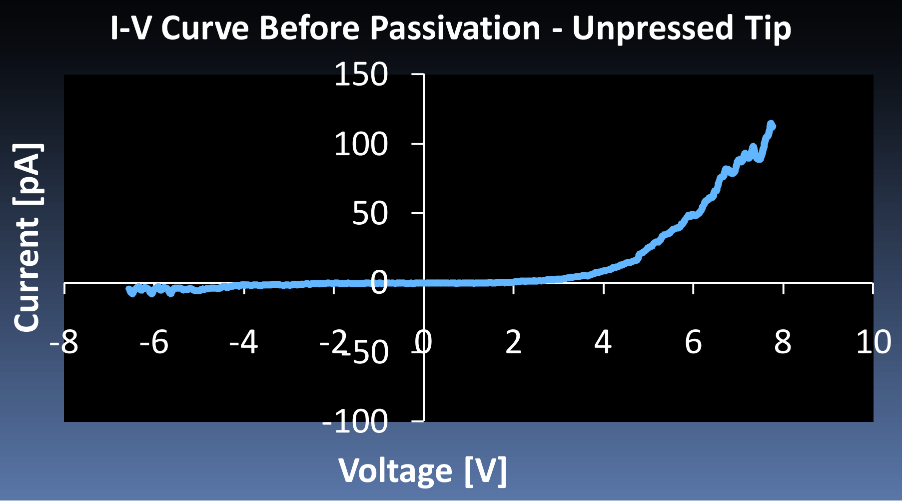
Measurement

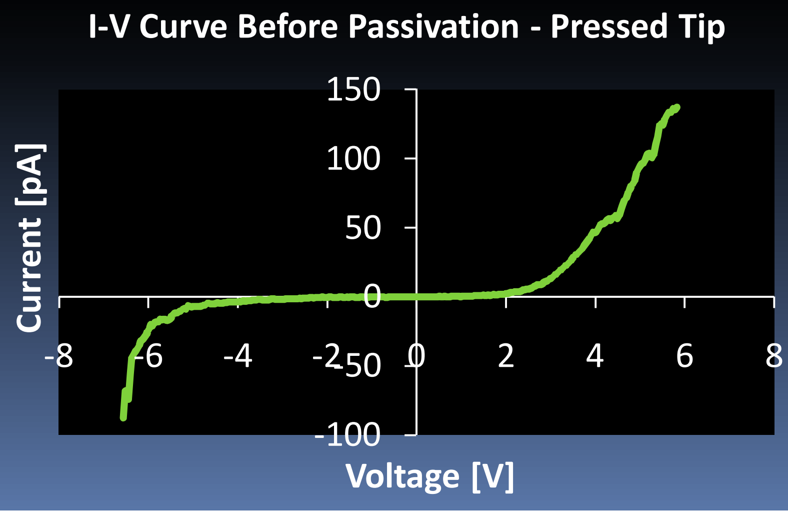
- Pillars measured using AFM
  - Contact-mode, Au/Pt-coated tip
  - Pillars still on growth substrate
- Current measured with tip voltage of -10 to +10 V
- Sample placed on metal disc with silver epoxy, top of pillar probed with tip



Results – No Passivation

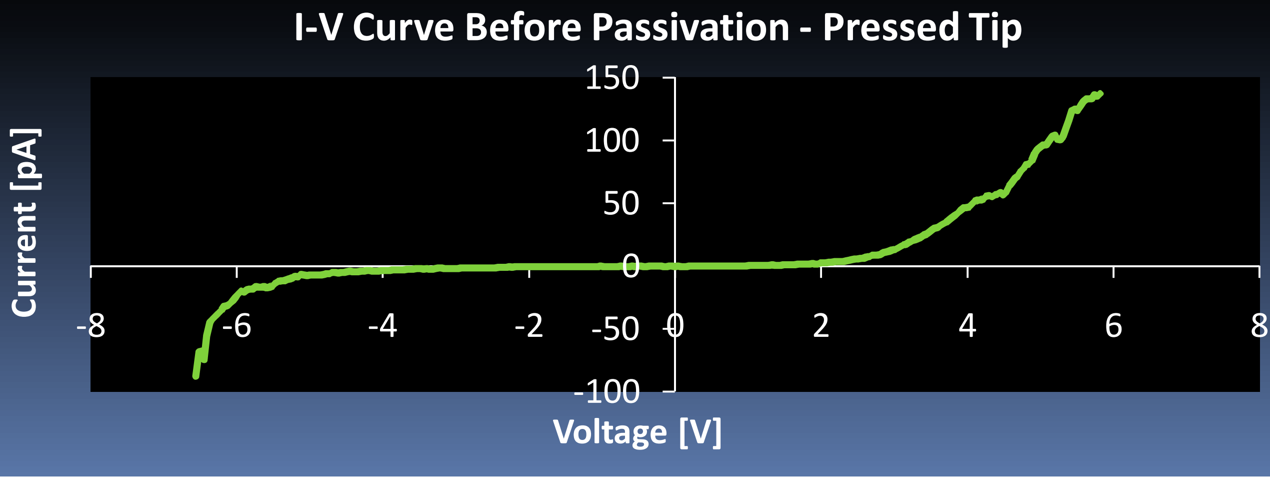
- Tip simply contacting pillar top creates rectifying I-V Curve (diode-like)
  - Injection-limited current
  - Exponential I-V curve only at forward bias
- Pressing tip into pillar created a I ∝ V^2 curve
  - Space-charge limited current, lower contact resistance
    - Possible destruction of native oxide, or curved tip creating a field enhancement


I-V Curve Before Passivation - Unpressed Tip


I-V Curve Before Passivation - Pressed Tip

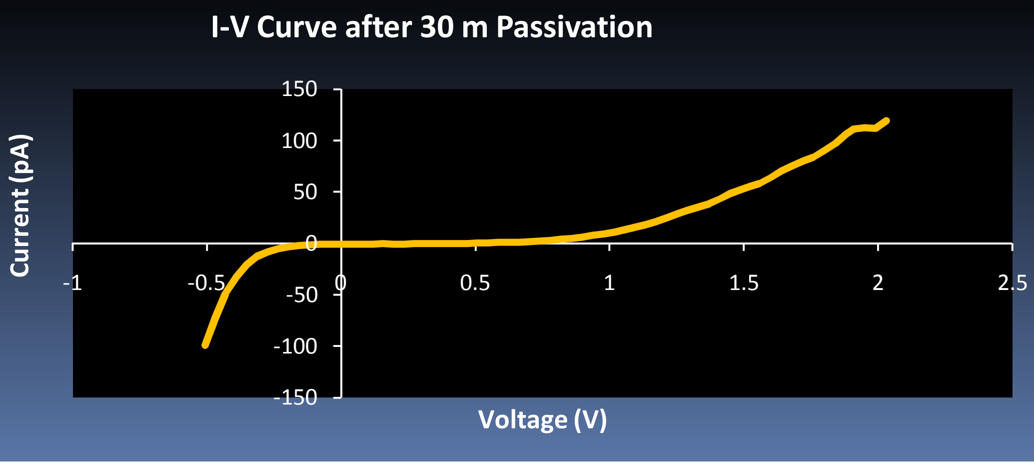
Results – No Passivation

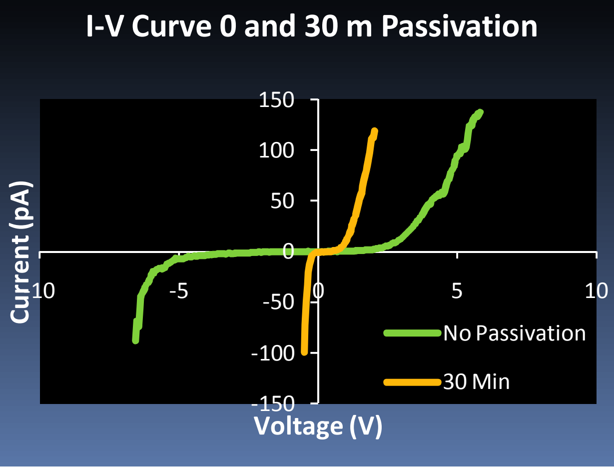
- Pressing tip in, average I-V measurements over 10 samples showed resistance of 44.9 GΩ
    - Using linear approximation of forward bias region
- Current flow begins at 2 V, reaches 50 pA at 4 V
- Maximum specific resisitivty of 8 x 10^5 Ω-cm
    - Average value of 3.9 x 10^5 Ω-cm
    - Schottky barrier height 1.159 eV
- Pillar's transport severely limited by both surface state density and Schottky barrier



Results – 30 Min Passivation

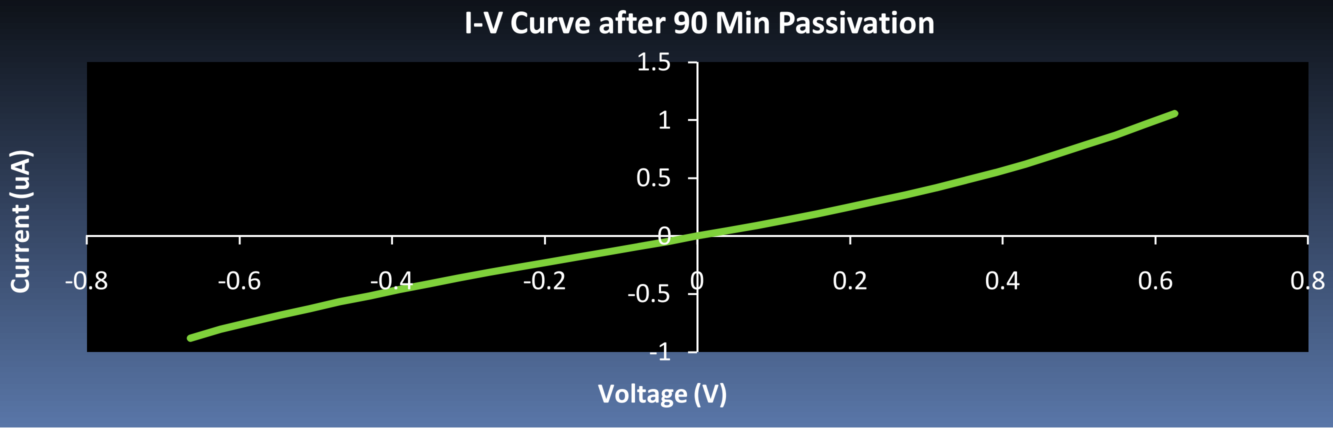
- Pillars were passivated in $(NH_4)_2S$ for 30 min
- Similar $I \propto V^2$ curve obtained, but current flows at a lower bias
  - Current flow begins at 0.75 V, reaches 50 pA at 1.5 V
- Contact resistance still exists
  - Still due to Schottky barrier
- Average resistance 17 GΩ
- Average resistivity 1.17×10^5 Ω-cm
- Further passivation needed to obtain a linear I-V curve


I-V Curve after 30 m Passivation


I-V Curve 0 and 30 m Passivation

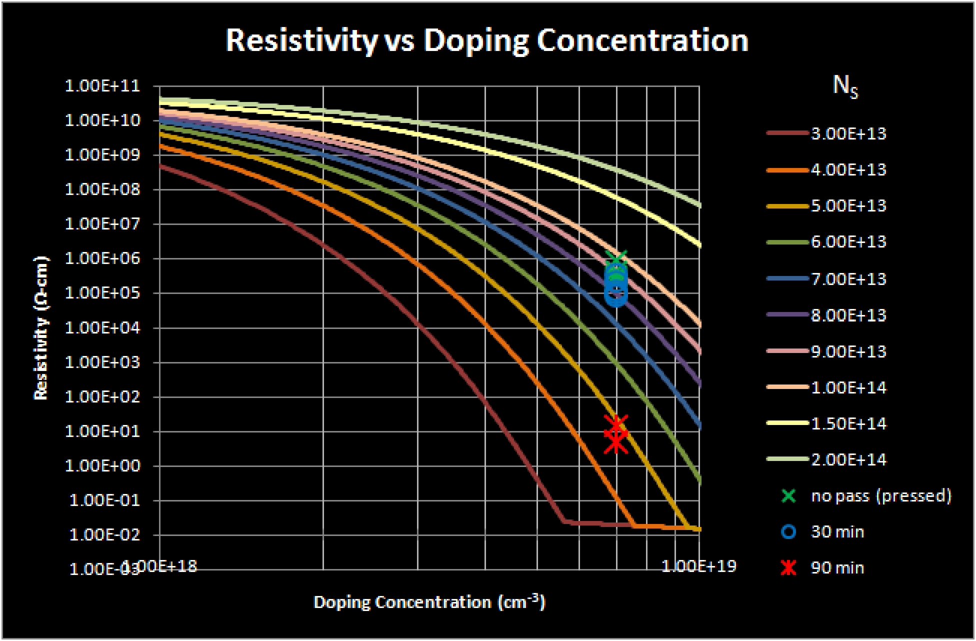
Results – 90 Min Passivation

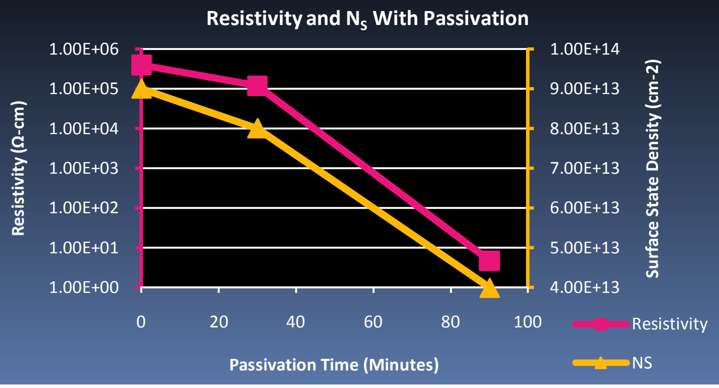
- After 90 min passivation, I-V curve becomes linear
- Much more current flows at a much lower bias
  - Current is 1.06 µA at 0.625 V
  - Much higher current than the 30-min and non- passivated pillars
  - Suggests transport is no longer hindered by depletion region
  - Schottky barrier height only 0.546 eV
- Average resistance 724 kΩ
- Average resistivity 4.7 Ω-cm



Overall Results – Surface State Density

- Surface state density is lowered with passivation
- 0 and 30 minute passivation densities overlap - slight decrease
- 90 minute passivation lowers by half an order of magnitude – large decrease
- High doping of 7 x 10^{18} cm^{-3} means small changes in N_S will be significant
- Resistivity approaches lowest possible calculated value of 10^{-2} Ω-cm





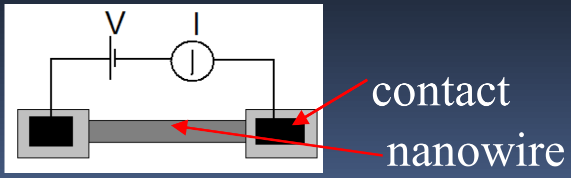
Passivation Time (min)	Resistance (Ω)	Resistivity (Ω-cm)	Surface State Density (cm^{-2})
0	44.9 x 10^9	3.9 x 10^5	**9 x 10^{13} – 1 x 10^{14}**
30	17 x 10^9	1.17 x 10^5	**8 x10^{13}**
90	724 x 10^3	4.7	**4 x 10^{13}**

Summary

- Devised a system of equations to relate resistivity to surface state density for *n*-doped GaAs nanopillars
  - Relationship with doping concentration, electronic radius, effective carrier concentration, resistivity
- Distinguished between physical radius and electronic radius
  - Depletion region created by surface states
- Used MATLAB to simulate these equations for nanopillars
  - Tied actual I-V data and resistivity from real nanopillars to model to determine their surface state density
- Observed and recorded the effects of passivation on nanopillars and their effect on surface states
  - Determined amount of surface state reduction
- A simple, fast and inexpensive method to determine the hard-to-measure parameter of surface state density

Future Work

- Further verify accuracy using a single-wire device
    - Single nanopillar off-substrate placed on metal contacts for Ohmic contact
    - Remove any possible effects from Schottky barrier created by AFM tip
- Fabrication and testing of device, passivated and non-passivated, is still underway



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