

LUND UNIVERSITY

THE PHYSICS OF LOW-DIMENSIONAL STRUCTURES AND
QUANTUM DEVICES

FFFN35

Nanowire Bandstructure

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1. Introduction

This project concerns bandstructure in a quasi-1D, cylindrical, infinitely long nanowire (figure 1). With a basis in the Schrödinger equation in cylindrical coordinates we calculated the subbands of the wires' lowest conduction band as well as the probability density of electrons in the wire. The energies found were then used to find the density of states for the conduction band electrons as well as the conductivity of the wire.

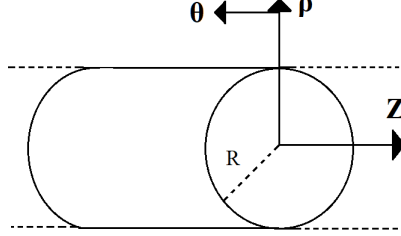


Figure 1: Sketch of our infinitely long wire with radius R , with the cylindrical coordinate system (ρ, θ, Z) .

2. Subbands

In an effective mass model, the Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 + V(\mathbf{r})\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \quad (1)$$

or, in cylindrical coordinates (ρ, θ, z) ,

$$\frac{-\hbar^2}{2m^*}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\theta^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + V(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \quad (2)$$

where the energy E is measured from the bottom of the conduction band. The potential $V(\mathbf{r})$ is modelled as $V(\mathbf{r}) = 0$ within the wire, and ∞ outside it. (Similarly to an infinite square quantum well, but with different geometry). Thus our wavefunction must be zero at the edge of the wire, at full radius R . Given the infinite extent of the wire, we can suppose plane wave solutions in the z -direction. Symmetry around the z -axis means that our wavefunction can be variable separated and take the form

$$\Psi(\mathbf{r}) = u(\rho)\Theta(\theta)Z(z). \quad (3)$$

where $Z(z) = e^{ik_z z}$, with k_z being the eigenvalue for wavenumber. Note that k_z is not constrained to discrete values, as electrons are not constrained in the z direction. Inserting the wavefunction in this form yields, after simplification and separation of variables,

$$\rho^2\frac{u''}{u} + \rho\frac{u'}{u} + \left(\frac{2m^*E}{\hbar^2} - k_z^2\right)\rho^2 = -\frac{\Theta''}{\Theta} = C. \quad (4)$$

where C is a constant that does not depend on the radius ρ or angle θ . (Both sides of equation (4) must equal this constant as the radial and angular dependence can be separated). $Z(z)$ notably falls away completely, which makes sense given the infinite extent of the wire. Solving the angular differential equation yields $\Theta(\theta) = Ae^{i\sqrt{C}\theta} + Be^{-i\sqrt{C}\theta}$. In order to fulfill the necessary periodicity with 2π , $\Theta(0) = \Theta(2\pi N)$, it follows that $\sqrt{C}$ must be an integer. Introducing l as $C = l^2$ yields $\Theta(\theta) = Ae^{il\theta} + Be^{-il\theta}$, where $l = 0, \pm 1, \pm 2, \dots$. We see that l can be interpreted as angular momentum. Further introducing $\varepsilon = E - \frac{\hbar^2 k_z^2}{2m^*}$ equation (4) can be rearranged into

$$u'' + \frac{1}{\rho}u' + \left(\frac{2m^*\varepsilon}{\hbar^2} - \frac{l^2}{\rho^2}\right)u = 0. \quad (5)$$

This is the familiar Bessel differential equation, and its solutions are well defined by the Bessel functions:

$$u(\rho) = aJ_l\left(\sqrt{\frac{2m^*\varepsilon}{\hbar^2}}\rho\right) + bY_l\left(\sqrt{\frac{2m^*\varepsilon}{\hbar^2}}\rho\right). \quad (6)$$

where a and b are constants. The second term makes little physical sense as its integral doesn't converge at zero, hence b must be 0. This leaves us with a full wavefunction

$$\Psi(\mathbf{r}) = aJ_l\left(\sqrt{\frac{2m^*\varepsilon}{\hbar^2}}\rho\right)(Ae^{il\theta} + Be^{-il\theta})e^{ik_z z}. \quad (7)$$

However, we have not yet considered our earlier boundary condition: $u(R) = 0$. This is fulfilled if the Bessel function is zero at radius R . Fortunately the roots of the Bessel function are well defined as $\alpha_{n,l}$: the n th zero of the Bessel function of order l . This imposes a restriction on our energies ε :

$$\sqrt{\frac{2m^*\varepsilon}{\hbar^2}}R = \alpha_{n,l} \iff \varepsilon = \frac{\hbar^2\alpha_{n,l}^2}{2m^*R^2} \iff E = \frac{\hbar^2\alpha_{n,l}^2}{2m^*R^2} + \frac{\hbar^2k_z^2}{2m^*}. \quad (8)$$

Equation (8) forms the basis of our subbands, where states are allowed. These form parabolas in k_z -space, shifted upwards by $\varepsilon_{l,n}$, which is determined by the Bessel zeros. As the Bessel functions J_l and J_{-l} have the same roots, $\alpha_{n,l} = \alpha_{n,-l}$, the states where $l \neq 0$ are degenerate in energy. The interpretation is that a state moving clockwise have the same energy as a state moving counter-clockwise. Figure 2 shows the first five parabolas for a GaAs ($m^* = 0.067m_0$) nanowire with radius $R = 10$ nm.

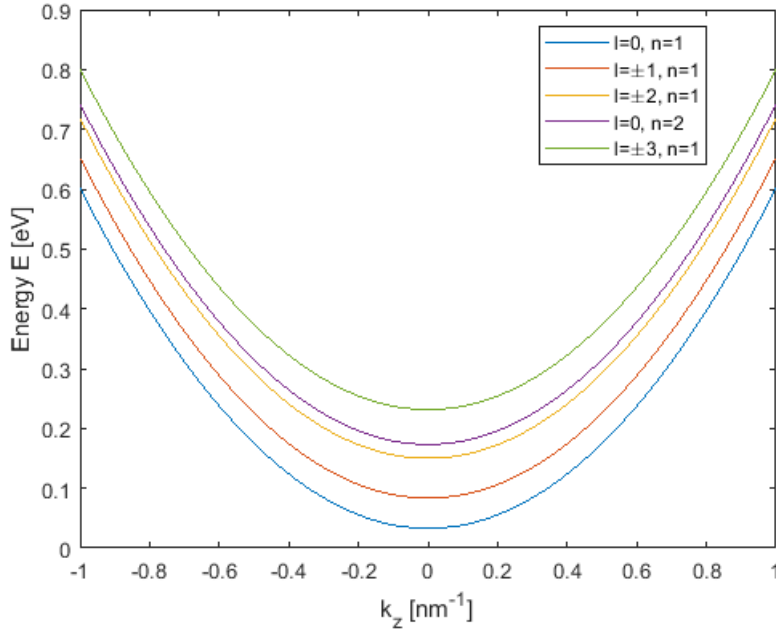


Figure 2: Energies E of the five lowest subbands as a function of k_z for a GaAs nanowire with radius $R = 10$ nm.

3. Probability Density

The probability density is the absolute value squared of the wavefunction. From equation (7) it follows that the probability density is on the form:

$$|\Psi(\mathbf{r})|^2 = a^2 J_l \left(\sqrt{\frac{2m^*\varepsilon}{\hbar^2}} \rho \right)^2 \quad (9)$$

Normalizing along a line from the center of the wire outwards to $\rho = R$ gives the constant a as:

$$a^2 = 1 / \int_0^R J_l \left(\sqrt{\frac{2m^*\varepsilon}{\hbar^2}} \rho \right)^2 d\rho \quad (10)$$

As the energies depend on the quantum numbers n and l , we get different wavefunctions and thus different probability densities depending on n and l (but still the same for positive and negative l as l is squared). Holding n fix at it's lowest value 1, the probability densities for the four lowest l are plotted in figure 3 for a GaAs nanowire of radius $R = 10$ nm. One finds that for $l = 0$ the electrons are most likely to be found at the centre of the wire, with decreasing probability as one moves outwards from the centre. Increasing the angular momentum l , the probability density shifts more and more towards the edge of the wire. For a non-zero value of l , the electron will never be found exactly at the centre of the wire. The probability densities' dependence on l thus agrees with the intuition from classical mechanics that a higher angular momentum should mean that the electrons are "pushed" outwards towards the edge of the wire.

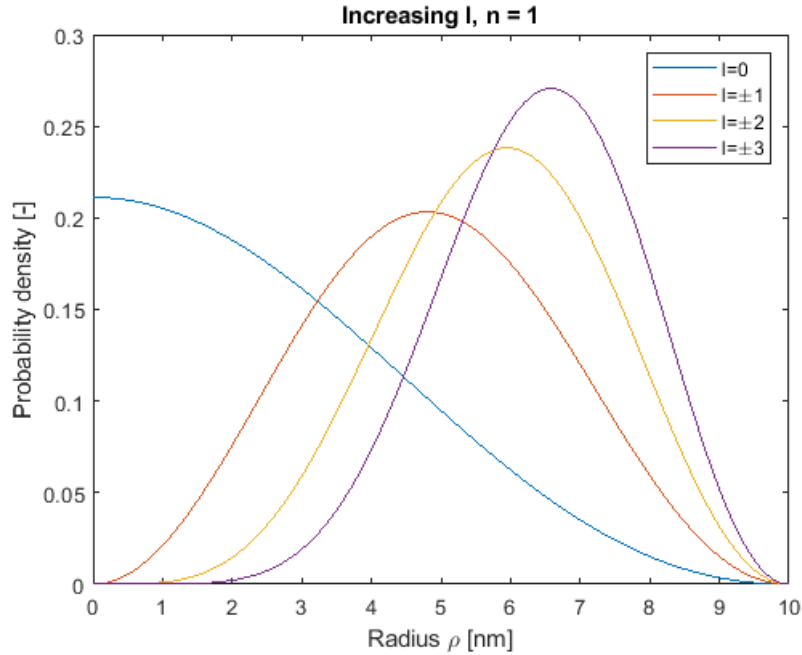


Figure 3: Probability densities as a function of radius ρ for a 10 nm GaAs nanowire. n set to 1 and l increased in increments of 1.

If we instead fix the angular momentum at $l = 0$ and study the four lowest n (for the same wire), we arrive at figure 4. We see that increasing n by one introduces one new node inside the wire, such that the total number of nodes radially can be expressed as $(n-1)$. Roughly, more nodes corresponds to a shorter wavelength and thus a higher energy. This is what we expect as a higher n means we have a larger $\alpha_{n,l}$, which by equation (8) gives a higher energy.

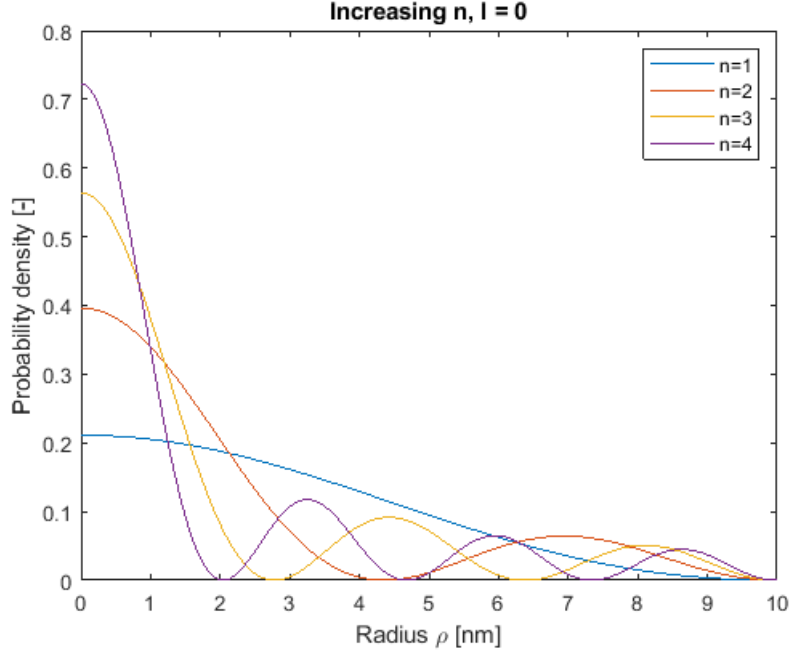


Figure 4: Probability densities as a function of radius ρ for a 10 nm GaAs nanowire. l set to 0 and n increased in increments of 1.

4. Density of States

The density of states per unit length along the wire, n_{1D} , can be derived similarly to Davies [1]:

$$n_{1D}(E) \frac{dE}{dk} dk = 2n_{1D}(k) dk \quad (11)$$

Davies shows $n_{1D}(k) = 1/\pi$. From equation (8) we find dE/dk :

$$\frac{dE}{dk} = \frac{\hbar^2 k_z}{m^*} \quad (12)$$

Also from equation (8), we can express k_z in terms of the energy E (assuming $E > \varepsilon_{l,n}$ for the subband we're considering). We find:

$$k_z = \sqrt{\frac{2m^*}{\hbar^2} (E - \varepsilon_{l,n})} \quad (13)$$

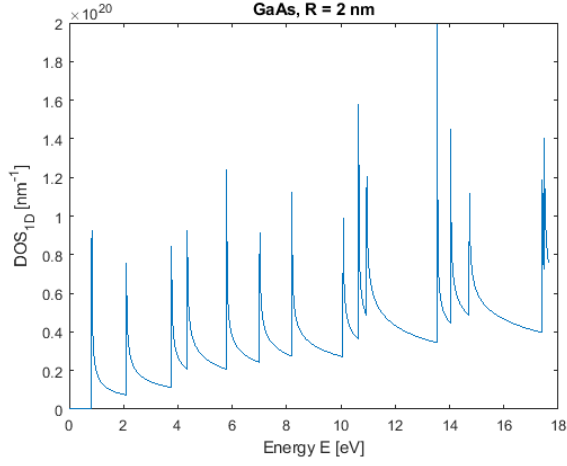
Substituting equations (12) and (13) into (11) one finds the DOS for one subband:

$$n_{1D}(E) = \sqrt{\frac{2m^*}{\hbar^2}} \frac{1}{\sqrt{E - \varepsilon_{l,n}}} \quad (14)$$

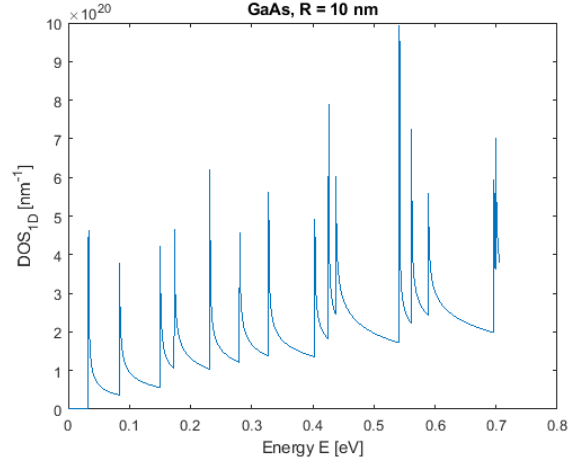
The total density of states at an energy E is the sum of all states across all subbands at that energy. From this and equation (14), with H as the Heaviside function, the total density of states is:

$$n_{1D}(E) = \sum_{l,n} \sqrt{\frac{2m^*}{\hbar^2}} \frac{H(E - \varepsilon_{l,n})}{\sqrt{E - \varepsilon_{l,n}}} \quad (15)$$

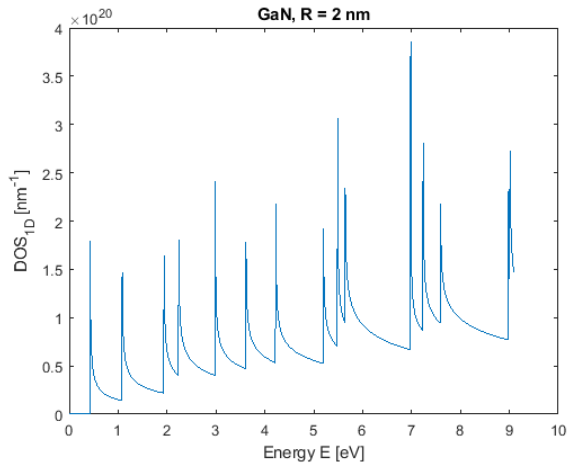
Figure 5 shows the DOS per nanometer for four different nanowires, consisting of GaAs and GaN with radii 2 nm and 10 nm. GaN has an effective mass of $0.13m_0$, which is about twice as large as GaAs' effective mass $0.067m_0$. (At first glance all subfigures of figure 5 look similar,



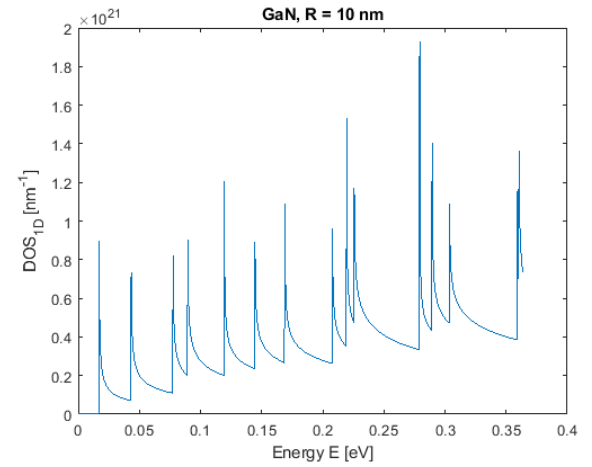
(a) GaAs wire with radius $R=2$ nm.



(b) GaAs wire with radius $R=10$ nm.



(c) GaN wire with radius $R=2$ nm.



(d) GaN wire with radius $R=10$ nm.

Figure 5: DOS per nm for 4 different nanowires made out of GaAs and GaN with radii 2 nm and 10 nm.

but this is only as we've chosen to draw the first 15 peaks - all axes have different scales). In general, the density of states decays proportional to $(\sqrt{E - \varepsilon_{l,n}})$, with a new peak appearing each time the energy enters another subband.

If we increase the radius R or the effective mass m^* , equation (8) shows that the subbands will come closer together (similarly to an infinite square quantum well). This explains why the GaN peaks are denser in energy compared to the GaAs by a factor of two. It also explains why the nanowires with larger radius has peaks closer together in energy.

Interestingly, the peaks seem to protrude from an underlying curve shaped like $\sqrt{E}$. That is also the shape of the density of states in a 3D system, a reminder that we are dealing with a three-dimensional wire that we have confined into a quasi-1D system.

5. Conductance

Like with the density of states, Davies provides a useful starting point for determining the conductance G of our wire, namely equation (16). With T denoting transmission and f the Fermi-function, we have [2]:

$$G = \frac{2e^2}{h} \int_{U_L}^{\infty} \left(-\frac{\partial f}{\partial E} \right) T(E) dE \quad (16)$$

This equation concerns the conductance of a potential barrier with a voltage applied over

it, but we can easily adapt it for our purposes. Firstly since we have no barrier in the wire, we can set the transmission coefficient to 1 (i.e. 100% chance of crossing the "barrier"). Secondly we can change U_L , which denoted the band edge to the left of the barrier, to ε for the bottom of a given subband. This will transform (16) into

$$G = -\frac{2e^2}{h} \int_{\varepsilon}^{\infty} \frac{\partial f}{\partial E} dE = -\frac{2e^2}{h} (f(\mu, \infty) - f(\mu, \varepsilon)) = \frac{2e^2}{h} (f(\mu, \varepsilon) - 0) = \frac{2e^2}{h} f(\mu, \varepsilon) \quad (17)$$

where μ is the chemical potential of the wire. Note that this is the conductance contributed by each subband! The total conductance will thus increase with chemical potential as

$$G_{Tot}(\mu) = \sum_{l,n} \frac{2e^2}{h} f(\mu, \varepsilon_{l,n}). \quad (18)$$

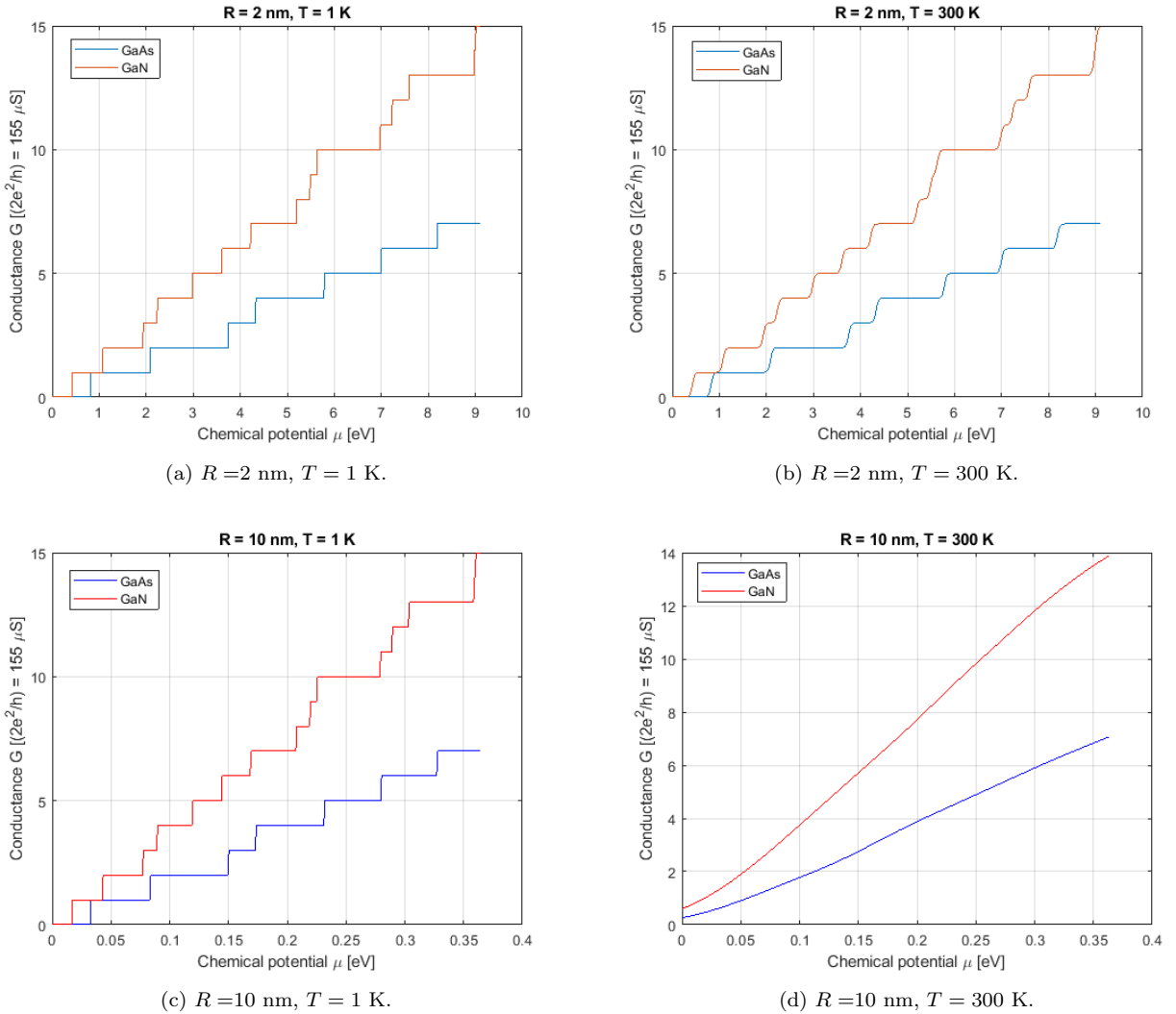


Figure 6: Conductance G as a function of chemical potential μ for GaAs (in blue) and GaN (in red). Radii $R = 2 \text{ nm}$ and $R = 10 \text{ nm}$, and temperature $T = 1 \text{ K}$ and $T = 300 \text{ K}$.

Using equation (18) the conductance G as a function of the chemical potential μ for GaAs and GaN nanowires with radius $R = 2 \text{ nm}$ and 10 nm at temperatures $T = 1 \text{ K}$ and 300 K were calculated. The result is shown in figure 6. Considering the case with a 2 nm wire at 1 K (figure 6a) we see that the conductance acts like a step-function, increasing with one quantum of conductance ($2e^2/h = 155 \mu\text{S}$) each time the chemical potential enters a new subband. As

GaN has a twice as large effective mass, its energy levels are twice as dense in energy, resulting in a quicker growth of conductance.

Comparing figure 6a to figure 6b, where the temperature has been raised to room temperature, we see a slight smearing of the conductance at energies close to the subband edges. This is as the thermal energy, $kT = 25.8$ meV at room temperature, allows some electrons to be thermally excited into the next subband even when the chemical potential is slightly below it. Increasing the radius of the wire to 10 nm, the energy levels come closer together as mentioned earlier. Comparing the conductance of the two wires at low temperature (figure 6a and 6c) the figures look similar except for the fact that the conductance increases quicker with chemical potential for the larger wire, as the energy levels are lower. When raising the temperature to $T = 300\text{K}$, the step-functions seem to disappear and we get a continuous behaviour. This is the same smearing we saw earlier due to thermal excitation. The only difference is that kT is now comparable to the energy range we are studying (in fact kT is around five times the largest energy difference between the subbands drawn!).

Bibliography

- [1] John H. Davies. *The Physics of Low-dimensional Semiconductors*, page 24. Cambridge University Press, 1997. ISBN 9780521484916.
- [2] John H. Davies. *The Physics of Low-dimensional Semiconductors*, page 165. Cambridge University Press, 1997. ISBN 9780521484916.