Model for Calculating the Density and Resistivity of Surface States in *n*-doped GaAs Nanopillars

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Objective

This project aims to study, understand and characterize the effects of the density of surface state charges on *n*-doped GaAs nanopillars. The effects on the pillar, the change of doping profile, resistivity, transport, and ionization energy caused by surface states at the nano-scale were investigated thoroughly through MATLAB simulations after fitting a model of a pillar to a circular-shaped ideal nanopillar. Experiments carried out afterwards supported the accuracy of our model through surface state density estimations via resistivity measurements of actual nanopillars. Much of the characterizations stem from the principle of charge-neutrality, which dictates the behavior of the doping profile and effective properties of the nanopillar, based on the changes in charges on the surface of the pillar. A model for this system was constructed that can help determine the electrical characteristics of the pillar, and possibly apply it to other systems.

Motivation

III-V semiconductor nanopillars have the potential to be realized as the building blocks for nextgeneration optoelectronic and electronic devices due to the intriguing properties of materials and devices at the nano-scale. However, as the dimensions decrease into the nano-scale, and with materials such as nanopillars when the surface-to-volume ratio increases, the role of charges on the surface of the material, or surface states, becomes more crucial. This is because the surface states can drastically influence the behavior of pillars and must be carefully studied and accounted for. With recent advances in III-V nanotechnology, specifically GaAs nanopillars, we begin to see a large effect on the characteristics of these pillars simply due to surface charges; as a result, a method of measuring these surface charges is desired that requires less expensive and complex procedures. Most of the research has been performed on nanopillars and other nano-scale structures using silicon technology, but there is comparably less literature and research on GaAs nanopillars. As such, we seek to apply and extend much of the principles investigated on silicon nanopillars to that of GaAs and other III-V material systems. In addition, with methods of reducing the density of surface states, such as passivation, an accurate method of measuring the change is desired in order to characterize the effectiveness of these processes.

With the nanopillars fabricated in our lab, and the equipment available it is not a simple task to measure the density of surface states; measurements such as photoluminescence, photoreflectance [1] and other methods are useful, but do not necessarily provide a hard value for the actual density of surface states. Using only the known doping concentration and a simple I-V curve, a method of easily and accurately determining the surface state density was desired. Using this method, a simple simulation could determine the surface state density of nanopillars given measurements of current and voltage. Due to the high volume of experiments and procedures being performed daily in lab environments, it is also optimal to find a way to investigate these methods and properties on currently running and already existing experimental data. Building upon existing techniques of characterizing effective carrier concentration in silicon nanopillars [2], such a model was created for our *n*-doped GaAs nanopillars.



Figure 1: GaAs nanopillars grown via catalyst-free selective area epitaxy

Background

Electronic states exist on the surfaces of the considered materials due to the abrupt transition from solid material to the outside, interrupting the periodicity of the lattice [3]. These states exist with energies in the forbidden gap between the valence and conduction bands of the bulk material. In bulk materials, the device as a whole can often neglect these charges because of their low nature. However in GaAs nanopillars, due to the charge neutrality condition and the high surface-to-volume ratio, the presence of these charges creates opposite charges within the device that serve to deplete the usable region in the material available for transport. This depletion region creates a smaller effective radius of the pillar, rendering the electronic properties of the device more dependent upon the existing surface states than on the physical dimensions themselves.



Figure 2: Example of the depletion region created by surface states, resulting in an effective radius smaller than the physical radius [4]

Surface states can alter nanopillar functionality in many ways. They create bands in between the bandgap and effectively act as carrier trapping centers which can detrimentally hamper the optical properties of the pillars. Furthermore, the surface states also affect the electronic characteristics by changing the effective carrier concentration and depleting the pillars, hindering transport of electrons. Studies have been reported for Si nanopillars that calculate the surface state density from the measured resistance [5], the effective area [6], as well as the effective electron concentration [4] in the partially and fully depleted nanopillars and finally the donor deactivation phenomenon and the effect of surface state density on Si nanopillars, little has been done to study III-V semiconductor nanopillars.

Stichtenoth *et al.* [2] have reported resistance measurements for *p*-doped GaAs nanopillars and their relation to hole concentration. However, the details of the effect of surface states on GaAs pillars as well as a complete theoretical study are still lacking. For simplicity and purpose of demonstration, *n*-doped GaAs nanopillars of a specific doping concentration have been studied. The idea is to be able to apply the model proposed in this paper to any type of doping and possibly to other material systems.

In addition to creating a depletion region within the pillar, surface states also causes Fermi level pinning at the metal-semiconductor interface, which is detrimental for measuring the pillar characteristics. The existence of surface states pins the Fermi level to a constant energy, bending the conduction and valence bands of the semiconductor upwards in the case of *n*-GaAs. This creates a high Schottky barrier at the interface, regardless of the type of metal used to contact the semiconductor.



Figure 3: Fermi level pinning and Schottky barrier caused by surface states in a metal-n-GaAs interface [8]

A method for decreasing the density of surface states on the nanopillars is via passivation. At the surface, the periodicity of the crystal is disturbed due to the termination of the interface; bonds become broken and end up as dangling bonds, and thus the surface can become very reactive. The vacancies of the surface bind and usually form an oxide with the available elements, such as air. Passivation creates a layer or film above this interface, bonding to the dangling bonds and creating a more stable surface such that the charges on the surface are lessened, and thus the surface state density decreases. An interface very close to an AlGaAs/GaAs interface can be created with sulfur passivation due to a strong chemical affinity between GaAs and sulfur [9].

Approach

The approach to this project was to create a model of a circular *n*-doped GaAs nanopillar using equations that characterize the effects of charges on the surface. This model could then determine certain properties of the pillar given others. These properties came down to the doping concentration N_D , physical pillar radius *r*, and surface state density N_S . Knowing two of the three would allow us to determine with certain accuracy of the third parameter. Here we have used MATLAB[®] to formulate our model. The main nanopillar considered in this case study has a radius of 82 nm, and an estimated acceptor doping concentration of 7 x 10¹⁸ cm⁻³. The surface state density is unknown, and will change throughout the process of passivation, but is assumed to be within the range of 10¹³-10¹⁴ cm⁻³ ([1], [10]), which decreases after passivation. For simulation purposes, we have performed sweeps of the parameters; the radius from 10 nm to 150 nm and the doping concentration from 10¹⁷ to 10²⁰ cm⁻³. The

model is based on several mathematical approximations of carrier behavior in nanopillars, which are outlined below.

In order to characterize the effects of surface states on the nanopillar and their carrier transport abilities, a good mathematical model of the was needed. As Figure 2 shows, an *n*-doped nanopillar will be subject to a positive sheet of charge on its surface, which was formed in order to preserve conservation of charge and charge neutrality. It will act as a parallel plate capacitor, imposing a fixed negative charge on the inner portion of the nanopillar. This depleted region is responsible for a change in the electronic transport properties within the nanopillar. Effectively, we see that the depletion region creates a second radius within the actual pillar that is capable of transport, while the depleted region is no longer useful. This gives rise to the two concepts of physical radius (r_{phys}), and electronic radius, considering the Poisson equation

$$\nabla^2 \psi(r) = -4\pi\rho \tag{1}$$

which, due to the circular approximation of the pillar and its symmetry, can be written in cylindrical coordinates

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

where *r* is the radial coordinate, *z* is the axial coordinate, ψ is the potential and ρ is the density of the charge. Neglecting the charge carrier diffusion between the depleted and non-depleted region, i.e., assuming a distinct transition between the two for calculation purposes, the charge density ρ can be shown as

$$\rho = \begin{cases} 0 & 0 \le r < r_{elec} \\ q(N_D - N_A), & r_{elec} \le r \le r_{phys} \end{cases} \tag{3}$$

By solving equation (2) with the abrupt assumption in (3), the potential within the nanopillar is

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

where ε_G is the dielectric constant of GaAs. Solving for the Poisson equation using polar coordinates [2], we can estimate the potential of the surface of the nanopillar at $r = r_{phys}$ as

$$\psi_s = \psi_0 - \frac{\rho}{4\varepsilon_s} \left(r_{phys}^2 - r_{elec}^2 \right) \tag{5}$$

The density of interface charges above and below the surface Q_{it} are given in terms of the surface state density N_s , and must satisfy the charge neutrality condition. This brings us to the following relations

$$Q_{it} = -q^2 N_s \psi_s \tag{6}$$

$$\pi (r_{phys}^2 - r_{elec}^2)\rho + 2\pi r_{phys}(Q_f + Q_{it}) = 0$$
(7)

Which, when solving for the electronic radius [7] gives us the final relation

$$r_{elec} = \sqrt{r_{phys}^{2} + \frac{2r_{phys}Q_{f} - 2r_{phys}N_{s}\psi_{0}}{q(N_{D} - N_{A})\left(1 + \frac{r_{phys}q^{2}}{2\varepsilon_{G}}N_{s}\right)}}$$
(8)

where N_D and N_A are the donor and acceptor concentrations, respectively, ε_s is the dielectric constant of the material (13.1 for GaAs), ψ_0 is the potential of the nanopillar at r=0, and N_s is the surface state density. From the above equations we can conclude that the size of the electronic radius is dependent on several factors, a few of which are controllable (N_s and N_D/N_A) via fabrication process of the nanopillars or post-fabrication procedures.



Figure 4: Cross-section view of a depleted nanopillar

As stated before, the electronic transport within the nanopillar is confined by the depleted region caused by the surface states (Figure 4), and the actual volume where the carrier transport takes place is of size $L\pi r_{elec}^2$. It thus becomes useful to define a threshold value of radius, the critical radius a_{crit} [2]. This value allows us to distinguish between the fully depleted and partially depleted states of the nanopillar, given the doping concentration and surface state density. This is defined as

$$a_{crit} = \frac{\varepsilon_G}{q^2 N_S} \left\{ -1 + \left[1 + \frac{4q^2 N_S}{\rho \varepsilon_G} (q^2 N_S \psi_0 - Q_f) \right]^{\frac{1}{2}} \right\}, \quad \approx \quad \frac{2}{\rho} (q^2 N_S \psi_0 - Q_f)$$
(9)

In this case, if the size r_{phys} is greater than the determined a_{crit} , then the nanopillar is partially depleted but still conductive in its center. However, if r_{phys} is less than a_{crit} , then the nanopillar is fully depleted and carrier transport no longer occurs due to the overwhelming surface state density's subsequent depletion region. We can see from this formula that the critical radius decreases with either increasing doping concentration (given in ρ) or decreasing surface state densities, because the depletion region width also decreases. Taking into account the depletion region, it is also necessary to adjust the actual doping concentration, depending on the actual doping N_D , the surface state density N_s , and the surface potential ψ_s . These factors all contribute to the critical radius, and so we come up with two equations for the effective carrier concentration n_{eff} which were determined by the actual radius r_{phys} and the critical radius a_{crit} . Remembering to consider the electron density of a normal bulk material:

$$n_0 = N_c \exp\left(-\frac{E_g}{2kT}\right) \tag{10}$$

Where N_c is the effective density of states in the conduction band, and E_G is the bang gap of GaAs. Combining the equation for electron density (10) with the potential of the pillar derived in (4), we can arrive at this equation with two cases:

$$n_{eff} = n_0 \exp(\beta \psi_0) \left\{ \frac{r_d^2}{a^2} + \frac{4\varepsilon_G}{\beta \rho r_{phys}^2} \left[1 - \exp\left(\beta \frac{\rho}{4\varepsilon_G} \left(r_{elec}^2 - r_{phys}^2\right)\right) \right] \right\}, r_{phys} > a_{crit}$$
(11)

$$n_{eff} = n_0 \exp(\beta \psi_s) \frac{4\varepsilon_G}{\beta \rho r_{phys}^2} \left[\exp\left(\beta \frac{\rho r_{phys}^2}{4\varepsilon_G}\right) - 1 \right], r_{phys} < a_{crit}$$
(12)

From here we can see that the actual doping concentration depends strictly on the surface state density, which is contained within the critical radius. With our model, using these equations we will be able to predict N_s or N_D given the other, and knowing the physical radius and dielectric constant of the material.

For the purposes of our experiments, due to the difficulty in quickly and easily measuring the actual surface states of the nanopillars, we are using the model to predict N_s while knowing the physical properties of the nanopillar, including r_{phys} and N_D . We can relate the resistivity of a nanopillar to its surface states density via the equations above, taking into account n_{eff} from (11) or (12), which accounts for N_D , which is known, and gives N_s as a result. The relation between the resistivity and n_{eff} can be seen through a simple relation with the electron mobility [11]:

$$R = \frac{\rho L}{A_e}, \quad where A_e = \pi r_{elec}^2 \tag{12}$$

$$\rho = \frac{1}{q\mu_k n_{eff}}, \quad \mu_k = \frac{\mu_0}{1 - \sqrt{\frac{n_{eff}}{10^{18}}}}, \quad where \ \mu_0 = 8500 \frac{cm^2}{Vs} \ (n - type)$$
(13)

where $\mu_0 = 450 \text{ cm}^2/\text{Vs}$ for GaAs. By performing a series of I-V measurements on our nanopillars, it is possible to extrapolate the resistance, and thus the resistivity, which corresponds to a specific surface states density given N_D within n_{eff} .

In order to describe the contact resistance within the pillar, it is also necessary to find an estimate of the Schottky barrier height created between the metal-semiconductor interface of the pillar and the measuring tip. This is done with a simple I-V measurement of the pillar, finding the saturation current density J_s and using the effective Richardson constant A^* and the following expression:

$$q\phi_B = k_B T \ln\left(\frac{A^* T^2}{J_s}\right), \quad A^* = \frac{m^*}{m_0} 120 \ A/(K^2 cm^2)$$
 (14)

MATLAB Model



Figure 5: Simulation of physical radius vs electronic radius for different surface state densities at a single doping

Figure 5 plots equation (8), which shows that as the surface state density increases, the point of full pillar depletion increases and we have a fully depleted, non-conducting pillar until that point. As such, the electronic radius r_{elec} is zero and acts as an insulator, a property not seen on larger-scale pillars due to the neglect of surface charges outside the nanorange. These charges are neglected because the surface-area-to-volume ratio is much smaller than in a nanopillar, and the depletion region created by a sheet of surface charges is very small compared to the conducting, non-depleted region. We can see that with higher surface state densities such as $N_s = 3 \times 10^{13} \text{ cm}^{-2}$, the critical radius lies at 66 nm and that a pillar less than that radius is fully depleted. As the surface state density reaches below the set doping concentration here of $7 \times 10^{18} \text{ cm}^{-3}$, the critical radius becomes smaller and thus transport ability is available to smaller radius pillars. The figure demonstrates the large effect surface states have on the transport abilities of nanopillars, and that changes in density even smaller than an order of magnitude have a large effect at this scale. We can also see that with the set doping concentration, surface states only have a real effect on our pillars at densities higher than 10^{13} cm^{-2} .



Figure 6: Critical Radius vs Doping Concentration

The relationship between the surface state density and the width of the depletion region is linear, and can be demonstrated by the charge neutrality condition described above and requires an equal and opposite charge for each surface charge. This is also shown by Figure 6, which gives the value of a_{crit} vs doping concentration for set values of surface state density. It also shows the effect of a higher doping concentration on lessening the impact of surface states, as there is a linear inverse relationship between

the two. As the doping concentration increases, the concentration of charges increases and the depletion region decreases due to charge neutrality, which dictates a specific amount of opposite charges in the depletion region that counter the surface states. With this plot we can also match the values of a_{crit} to those seen on Figure 5, where the electronic radius r_{elec} begins.



Figure 7: Effective carrier density as a function of N_D; the curves turn linear once the critical radius value reaches the physical radius

The effective carrier concentration n_{eff} can be plotted by the model over a range of doping concentrations. Due to the variation in the size of the pillar and the surface state density and a_{crit} , we have different values for n_{eff} , which changes as the doping increases and has reached r=82nm, the physical pillar radius. Figure 7 shows a sweep of these values. It can be seen that once the critical radius is reached, the relation between n_{eff} and N_D becomes linear as the pillar is no longer fully depleted and can now conduct. This figure shows that while the pillar is in a condition of full depletion, the effective hole concentration is drastically different than expected of a normal bulk semiconductor; after a_{crit} is reached, the pillar is able to conduct because the surface charges no longer create a fully depleted pillar. At this point, the effective carrier concentration approaches the value of the actual doping concentration. We can also see on the opposite end, at the lower doping concentrations we see that the effective carrier concentration approaches the intrinsic value for GaAs of 2.25 x 10^6 cm⁻³.



Figure 8: Effective carrier concentration vs surface state density

Figure 8 shows that an increase in surface states can cause a portion of the pillar to actually allow carrier transport. Other pillar radii are shown for reference. With our physical pillar of radius of 82nm, we see that the effect of surface states on the pillar do not adversely affect the carrier concentration (meaning

cause full depletion in the pillar) until we reach a high surface state density of around 3 x 10^{13} cm⁻². Below this point, decreasing the surface state density does not affect n_{eff} , whereas increasing N_s past this point beings a drastic, non-linear decrease in the usable carrier concentration of the pillar. Increase of N_s by less than an order of magnitude can drop the effective carrier concentration by several orders of magnitude.



Figure 9: Resistivity vs surface state density and doping concentration

We can now apply these models of the effective carrier concentration to map out the resistivity of a nanopillar given its doping concentration, size, and surface state density. Using equation (13) above, the relationship between resistivity and effective carrier concentration is quite simple, and thus the plot of a nanopillar's expected resistivity due to changes in surface state density and doping concentration are shown in figures 9a and 9b respectively. The relationship between n_{eff} and ρ is inversely linear, so we see the same type of steep non-linear increases in the resistivity with increasing surface states, or non-linear decreases in resistivity with increasing doping concentration. These simulations will become the core of our determination of surface state density given experimental data.

Device Fabrication

The device used for the first experiment was an array of hexagonal *n*-doped GaAs nanopillars, which were grown through a catalyst-free method via selective-area epitaxy using MOCVD, on an *n*-type GaAs substrate as shown in Fig 10. Although the pillars are hexagonal, we will use as a first approximation the circular approximation for the models. The pillars were grown in groups of different height and decreasing radius, using a SiO₂ growth mask to determine the patterns. The height and radius ranged from 265-626 nm and 27-82 nm, respectively. Si is used as an *n*-type dopant for GaAs. The pillars were grown at a temperature of 700° C, with a V-III ratio of 10:1, a growth time of 20 minutes and a planar growth rate of 1 A/s. For our measurement purposes we concentrated on a single array with height 306 nm, and radius 82 nm.



Figure 10: SEM images of a) SiO₂ mask, b) arrays of nanopillars and c) close-up of nanopillar array

Doping of this device was determined through empirical testing and calculated simulation. The doping on planar growth was measured with Hall measurements within the MOCVD machine, and the recipe for growth was modified for other dopings higher and lower in order to roughly calibrate the concentration. Taking into account the pillar height, width, and I-V curves given both from passivated and unpassivated pillars of the same sample, and fitting them to a simulation of doping done in the lab, the doping level for these pillars was determined to about 7×10^{18} cm⁻³.

Passivation was done using a concentration of ammonium sulfide, $(NH_4)_2S$. The ammonium sulfide was a 22% concentration liquid, and the GaAs samples were immersed into the solution for various amounts of time, in order to measure different amounts of passivation. Afterwards, they were removed from the solution and rinsed with water and dried with nitrogen gas. This process creates one monolayer of sulfur atoms on the surface, capping the surface states of the dangling bonds. Measurements of the pillar's resistance were taken for the pillars passivated for 0, 30, and 90 minutes. In all cases, the pillars were removed from the solution and measured using an AFM using the process outlined below. Results have shown that with an As-terminated surface, using an $(NH_4)_2S$ solution bonds the As atoms a sulfur atom, creating a much more stable material surface and reduced amount of surface states that agrees with literature [12].

The nanopillars' electrical characteristics were measured using an atomic force microscope. Due to the small size of the AFM's probing tip and its measurement method using electrical current to image, it was the ideal choice in measuring the I-V characteristics of the pillar. The sample containing the nanopillar arrays was placed on a metal disc with a very low resistivity for measuring, and was adhered using a silver epoxy that served as the back contact. The AFM was outfitted with a gold and platinum coated tip. In contact mode, the tip was placed on the top of the pillar and the output current generated at set voltages was recorded from -10V to +10V.



Figure 11: a) close-up of nanopillars being measured. b) Au/Pt tip contacting the top of a hexagonal nanopillar for I-V measurement

Experimental Results

The first experiments were carried out the first device where array of nanopillars was still situated on the *n*-GaAs substrate. The measurements of resistivity were carried out at three points: non-passivated, passivated for 30 minutes, and passivated for 90 minutes. The non-passivated measurements showed a large amount of contact resistance due to a significant Schottky barrier height. Initially the I-V curve was rectifying and resembled that of a diode rather than a conductive pillar (Fig 12a), with an exponential I-V characteristic only at forward bias. However, when the tip was pressed into the pillar, an $I \propto V^2$ curve (Fig 12b) is observed instead. This change from a rectifying curve to a quadratically symmetric I-V curve can be explained by a transition between injection-limited and space-charge-limited current. It shows that the contact resistance is lessened and that the $I \propto V^2$ curve is due to the transport in the nanopillar itself, rather than the tip-pillar contact. Reasons for this have been hypothesized, including destruction of a thin native oxide layer on the pillar due to the pressure, or the curvature of the tip creating a field enhancement [13].



Figure 12: I-V curves of non-passivated nanopillars, first (a) without the tip pressed and then (b) with the tip pressed in

Averaging I-V measurements, from 10 samples the non-passivated case was found to have a large resistance value when of 44.9 G Ω , taken by a linear approximation of the forward linear region of the pressed-IV curve over a positive voltage window as shown in Fig 12(b). Current flow did not begin until the bias reached 2 V, and reached 50 pA at about 4 V. At this point the current-voltage characteristic appeared to become linear, much like a diode. This gives a maximum specific resistivity of about 8 x 10⁵ Ω -cm, and an average value of 3.9 x 10⁵ Ω -cm. At this state, however, the pillar's transport is severely modified by both the surface state density and the Schottky barrier that still exists. In this case, the

Schottky barrier height was calculated to be about 1.159 eV. The resistance here, when matched up to the predicted values from the MATLAB model, and assuming the estimated doping concentration of $N_D = 7 \times 10^{18}$ cm⁻³, corresponds to a surface state density around $9 \times 10^{13} - 1 \times 10^{14}$ cm⁻². This high value, which has been characterized in other literature for non-passivated GaAs as well [10], prevents carrier transport which results in the very high resistivity measured.



Figure 13: (a) I-V curves of the 30-minute passivated pillars, (b) compared to the non-passivated pillars

The next step was to passivate the pillars and re-measure their resistance. After a 30-minute passivation, the pillar resistance was measured again. An I-V curve similar to that of the non-passivated case was apparent, but less drastic. It followed a quadratic $I \propto V^2$ curve as well, as shown in Fig 13(a). Here, however, the current begins to flow at a lower voltage. Current begins to flow at about 0.75 V, and hits the 50 pA mark at about 1.5 V, a good improvement compared to the non-passivated case. The curve, however, is still not linear, and similar in shape to the non-passivated curve (Fig 13(b)), which means a large Schottky barrier still exists and provides a contact resistance. From these curves, the average resistivity is seen to be about 17G Ω , and ranges from 14.4 to 30.8 G Ω . Thespecific average resistivity of the 30-minute passivated pillars is still high, and close to the value of the non-passivated pillars, with an average value of $1.17 \times 10^5 \Omega$ -cm. The amount of current it passes is close to that of the non-passivated case, but transport begins with less voltage. This resistivity corresponds to a slight drop in the surface state density to about 8 x 10^{13} cm⁻², which is not significantly lower than the unpassivated pillars. This concludes that 30 minutes of passivation does not make a significant difference in suppressing the surface states on the pillar, perhaps because there is not enough time for the sulfur atoms to bond to the Ga or As atoms on the suface.



Figure 14: I-V curve of a 90-minute passivated pillar, showing linear characteristics and high current

Finally, pillars that have been passivated for 90 minutes were tested. With longer passivation times, the sulfur atoms should have had adequate time to bond to the broken surface bonds of the pillar, and decrease the amount of surface states that create depletion within the pillar. The results shown in Figure 14 confirm just that. The actual I-V curve of the pillar has become just like that of a resistor, linear and increasing current with voltage in both directions, starting at V = 0. It can also be seen that a much larger current is able to flow through the pillar, with a current of 1.06 µA at the highest measured voltage of 0.625 V. We see that a high amount of current is reached before the point where the 30-min and non-passivated pillars even begin to have transport. This high conductibility of the pillar suggests that transport is no longer hindered (or only very slightly so) by the depletion region created by the surface states as compared to the 30 minute case. The resistance and resistivity for these pillars is quite low, at an average value of around 724k Ω and 4.7 Ω -cm, respectively. This corresponds to a Schottky barrier height of 0.546 eV, and surface state density slightly above 4 x 10¹³ cm⁻², which for a pillar with a doping of 7 x 10^{18} cm⁻³ is enough to almost negate the size of the depletion region created by the surface states for transport purposes. The actual resistivity of bulk GaAs at a doping level of N_D = 7 x 10^{18} cm⁻³ is still lower, at around 10^{-3} cm⁻³ [11], but as the plot of electronic vs physical radius in Figure 5 as well as n_{eff} vs N_D in Figure 7 shows, the carrier concentration will not completely equal the doping concentration due to the nature of the nanopillar's size.



Figure 15: Estimation of surface state density given the resistivity of the three samples

Figure 15 above reiterates the predictions of surface state density for the nanopillar after different stages of passivation. From the figure, we can see that there is not much difference between the non-passivated pillars and pillars passivated for 30 minutes. There is a slight discernible decrease in the 30-minute minimum as compared to the non-passivated maximum, but the ranges still overlap. This places the surface state density for the first two samples between 8 x 10^{13} and 1 x 10^{14} cm⁻². We see a large decrease in surface states with 90 minutes of passivation, lowering the resistivity to below 5 Ω -cm and a surface state density slightly above 4 x 10^{13} cm⁻². While this is not a decrease over a full order of magnitude, the high doping concentration presumably gives way to large changes in transport ability

with changes in surface state density less than an order of magnitude. While the resistivity of the 90minute passivated pillar does not reach the lowest possible simulated value of about $1 \times 10^{-2} \Omega$ -cm or the GaAs intrinsic resistivity of ~6 x $10^{-4} \Omega$ -cm, it then appears that there is still room for further passivation of the pillars to decrease the surface state density even more. However, further research done on quantum dot passivation has shown that the passivation benefits begin to plateau at this range, and thus further immersion in the passivation solution may not be as effective.

Summary and Future Work

From the given equations and relations we were able to construct a MATLAB model of *n*-doped GaAs nanopillars with specific parameters N_D , N_s , and r_{phys} . With this we were able to extract a relationship between surface state density and several characteristics – donor concentration, electronic radius, effective carrier concentration, and resistivity. We were able to distinguish between two different radii, the physical and electronic radius, and how each comes into play when considering the effect of surface state density at sizes in the nanoscale. We also saw the change in the effective carrier concentration from the actual donor concentration. Through I-V measurements of actual nanopillars, we were able to use the resistivity to determine the amount of surface states on the pillars. The non-negligible existence of surface charges on nanostructures have been illustrated by these measurements and have shown a difference between materials in bulk and nanoscale. We also showed that while the presence of surface states is detrimental, they can be controlled and reduced via passivation. This passivation process showed how simple it is to cap the dangling bonds on the surface with sulfur and effectively return the nanopillar to a usable structure for electron transport.

The next steps with this model would be to further verify the accuracy of the surface state density prediction using single-wire devices placed on metal contacts, to lessen or eliminate the Schottky barrier created by the AFM measurement setup and remove any possible effects from the pillar being in an array or still attached to its substrate. Such a device is still being actively fabricated, in both passivated and non-passivated forms.

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