

# Finite element modeling of strained nanowire heterostructures

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## Abstract

When two materials with different lattice constants are grown together, this generates stress between them, and therefore strain. This strain causes them to have different thermal and electrical properties, and this is especially important on the nanoscale where changes have large impacts.

This project is intended to see if COMSOL can be used as a tool to model how materials respond to lattice mismatch induced strain. One nanowire consisting of three segments was generated. One middle segment of indium phosphide surrounded by indium gallium phosphide, based on locally made nanowires. It is also intended to serve as a base point for further direct research based on data points generated from the project's simulations.

The COMSOL Multiphysics' engine is used to generate simulations of nanowires using a Finite Element Method. The goal with this work is as a demonstration of how this can be easily replicated in the future. The variables tested were wire radius, the thickness of the middle InP, and percentage gallium in the InGaP segments.

The results of the simulations match the theory well, but due to time and scope constraints they could not be compared to the experimental nanowires used as a foundation for the project, so this should be treated as a first step in determining how useful COMSOL is for practically modelling nanowires.

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# 1 Introduction

In just about every modern computing device, from a simple calculator to a supercomputer, transistors are the most vital, basic component. Since the transistors used in the first computers, there have been many innovations regarding material, size, and function. These innovations have reduced the size of a computer from what might fit in a room to what can easily fit in a pocket. The computer industry is approaching the limit of what size reduction can do, and material science seems to be the most likely path forward; using new materials or new forms with useful properties.

Strain is of interest to this as it affects how all transistors behave. Strain is caused by a lattice mismatch, or differences in how the atoms are spaced, that can occur when combining two different materials, and this affects the electrical and thermal properties of the components. Knowing what temperature and currents a transistor can handle before performance starts declining is of course of great importance when making a device.

Strain is also highly relevant in strain engineering, which aims to induce strain in semiconductors to improve performance.

The idea behind this work is examining if there is a natural and straightforward way to simulate the strain caused by lattice mismatch. This is done in an attempt to mimic lab-grown nanowires. These are structures on the scale 10-1000 nm where it extends further into one dimension than it does the two others. The simulations of the nanowires can be compared to theoretical models and the behavior of the actual lab nanowires to determine the accuracy of the model.

The program COMSOL is used to generate a model, and MATLAB is then used to process the results. COMSOL was chosen because of the ease with which models can be produced and altered to test additional variables, and because it can serve as a platform for examining things like heat dependency if anything is built on this project. MATLAB is used because COMSOL only treats the continuous case. The data is exported into MATLAB and each point can then be handled discretely, allowing future examination as to whether these points can be treated like atoms when it comes to diffraction patterns.

The specific model being generated is an 800 nm long nanowire consisting of three segments, arranged as InGaP, InP, InGaP. This configuration was chosen because this kind of wire has been grown locally, and would therefore be simple to compare to.

## 1.1 Acronyms and Abbreviations

QM - quantum mechanics

InP - indium phosphide

InGaP - indium gallium phosphide

FEM - Finite Element Method

PDE - Partial Differential Equation

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## 2 Theory

Classically, materials are described as consisting of atoms taking up discrete points in space. With the advent of quantum mechanics, a description which was much more complicated and accurate was formed. This work avoids the quantum interpretation and aims at simplifications by assuming the materials are classical, and through the use of numerical approximations. In the case of strain, there are no significant quantum mechanical effects within the material, which means the classical case can be considered without any noticeable information loss. In the classical assumption, atoms are discrete and interact only with the closest neighbours. In the one-dimensional case, this could be analogous to a string of beads, as has been depicted in figure 1. The simulations treat only the three-dimensional case. The one-dimensional case is used for explaining the underlying theory, and the two-dimensional case is used to illustrate the effects of a lattice mismatch and strain. This is done for simplicity of presentation, and their implications extend into further dimensions.



Figure 1: Classical atoms in one dimension

### 2.1 Stress and strain in one dimension

Stress in a solid leads to its deformation or strain. If stress is applied, a point in the material  $x$  is displaced by  $u$  depending on the amount of stress applied to the material by for example pulling one end while keeping the other stationary. This is illustrated in figure 2, where a section of length  $X$  is strained to length  $U$ , making the relative length of the section  $e = \frac{dU}{dX}$ . The strain  $e$  is unitless and measured as difference relative to the original length of the strained object.

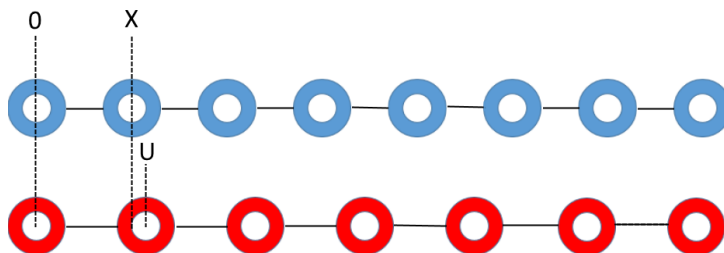


Figure 2: Example of one-dimensional strain, where a one-dimensional chain of atoms are strained by a factor  $u$ .

### 2.2 Stress in three dimensions

In three dimensions, the stress  $\sigma$  (force per unit area) can be described with a symmetric second-degree tensor representing the stress along different axes. This tensor is displayed in equation 1.



$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} \quad (1)$$

Stress can be described using only three components; uniaxial, shear and hydrostatic stress. Uniaxial stress is stress along the first, second, and third axis, represented by  $\sigma_{11}$ ,  $\sigma_{22}$ , and  $\sigma_{33}$  in the matrix, and  $\sigma_1$ ,  $\sigma_2$ , and  $\sigma_3$  in the column vector. Shear stress is stress along a plane spanned by two axes, represented by  $\sigma_{12}$ ,  $\sigma_{23}$ , and  $\sigma_{34}$ . Hydrostatic stress, or pressure, is uniaxial stress over all three axes at the same time, where the components are identical  $\sigma_{11} = \sigma_{22} = \sigma_{33}$ . The equation describing strain then becomes 2.

$$\sigma = \begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{11} & 0 \\ 0 & 0 & \sigma_{11} \end{bmatrix} = \begin{pmatrix} \sigma_1 \\ \sigma_1 \\ \sigma_1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (2)$$

### 2.3 Strain in three dimensions

Strain is a direct result of stress on a material, and is the deformation that alters the properties of a material. The strain generated by uniaxial stress ( $\sigma_1, \sigma_2$  or  $\sigma_3$ ) is either compressive strain, which is a decrease in length parallel to the direction of compression, or tensile strain, which is an increase in length parallel to the tension. The strain corresponding to shear stress is called shear strain. A rectangular object being deformed through shear strain would take on the shape of a parallelogram. In this case, the ratio of deformation is measured perpendicular to the surface being considered.

To describe the strain another tensor is needed, similar to the stress tensor. The strain tensor is described by equation 3, and each element  $e_{ij}$  of the matrix is described by equation 4. In this equation,  $i, j = 1, 2, 3$  represent the first, second and third dimension respectively, and  $\frac{du_i}{dx_j}$  is an extension from the one dimensional case.

The tensor can be simplified into a column vector with six components, the same number of independent components the tensor has. As before, the diagonal components  $e_{11}$ ,  $e_{22}$  and  $e_{33}$  correspond to  $e_1$ ,  $e_2$  and  $e_3$  in the column vector.  $\frac{1}{2}(e_{32} + e_{23})$  corresponds to  $e_4$ ,  $\frac{1}{2}(e_{13} + e_{31})$  corresponds to  $e_5$ , and  $\frac{1}{2}(e_{12} + e_{21})$  corresponds to  $e_6$ .

$$\begin{bmatrix} e_{11} & \frac{1}{2}(e_{12} + e_{21}) & \frac{1}{2}(e_{13} + e_{31}) \\ \frac{1}{2}(e_{12} + e_{21}) & e_{22} & \frac{1}{2}(e_{32} + e_{23}) \\ \frac{1}{2}(e_{13} + e_{31}) & \frac{1}{2}(e_{32} + e_{23}) & e_{33} \end{bmatrix} = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \\ e_6 \end{pmatrix} \quad (3)$$

$$e_{ij} = \frac{1}{2} \left( \frac{du_i}{dx_j} + \frac{du_j}{dx_i} \right) \quad (4)$$

For  $i = j$ , or  $e_{xx}, e_{yy}, e_{zz}$ , this is the tensile or compressive strain. The sum of these gives the change in volume  $V$ .

$$\frac{\Delta V}{V} = \sum_{i=1}^3 e_{ii} \quad (5)$$

$e_{ij}$  when  $i \neq j$  is the resulting rotation around the axis not used.  $e_{12} = -e_{21}$  is the counter-clockwise rotation around the z-axis.

## 2.4 Poisson's ratio

Compressive and tensile strain both go under the term linear strain, caused by uniaxial stress. Lateral strain is the strain resulting from the same uniaxial stress, in all direction perpendicular to the stress. Poisson's ratio  $v$  is unitless and tells us the ratio between lateral strain  $e_l$  and axial strain  $e_s$ , and is expressed in equation 6. The minus in the equation is convention to make Poisson's ratio positive. Most materials vary between  $0 \leq v \leq 0.5$ , with cork  $v \approx 0$ , showing little expansion when compressed. Rubber has  $v \approx 0.5$  and expands laterally at a much greater rate. Some auxetic and anisotropic materials display a negative and greater than 0.5 Poisson's ratio respectively, but this project restricts itself to  $0 \leq v \leq 0.5$ .

$$v = -\frac{e_l}{e_s} \quad (6)$$

## 2.5 Young's modulus

Axial stress gives rise to axial strain. The axial strain of an object tells us the change in length compared to the original length of the material. Young's modulus  $E$ , described in equation 7, tells us the ratio between the axial stress  $\sigma$  (force per unit area) a material is experiencing, and the resulting axial strain  $\epsilon$ . It is in a sense an expression of the stiffness of a material, where the larger Young's modulus is, the stiffer and more resistant to the effects of stress a material is.

$$E = \frac{\sigma}{\epsilon} \quad (7)$$

## 2.6 Describing a crystal structure

Crystals are materials with a regular, periodic arrangement of atoms. One way to formalize the periodicity description is through a Bravais lattice  $\mathbf{B} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$ , where  $n_i$  is an integer, and  $\mathbf{a}_i$  is a primitive vector, where all three form a three-dimensional lattice. In figure 3, a two-dimensional example can be viewed. If extended into three dimensions the third vector  $\mathbf{a}_3$  would be extruding towards the viewer.

For this work, only a cubic lattice is considered, where all angles  $\theta = 90^\circ$ , and the vectors  $a_1 = a_2 = a_3$ .

The smallest possible repeating pattern in a cubic lattice does not necessarily correspond to a pattern with one particle in each corner, as in the case of figure 3. The internal structure of particles within the smallest repeating pattern can be much more complicated but is not directly described through a Bravais lattice.

The description used for crystalline materials is all under the assumption that there are no anomalies or structural defects. The perfect Bravais lattice spans all directions

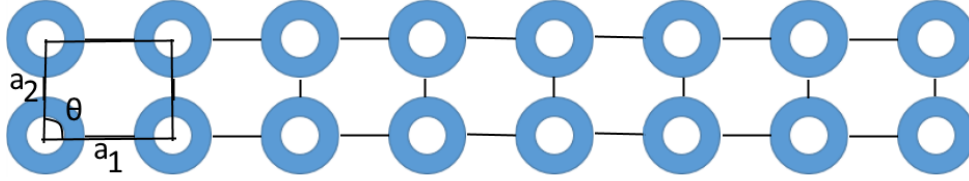


Figure 3: A two-dimensional Bravais lattice where the angle  $\theta = 90^\circ$  and the primitive vectors  $a_1 \neq a_2$

to the edge of the material, with no abnormalities. If there is a defect in a crystal, its properties are altered from the idealized version, especially regarding the change in properties that emerge from strain. Imperfections can be a foreign atom that does not fit into the otherwise perfect lattice or more macroscopic effect such as cracks or edges. The materials examined in this work is assumed not to have any such defects.

## 2.7 Lattice mismatch

Different crystals have different lattices dependent on its atomic properties, for example size and how its constituent atoms bond.

A lattice can have three lattice constants as they need to be described in three directions, much like the Bravais lattice. In the simplest and most common case of a cubic lattice, they can be described using only one constant as  $n_1 = n_2 = n_3$ . Both InP and InGaP are cubic crystal systems and therefore have only one lattice constant. The difference between the InP and InGaP lattice constant is linearly dependent on the percentage of indium and gallium in a sample, varying between  $5.8687 \text{ \AA}$  for pure indium phosphide and  $5.4505 \text{ \AA}$  for pure gallium phosphide.[1]

Heterostructures are created when a material is grown on another. This process is called heteroepitaxy. One material functions as a base for deposition of another layer through a variety of methods employed in the field of nano-science. The interface between two materials forming a heterostructure is referred to as a heterojunction.

When two materials with different lattice constants form a heterostructure, both materials try to adapt to each other's lattices. This generates stress along the heterojunction, which results in the materials being strained. An example of this can be seen in figure 4, where the strain causes some atoms in the lattice to be uncoupled, leading to an edge dislocation. A change in temperature can also generate stress. If two materials bonded together expand at different rates, the differences between their lattices increase with temperature, leading to strain.

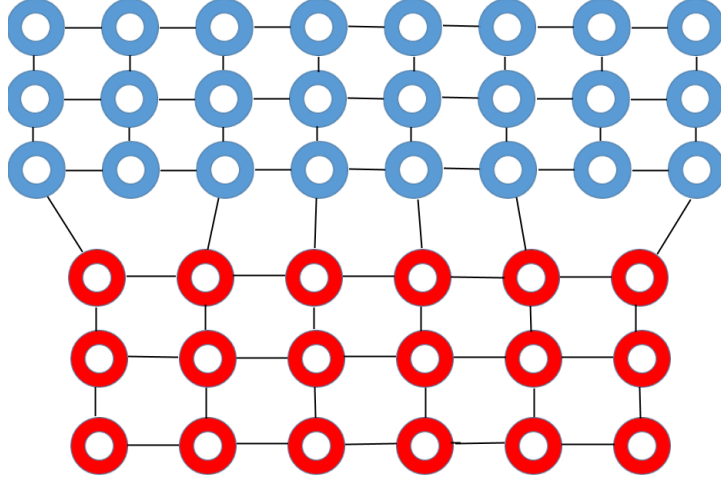


Figure 4: Lattice mismatch illustration with edge dislocations

## 2.8 Finite Element Method

Physical problems dependent on several variables can be described well using Partial Differential Equations (PDE's). A PDE of the function  $f(x_1, \dots, x_n)$  has the general formula 8.

$$F(x_1, \dots, x_n, f, \frac{du}{dx_1}, \dots, \frac{du}{dx_n}, \frac{d^2u}{dx_1 dx_1}, \frac{du}{dx_1 dx_n}, \dots) = 0 \quad (8)$$

COMSOL solves a time-independent PDE displayed in equation 9, based on Hooke's law, where  $\nabla \cdot S$  is the divergence of the stress tensor displayed in equation 1,  $F$  is body force per unit volume,  $\rho$  is the mass density, and  $u$  is the displacement.

$$\nabla \cdot S + F = \rho \frac{d^2u}{dt^2} = 0 \quad (9)$$

The  $S$  in equation 9 is composed of the stresses and strain present in the material, displayed in equation 10.

$$S = C : \epsilon_{el} \quad (10)$$

$C$  is a 4th order 6 by 6 stiffness tensor unique to each material and  $\epsilon_{el}$  denotes the tensor of initial strain the wire is experiencing. In this work, the initial strain is only dependent on the difference in lattice constant between the two materials.  $A : B = A_{ij}B_{ij}$  denotes the inner product of two tensors.

In general PDE's are not solvable analytically except for very simple cases, and this is the case with this equation as well. The Finite Element Method (FEM) is used to reach a numeric approximation. The geometry over which we wish to calculate the displacement gets divided into simple subdomains and equation 9 is solved for each individual subdomain.

## 3 Method

The physics modelling software COMSOL was used to generate a model of a nanowire and perform calculations on this geometry. MATLAB was then used to process the results and generate graphs.

### 3.1 COMSOL

In COMSOL Multiphysics', there is a standard workflow for creating a model. Using the Computer-Aided Design software (CAD), you start by designing the geometry of the object by assigning parameters such as height, width or radius. Then the material parameters are added, such as density or heat capacity.

There is already an extensive material database included in the COMSOL packages, but the materials used in this project were not included in the database, so the values used were found online[1]. The three parameters that a strain and deformation model needed were density, Young's Modulus, and Poisson ratio. More parameters can be added depending on the type of study you are designing.

There also needs to be some initial values, such as which parts are free to move or expand, depending on if something counts as locked to another section or simply locked in space. As the FEM requires at least one part of the object to be spatially locked, the base of the wire was fixed in place. The study was performed under the assumption that the strain is not time-dependent.

The geometry created for the study is split up into smaller elements, called a mesh. The mesh is used to perform the calculations with the FEM. The mesh is highly adaptable regarding size and shape of sections, allowing for some areas to be solved in greater detail. Selecting the shape of the mesh is an important balancing act, as an extreme towards either too small or too large elements can cause the calculations not to converge.

### 3.2 COMSOL Recipe

#### 3.2.1 Geometry

The first thing COMSOL needed to operate was model parameters. The geometrical parameters specified were the radius and length of each wire segment. A wire consisted of alternating segments of InGaP, InP, InGaP, with the specific values used viewable in table 1. The InP segment length was made variable to keep the wire a constant length and therefore more easily comparable. All wires started growing at  $z = 0$  and expanded height-wise in the positive  $z$  direction, and radially from  $(x, y) = (0, 0)$ .

Several versions of the model were created in COMSOL, varying wire diameter, the percentage of gallium in the outer sections, and length of the midsection. Versions were created where there were two InP sections to see how much they affected each other, as the wires the simulations were shaped after had several sections of differing length on the same wire. As the distance between these segments in the experimental wires was several 100 nm and the strain from the InP segments did not affect each other until close to 50 nm, it was determined that they could be treated as isolated segments. As the results for modelling only one at a time were accurate and provided a significantly reduced computation time, the only variations with multiple segments of InP that were attempted were done to confirm that their effect was negligible. Therefore each simulation featured only contains one midsection of a different material.

|                      |                 |
|----------------------|-----------------|
| Wire radius          | 88 nm           |
| Total length         | 800 nm          |
| InP segment length   | 45 nm           |
| InGaP segment length | (Total-InGaP)/2 |

Table 1: Values used for the geometry

Two work planes were defined in the model, spanning the XY plane, located 50 nm from either side of the middle segment. These are later used to broaden the fine area in the mesh. To allow easy comparison between samples the total length of the sample was kept constant between runs, and to do this while varying the middle segment length the two InGaP segment lengths had to be defined as the difference between the middle segment length and the total length.

### 3.2.2 Material parameters

The InGaP's percentage of Germanium ( $x=15\%$ ) was used in the formula for determining density, Young's modulus and Poisson ratio with the highest possible accuracy.[1]

|                 | InGaP                          | InP                  | Unit       |
|-----------------|--------------------------------|----------------------|------------|
| Density         | $4.81 - 0.67 \cdot x$          | 4.81                 | $g/cm^3$   |
| Young's Modulus | $(6.11 + 4.19 \cdot x)10^{11}$ | $6.11 \cdot 10^{11}$ | $dyn/cm^2$ |
| Poisson's ratio | $0.36 - 0.05 \cdot x$          | 0.36                 | 1          |

Table 2: Values used for the Base case

When comparing the effects of the gallium percentage in the InGaP segment, the InP segment was assumed to have a lattice constant of 5.8687 Å, and the InGaP segment  $5.8687-0.4182x$  Å, where  $x$  is the % gallium in the segment.[1]

### 3.2.3 Mesh

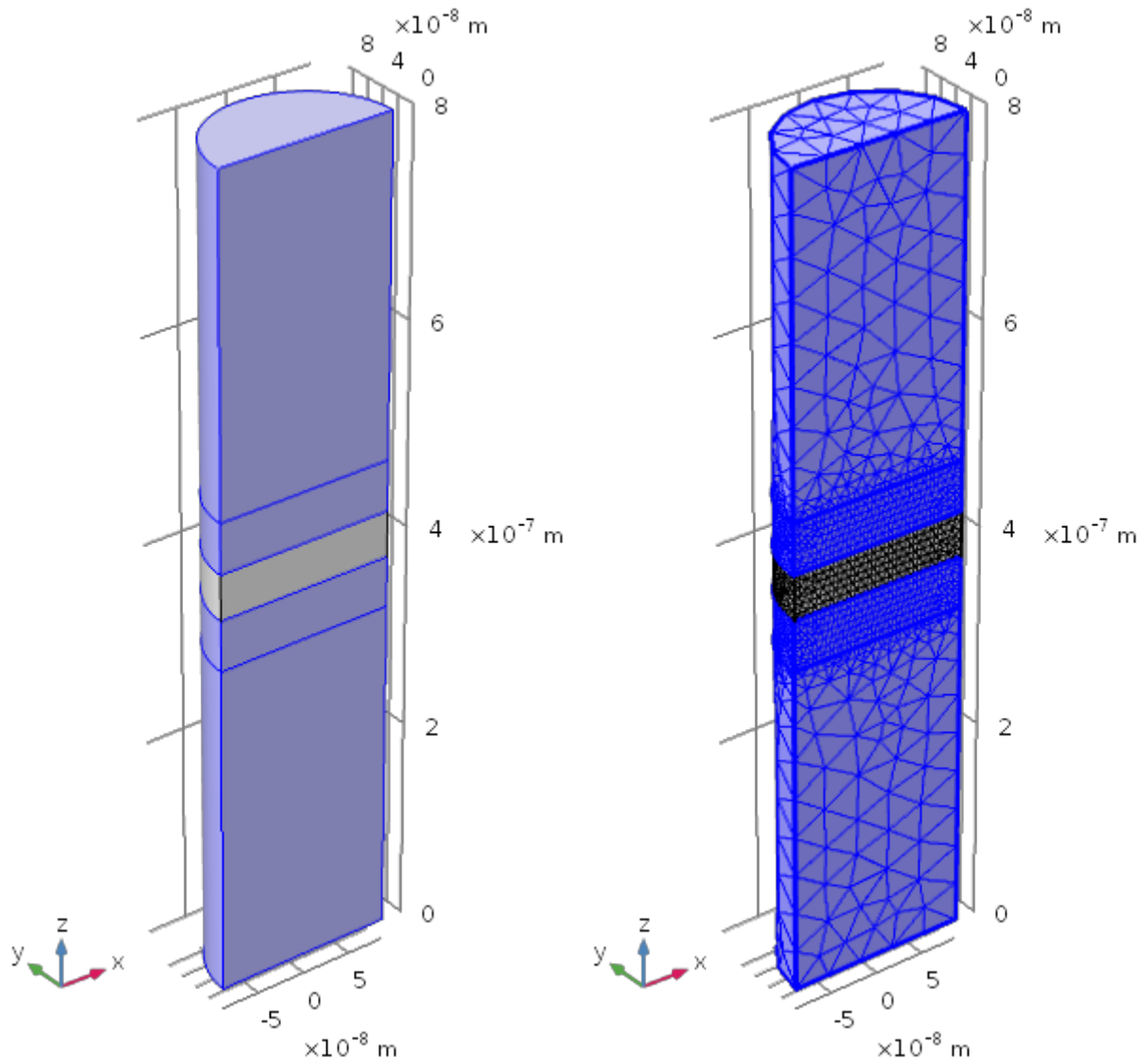
A rough and a fine mesh were created during the model creation. The rough mesh was created to get a ballpark estimate of how the results would look without having a computation time of 10-20 minutes per variation using the finer mesh. This turned out to be a balancing act because if the mesh is too rough the results never actually converge. COMSOL still attempts the calculation and gets stuck in a seemingly infinite loop. Once everything had been tested and determined to work, only the fine mesh was used to generate results.

For the fine mesh used, the maximum element size was 40 nm. The minimum element size was the radius/10. This was done to keep the number of data points consistent when doing iterations with different radius, as maintaining a constant element size meant the number of elements along the nanowire varied. The area of the InGaP segment, as well as 50 nm around the segment, had a geometry scaling of 4.5 in all direction, making it finer. A maximum element growth rate of 1.5 controlled the transition between the coarser and finer parts of the mesh and allowed for coarser mesh sizes in the less interesting areas. There was no need to have an extra fine transition as the areas around the segment were designed to be finer already. The curvature factor was 0.6, where the lower the value the finer the mesh along curvature. This offers a higher resolution of the curved areas which

in the cylindrical case is along the entire geometry. The resolution of narrow regions controls the number of layers in the mesh in narrow regions. This was set to 0.5 as there were no narrow regions of interest within the structure.

The model geometry generated and used can be viewed in figure 5a. Along the wire, four XY planes are defined. The two center planes define the middle segment, and the two outer planes define the area of greater interest. In figure 5b, the mesh can be viewed. When the radius and middle segment thickness were altered for the study, the mesh necessarily had to adapt to fit these new shapes, and therefore the mesh is not microscopically identical in all cases.

As the results did not have the same geometry, the data points generated did not have the same spatial distribution. It was therefore not possible to export the data into a single file except in the case of varying percentage gallium in the sample, where the geometry of the mesh was identical.



(a) A slice of the base sample's geometry.

(b) A slice of the base sample's mesh.

Figure 5: Nanowire model generated in COMSOL Multiphysics. The blue sections are InGaP, the grey sections are InP.

## 4 Results

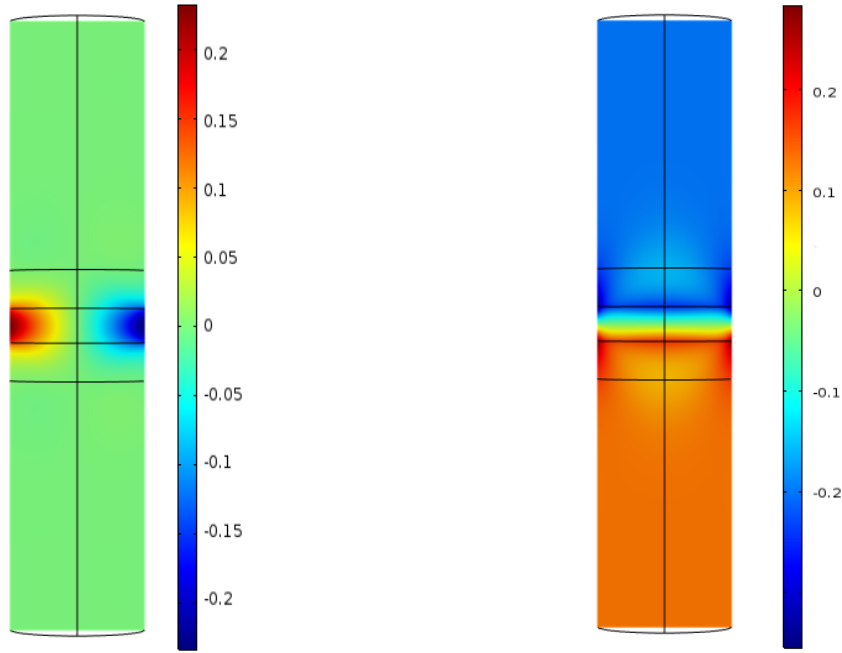
MATLAB was chosen as a processing tool because it was of interest to continue with a discrete model. COMSOL provides a good model creation tool, but comparing results leaves something to be desired. Having individual data points and several ways to plot and overlay them means it is easier to construct a good visual representation of the results in MATLAB. MATLAB also allows you to examine the values and properties at different points whereas COMSOL is limited to visual comparison.

In figure 6 the results from the strain on a 45 nm midsection, 15% gallium, 88 nm radius sample are visible. This is the "base" sample, used as a reference point for when altering variables. When varying midsection thickness, gallium percentage or radius, all but the chosen variable remain those of the base sample. The results are consistent with previous similar simulations[4] and expectations of symmetry about the origin. The magnitude of displacement is as expected given a strain around 1.2%. All simulations were made with the wire growing along the positive Z-axis. As there was no meaningful distinction between the symmetrical X and Y axes, the Y-axis was omitted from the graphical results. In COMSOL, a slice of the geometry was extracted at  $y = 0$ , and the resulting displacement heat maps can be seen in figures 6a and 6b.

Heat maps of the same sample were generated in MATLAB for the sake of comparison in figure 6c and 6d. In these figures, each data point is a point in space associated with three displacement values. Comparing the MATLAB figures to the COMSOL figures shows that MATLAB can generate an accurate representation of the data exported from COMSOL. What MATLAB makes clearer is how few data points there are outside the area of interest. This is because one point of data is generated for each element in the mesh, see figure 5b. COMSOL does not display this, and instead gives the illusion of fully continuous data.

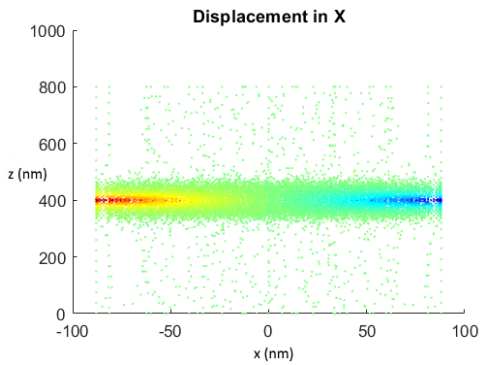
For clarity, the graphs have been split into the X (figure 6a and 6c) and Z (figure 6b and 6d) components of the displacement when generating this heat map.



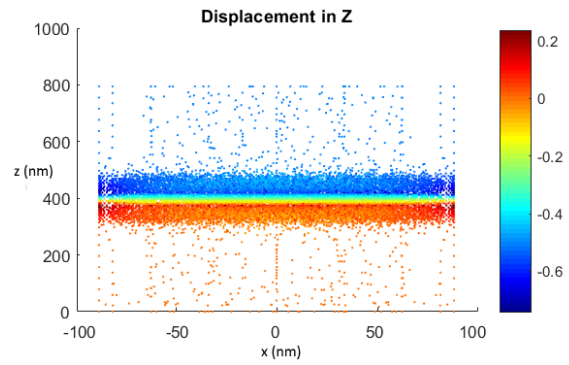


(a) Displacement in the x direction in the  $y=0$  plane of a nanowire. The displacement is symmetric about the center of the plane. The figure is exported from COMSOL, where the nanowire was simulated

(b) Displacement in the z direction in the  $y=0$  plane of a nanowire. The displacement is symmetric about the center of the plane. The figure is exported from COMSOL, where the nanowire was simulated



(c) Displacement in the x direction from the same data as (a), but plotted using MATLAB's scatter plot function



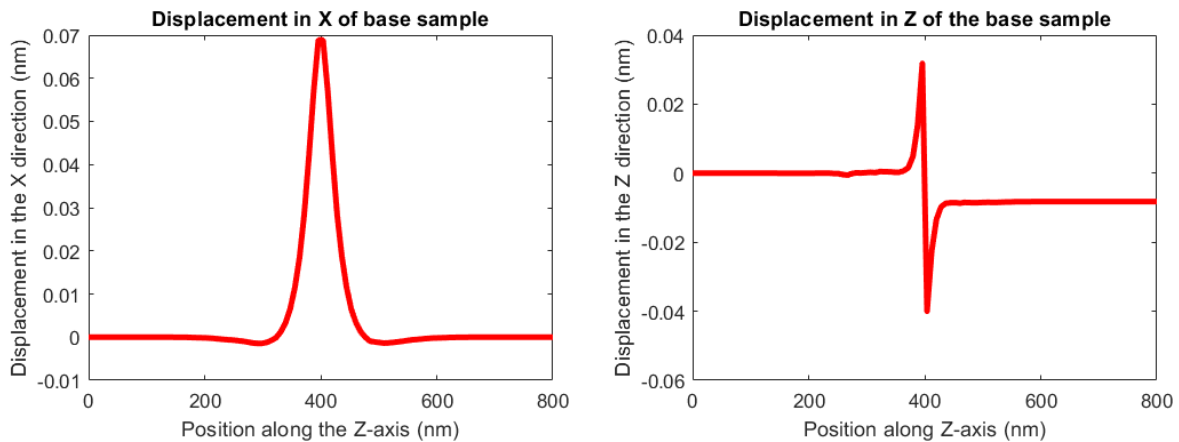
(d) Displacement in the z direction from the same data as (b), but plotted using MATLAB's scatter plot function

Figure 6: Simulation of displacement in a nanowire with length 800 nm and radius 88 nm, in the x and z direction as represented by COMSOL and MATLAB

## 4.1 Reference sample

Figure 7 shows the behavior of the reference sample, where 7a is the displacement along the X-axis, and 7b is the displacement along the Z-axis. This does not represent the maximum displacement in the sample, but the displacement generated along the 1/4 point in the x and y dimensions. The data is therefore gathered around  $(44,44,z)$  (nm). As the measurements are taken on both sides of the center (400 nm) along the z direction,

but only on the positive side of the center in the x direction, both the positive and negative displacements are visible in the z direction, but only the positive in the x direction. A measurement taken along  $(-44,-44,z)$  would have an identical graph of displacement in z, but inverted in x. Along the  $(44,44,z)$  line the displacement in the x-direction peaks at 0.07 nm in the middle of the nanowire, and the displacement in the z-direction has one peak on either side of the middle, at 0.03 nm closest to the base of the wire, and -0.04 on the other side. These peaks are the regions of interaction between the two materials and contract sharply, leading to a positive peak to the left of the center and a negative peak to the right of the center. The point of symmetry between these peaks is located at around -0.005 nm as the nanowire is spatially locked in one end. When it then contracts it moves all matter outside the middle a tiny bit, yielding a displacement of the same magnitude at all points to the right of the middle.



(a) Simulated displacement in the x direction of a nanowire grown in the z direction

(b) Simulated displacement in the z direction of a nanowire grown in the z direction

Figure 7: Reference nanowire, a simulation with a radius of 88 nm, a middle segment thickness of 45 nm, and the InGaP segments containing 15% gallium, measured along  $(44 \text{ nm}, 44 \text{ nm}, z)$ .

## 4.2 Varying the radius of the sample

Increasing the radius of the sample means that there is a larger area over which the different materials interact, which causes more strain and therefore more displacement. The amount of displacement is proportional to the area of the sample, and so is not linear but follows the radius squared.

The displacement in the x-direction has a narrow peak with the same general shape as the reference sample, as can be seen in figure 8a. There is no significant widening of the peak relative smaller radii. The effect of increasing the radius gets less pronounced the more the radius increases, where the difference between 40 nm and 20 nm is much greater than between 140 nm and 100 nm.

The z-direction displacement also behaves similarly to the reference sample, as can be seen in figure 8b. As the radius increases, the peaks get larger, and the point of symmetry gets more negative.

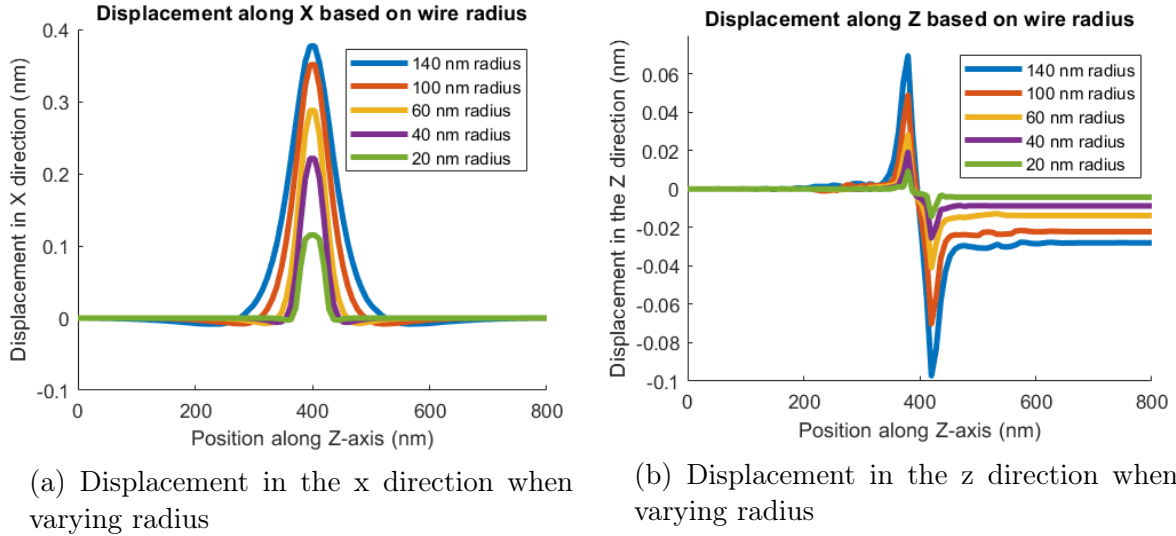


Figure 8: Simulated displacement of a nanowire grown in the z direction. All values apart from the radius were kept constant, and measured along (44 nm, 44 nm, z).

### 4.3 Varying segment thickness

When varying the thickness of the middle segment, the greatest change is the width of the area affected, as can be seen in figure 9. At a heterojunction, the materials attempt to adapt to each other, and the more support behind it a material has the more resistant it is to adapt, which leads to an increased strain. The thicknesses for the middle segments were chosen because these were the values from the nanowires the study was based on.

The displacement in the x-direction has a wider peak the thicker the sample is, as can be seen in figure 9a. This is not so much that the effects penetrate deeper out from the heterojunctions, but because the heterojunctions themselves are pushed away from the middle of the nanowire. The magnitude of displacement increases with thickness, but the effect eventually tapers off. The displacement difference between 170 nm and 80 nm is smaller than between 80 nm and 45 nm. At some point, there will be no appreciable difference when increasing the thickness, as this means there is just more material unaffected in between the heterojunctions.

The displacement in the z-direction follows similar patterns where the displacement locations are pushed away from the middle, as can be seen in figure 9b. A more gentle slope is introduced between peaks as the heterojunctions affect each other less, and the strain can be distributed over the distance. The difference in magnitude is much less pronounced than in the case of radius as a variable. At 80 nm thickness, the magnitude of displacement is smaller than for 45 nm and 19 nm thickness.

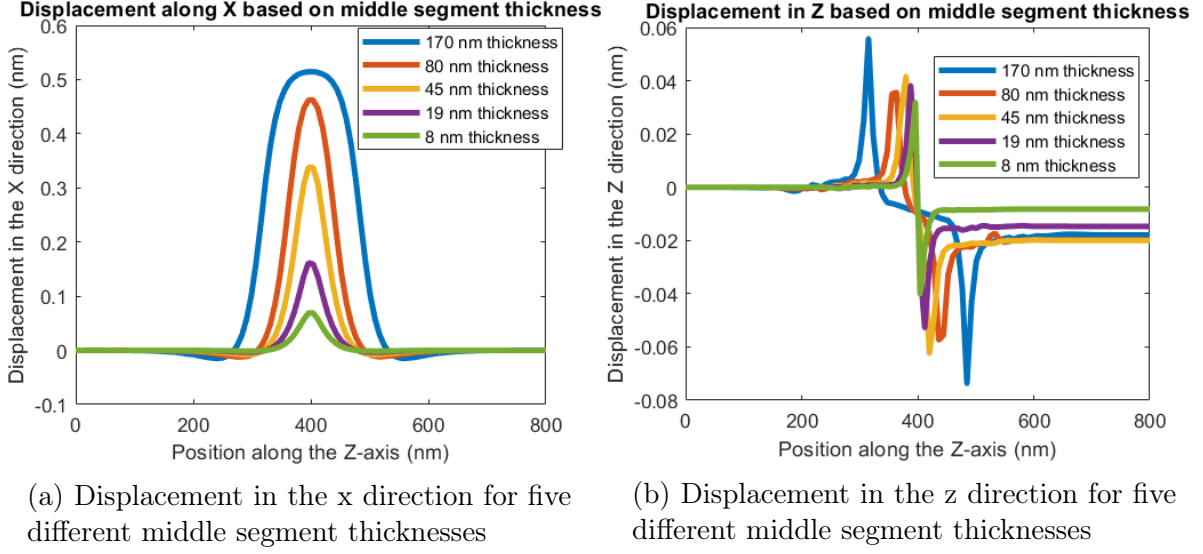


Figure 9: Simulated displacement of a nanowire grown in the z direction. All values apart from the thickness of a middle segment of InP and the surrounding InGaP segments were kept constant. The displacement was measured along (44 nm, 44 nm, z).

#### 4.4 Altering percentage of gallium

Varying the percentage of gallium in the sample showed the greatest effects, compared to radius and middle segment thickness. With 0% gallium, the wire is essentially only one long segment of InP, with no difference in the lattice constant and therefore no strain. As the percentage of gallium in the sample increases, the lattice constant for the outer segments increases, and the rising difference between the two lattice constants give rise to a linearly increasing strain.

The magnitude of displacement reached up to 2.5 nm in the x-direction (figure 10a), and 4 nm in the z-direction (figure 10b) with 100% gallium in the outer segments, compared to 0.07 nm and 0.04 nm respectively for the reference sample. The displacement in both the x and z directions behave similarly to the displacement when varying thickness of the middle segment and radius, only much larger. Like previously, when looking at displacement in the z-direction, the magnitude of peaks and center point location vary, but the most important effect is the displacement of the sample as a whole occurring to the right of the middle, which completely dwarfs any differences in peak magnitude.

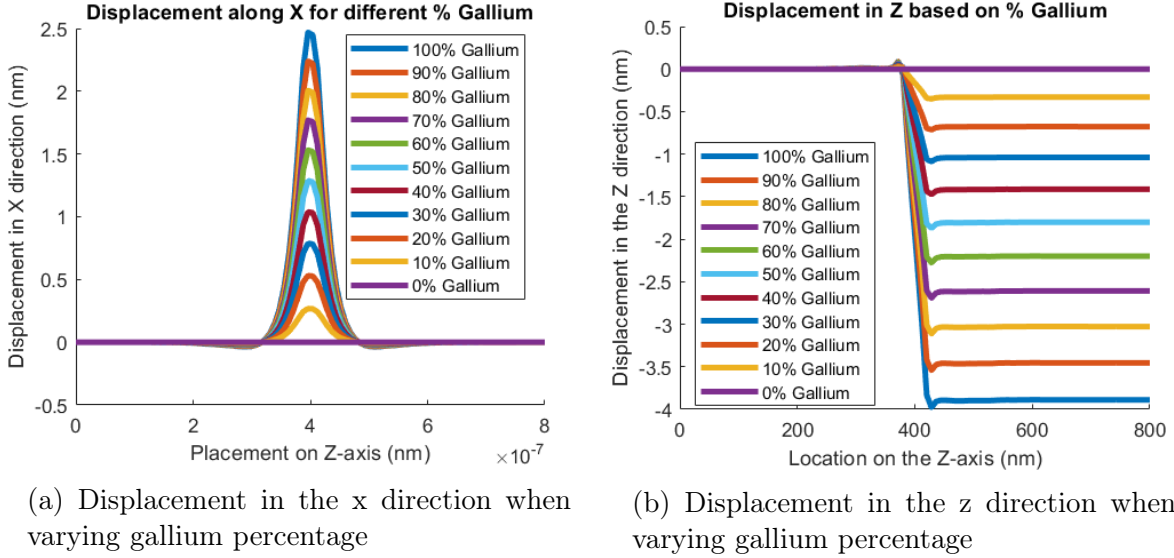


Figure 10: Simulated displacement of a nanowire grown in the z direction. All values apart from the percentage gallium in the outer segments were kept constant. The displacement was measured along (44 nm, 44 nm, z).

## 5 Conclusions

At the level of growth and precision involved in making nanowires, it is not only possible but rather straightforward to make a simulation of them. As there is no issue with impurities the flawless simulation model is closer than what might be achievable when creating structures on a macro scale; this means COMSOL and its uniform handling of materials is applicable for this specific scenario. COMSOL is therefore most useful when predicting results from the slower more expensive methods of creating nanowires, which are used because they produce better results. The results have not been compared to experimental nanowires as this was outside the scope of this work. There is still the possibility that the FEM has a large enough difference to reality as to not make it viable. The continuous elements of matter making up the mesh is different enough from the atomic model that this may play a role at this scale.

Most of the results were as expected from established theory. Varying the segment thickness generated one abnormal result where the displacement magnitude was reduced with increasing thickness. This could be due to an anomaly along that particular part of the nanowire, but this was not examined further due to time constraints. The anomaly cannot be easily spotted when examining the data in a more complete but less easily displayed way.

The limiting factor in producing results with this method was time, as this project was limited in scope and computing power. A finer mesh would assuming convergence of results always mean a more accurate picture presented.

## 6 Outlook

The aim of this work was not to challenge previously established findings or to be a giant leap in the progress of material physics. The question is whether this software combination is a useful tool for the future, and to serve as inspiration for what worked for

future inquiries along the same lines. The models generated proved to follow established theory and leaves several questions to be investigated for the future. How useful is the discrete data for further simulations? Can this method be effective for more simulation space, like varying materials or temperature of the sample? This could all be answered in time but was not due to the limitations of the project.

The recipe and methods used are included in such detail to allow easy replication, so the hope is that future research gains something useful from what is used in this work and that it can allow further questions to be both asked and answered in the future. The theory included is kept focused and simple so that no outside reading apart from COMSOL documentation is necessary for project reproduction.

Apart from the general hope that this inspired future research, the data generated is also going to be used as a foundation for further studies. Under the assumption that the data points extracted from COMSOL behave atomically, can X-ray diffraction be accurately simulated?

## 7 Acknowledgements

I would like to thank my supervisors, Jesper and Sanna, for showing me how research gets done and helping me grow. I would also like to thank my family, who believed in me and always showed interest in the dullest of material, and my girlfriend Rebecca, who kept me sane when all hope seemed lost, and also my friend Julie, who inspired and believed in me even though she did not need to.

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