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RESEARCH ARTICLE

REVISED Machine Learning Inspired Nanowire Classification Method based on Nanowire Array Scanning Electron Microscope Images

[version 2; peer review: 2 approved, 1 approved with reservations, 1 not approved]

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Abstract

Background

This article introduces an innovative classification methodology to identify nanowires within scanning electron microscope images.

Methods

Our approach employs advanced image manipulation techniques in conjunction with machine learning-based recognition algorithms. The effectiveness of our proposed method is demonstrated through its application to the categorization of scanning electron microscopy images depicting nanowires arrays.

Results

The method's capability to isolate and distinguish individual nanowires within an array is the primary factor in the observed accuracy. The foundational data set for model training comprises scanning electron microscopy images featuring 240 III-V nanowire arrays grown with metal organic chemical vapor deposition on silicon substrates. Each of these arrays consists of 66 nanowires. The results underscore the model's proficiency in discerning distinct wire configurations and detecting parasitic crystals. Our approach yields an average F1 score of 0.91, indicating high precision and recall.

Conclusions

Open Peer Review

Approval Status ✗ ✓ ✓ ?

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Any reports and responses or comments on the article can be found at the end of the article.

Such a high level of performance and accuracy of ML methods demonstrate the viability of our technique not only for academic but also for practical commercial implementation and usage.

Keywords
computer vision, nano-materials, nano- wires, image segmentation, machine learning, microscopy imaging, scanning electron microscopy



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REVISED **Amendments from Version 1**

A series of modifications to the article's main body were made following the feedback received from the reviewers. Mentions of the materials used in the nanowires and the types of challenges encountered with electrical interconnects were added, as well as a description of the advantages of using our growth regimen. The maximum tilt angle for the nanowire arrays to be correctly pre processed with our algorithm was specified, as well as the initial composition of the dataset. A statement about the potential of our approach was added to the conclusion. Regarding the supporting information, changes were made to the repository containing the code in an effort to provide comments in the code itself as well as documentation.

Any further responses from the reviewers can be found at the end of the article

Introduction

The size of current transistors is in the range of tens of nanometers, and such ultra-scaled dimensions pose many fabrication challenges[1,2]. One challenge is finding the best way to connect the transistors, as in the best interconnect material and mode. The current industrial standard is to fabricate the interconnect using many conducting layers of metals and their alloys (*e.g.* Cu and Ru)[3,4]. However, metal interconnects offer their own challenges at such small scales such as being bound by the aspect ratio limit in bit rate capacity and cross talk between different electrical lines[5].

To overcome some of these issues, there is growing interest in substituting metal with miniaturized active photonic components for short-range optical interconnects[5–7]. Materials such as III-V semiconductors are known for their superior light adsorption and emission qualities[8,9]. They are currently integrated on silicon (Si) substrates with pick-and-place[10] or wafer bonding methods[11]. This allows manufacturers to avoid defects related to lattice mismatch but limits integration density and alignment precision[12,13]. Monolithic growth of III-V semiconductors on Si can achieve quick, high-precision, simultaneous integration on large wafer scales.

Template assisted selective epitaxy (TASE) allows high defect control when growing III-V nano- and microstructures monolithically on silicon[14,15]. Analysis of the evolution of the growth front in TASE-grown heterostructured III-V nanowires is fundamental to ensure homogeneous heterolayer thickness[16] and composition, in the case of ternary III-V compounds[17]. Achieving high uniformity across the entire wafer surface is critical, as these factors affect the optical behavior of the device.

Heterostructured III-V micro- and nanostructures are usually analyzed using scanning transmission electron microscopy (STEM) to determine the evolution and stability of the growth front[18,19], as well as the presence of crystalline defects[20,21]. STEM analysis has shown[19] that stabilization of the growth front tends to occur early in the growth process. This stabilisation improves the growth rate and geometry uniformity in TASE grown III-V nanowire. As a result, contact design is simplified, compared to previous experimental results where the metallic deposition area had to be defined on a wire by wide basis[16]. However, sample preparation for STEM is long and destructive[22], making scanning electron microscopy (SEM) preferable for yield and reproducibility studies.

For the samples presented in this work, we selected growth conditions that stabilize a single {1 1 1} facet as a growth front perpendicular to the wafer surface for nanowires containing heterolayers of InP and InGaAs grown directly from a silicon seed[19,23]. From this knowledge, it is already possible to classify the wires as perfect from an SEM top-down view of the wire if the seed facet and the end facet are parallel along the growth direction and as defective otherwise.

When growing densely integrated submicrometer-sized III-V crystals, the current approach of manually cataloguing different growth outcomes on even a 2 cm × 2 cm chip becomes a very time-consuming and tedious process. One way to decrease the time requirements of such a study is to use machine learning (ML) methods. ML is a powerful tool for handling large amounts of data and has found application in materials science for various tasks. Classification[24,25] and segmentation[20] of electron microscopy images can be used to deduce device properties, if the images contain sufficient information[26]. ML models for identifying different types of nanostructures, such as the difference between nanowires, nanoparticles, and nanoporous substrates, have been shown to have extremely high accuracy[27]. However, models that are tasked with segmentation often do not perform as well[28].

Classifying images containing multiple objects with fine differences is complex because the variability between nanowire images is of the same magnitude and quality as the target imperfections. Additionally, SEM images contain a high degree of noise that impedes the performance of traditional classification methods[29]. Due to the large number of images, this process can benefit from automatization[30], especially when the need to use a less resolved and time-consuming characterization method arises[31].

Hence, to tackle some of the abovementioned problems, we describe a novel ML-based approach in this paper. For the purpose of this work, we introduce and characterize a new dataset for nanowire classification. Finally, we evaluate the performance of our method on the aforementioned dataset and discuss future research areas.

This article makes the following contributions to the current state of the art:

1) To the best of our knowledge, this work shows the first kernel-based splitting algorithm for III-V nanowire array SEM images.

2) Our work provides a new nanowire classification dataset containing annotated images of III-V nanowire arrays.

3) In this work we demonstrate the performance of a compact convolutional neural network (CNN) classifier on the aforementioned dataset.

Methods

To extract individual nanowires for classification from each SEM image, we developed a novel algorithm that finds the location of each nanowire and extracts it[32]. The following algorithms were written in Python 3.9[33], using OpenCV[34,35] as the image manipulation package. The algorithm locates the nanowires and is based on two kernel operations applied to an image. These operations minimize the effects of noise and enhance wire edges. The kernel manipulations used are similar to, but distinct from, the typical definition used in machine learning. In this approach, the kernel operates *in situ* and transforms an image into a filter to locate feature edges. Once the edges are located, we split the image into granular blocks and condition each image through histogram equalization. This produces the final input to the ML model. The entire pipeline of operation is shown in Figure 1.

A. Kernel operations

As already discussed, our algorithm is based on two kernel operations. Both kernel operations are functions which act similarly. Each kernel searches for an extremum in a section of the image and then overwrites the whole section with the extremum value. Afterwards, the kernel moves along its row, ensuring an overlap between the previous and current window. At the end of a row, the kernel moves down the image and repeats the process without vertical overlap. This creates hard edges in the SEM image, removing any noise. Therefore, these operations find the rolling extremum in a row and propagate it forward. The two kernels find the minimum and maximum and are termed MinKernel and MaxKernel, respectively. The effect of these kernels on a noisy image is shown in Figure 2. There, it can be seen that the pixel values with the most extreme values are applied to the entire kernel and, due to the overlap, are extended to the end of the image.

Algorithm

The algorithm splits up an image of an array, as in Figure 4, into its constituent nanowires by combining rotation, cut, split, and mirror operations. To simplify the nanowire isolation process, we have improved the cut operation to detect feature edges to cut around automatically. The operation is performed using information derived from MinKernel and MaxKernel. We devised a smart image paradigm that allows us to map a subsection of the visual domain onto its original coordinates and ultimately apply the cut on the original image for extraction. In this way, we can freely perform modifications, and once we determine the correct boundary, we can map back onto the original image and extract the nanowire picture. MinKernel and MaxKernel are used with gradient methods to identify where the cut point should be placed. The complete cut algorithm is shown in Algorithm 1.

Algorithm 1. Cut algorithm

Require: MinKernel
Require: MaxKernel
Require: Split(image, location or number of outputs)
Require: *img* - input image
  images are treated as 2D arrays following right hand coordinate system
  for each side **do**
    minImg ← MinKernel(*img*)
    maxImg ← MaxKernel(*img*)
    for each *col* in maxImg **do**
      maxV ← max(*col*)
    end for
    for each *col* in minImg **do**
      minV ← min(*col*)
    end for
    maxGrad ← $\left|\frac{\partial\, maxV}{\partial x}\right|$
    minGrad ← $\left|\frac{\partial\, minV}{\partial x}\right|$
    cutPoint1 ← arg $\max_x$(*maxGrad*)
    cutPoint2 ← arg $\max_x$(*minGrad*)
    img ← Split(*img*, min(cutPoint1, cutPoint2))[1]
    rotate *img* by 90°
  end for
  return *img*

The full algorithm used to isolate a nanowire is shown in Algorithm 2. It involves cutting and rotating the image to isolate the main three-column array. Afterwards, one can split the array symmetrically into six parts. Then, each part is split again into eleven equally spaced rows. The base images are not perfectly aligned with the horizontal axis. Regardless, the algorithm works effectively for small degrees of tilt, up to 5°. For larger tilts, the methodology fails; however, as the environment is heavily controlled, the tilt in the images is significantly limited. Thus making our methodology suitable for use. Additionally, the rotation should not affect the classification accuracy since a wire's features, which determine its class, are rotation-independent up to some allowable limit. The main features are how parallel the wire fronts are and the presence of a parasitic crystal growing on the surface of the wire.

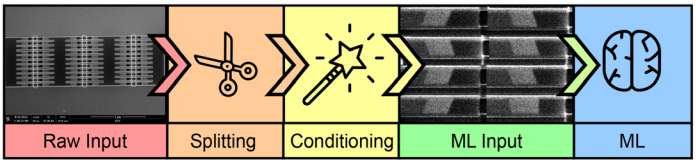

Figure 1. Process flow of classification method. The raw input consists of scanning electron microscope (SEM) images divided into individual wires through a splitting algorithm. The wire images are conditioned and later used as the input for a convolution neural network (CNN) classifier in our machine learning (ML) method.



Figure 2. Mode of operation of kernel min and kernel max. The application of the MinKernel is shown on the top row. The raw input from the left is transformed into the image on the right. The section with the darkest pixel value is highlighted. The application of the MaxKernel is shown on the bottom row. The raw input from the left is transformed into the image on the right. The section with the lightest pixel value is highlighted.

Algorithm 2. Process algorithm

Require: MinKernel
Require: MaxKernel
Require: Cut(image)
Require: Split(image, location or number of outputs)
Require: *img* - input image of nanowire array
  img ← Cut(*img*)
  imgs ← Split(*img*, 6 columns)
  wires ← empty list of nanowire images
  for *i* in *imgs* **do**
    i ← Cut(*i*)
    tmpWires ← Split(*i*, 11 rows)
    for *j* in *tmpWires* **do**
      tmpWire ← Cut(*j*)
      tmpWire ← Histogram equalization of *tmpWire*
      Append *tmpWire* to *wires*
    end for
  end for
  return *wires*

Machine learning model

The primary objective of this research paper is categorizing diverse visual representations depicting heterostructured nanowires. As previously mentioned, the pivotal impediment within this process pertains to the precise separation and extraction of nanowires from the base image. To demonstrate the efficacy of our pre-processing methodology, we have chosen to employ a compact image classification architecture implemented in the PyTorch framework (RRID:SCR 018536)[36,37]. The architectural configuration comprises a pair of convolutional layers succeeded by a trio of linear layers. The model structure is shown in Figure 3. The optimization process integrates the cross-entropy loss function with the Adam algorithm. Training was carried out for 100 iterations until loss saturation

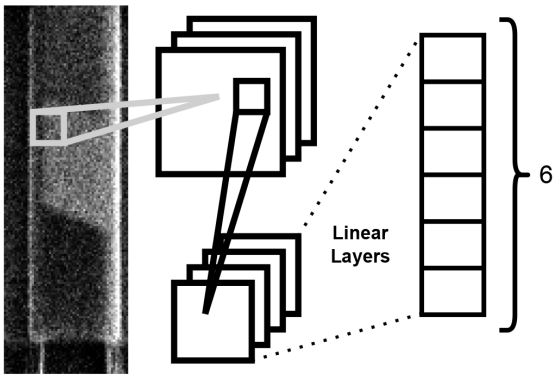

Figure 3. Diagram of the operation of the ML model used for nanowire classification. Each nanowire image is fed through to two convolutional layers followed by three linear layers producing a final output of six probabilities.

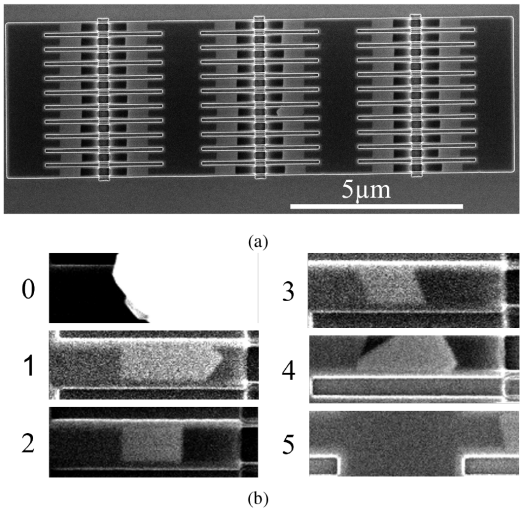

Figure 4. Scanning electron microscopy (SEM) images of two 11 × 6 nanowire arrays. a) 210nm wide wires in a template parallel to a ⟨1 1 1⟩ in-plane direction. The wires appear as light grey segments. **b**) image portions representing each of the classes as cut by Algorithm 1.

was achieved. The model uses a standard convolution approach, which has been used successfully to identify the class of images from popular datasets such as the CIFAR-10[38].

Dataset

The dataset consists of 240 images containing arrays of 66 nanowires such as that presented in Figure 4a[39], therefore, a total of 15840 nanowire nucleation sites are available in the dataset. 60% of the images contain arrays for the growth of wires in the "parallel" configuration and the remaining 40% consists of images of arrays in the "tilted" configuration. The wires were grown using TASE[14,19,23]. The images were captured with the electron beam of a FEI Helios NanoLab 450S in SEM mode. The arrays are made of different nanowire widths, with four sizes present: 70nm, 140nm, 210nm, 280nm, and in

orientation with respect to the in-plane ⟨1 1 1⟩ directions. As the Si crystal determines the seed surface and the final facet orientation, changing the template orientation will produce a tilted seed and end facet (Figure 4b, class 3). SEM images are used for quality control in nanofabrication, as they allow for high magnification and survey speeds. Traditionally, once an SEM image is taken, the operator determines whether the nanowires contained in it are defective. We have surveyed the nanowire arrays and labelled them to produce the dataset used in this paper[39].

The examples shown in Figure 4b provide an idea of what each class looks like. The wires were labelled using LabelMe[40], with four classes used to capture the differences between the wires grown along a ⟨1 1 1⟩ direction and those grown tilted away from it (Table I). This produced the first four classes: "Wire Parallel Perfect", "Wire Parallel Defect", "Wire Tilted Perfect", and "Wire Tilted Defect". They represent 49.7%, 2.4%, 21.6%, and 1.6% of the dataset, respectively. Therefore, an imbalance exists between the number of defective and perfect wires, with the latter greatly outnumbering the former and an overall prevalence of the "Wire Parallel Perfect" class in the dataset.

A fifth class is necessary because of the presence of parasitic growth on the surface of some arrays. Parasitic growth occurs on the rare occasion when III-V material nucleates on the walls of the template SiO_2. As there is no template to contain the growth of this parasitic crystal, it expands faster, covering a large number of templates.

A "Null" class is introduced to take into account the possibility that the pre-processing algorithm could have sliced the image incorrectly. This can be due to a number of factors, such as a tilt of a few degrees of the structure in the image or the influence of a large parasitic growth crystal in the cutting of the array contours. The percentage of "Null" class images in the dataset was calculated at 12.6%.

Experiment set-up

We divide the data set into training and validation sets with a 70/30 split. We trained the model for 100 epochs. The training loss is shown to saturate around 100 epochs in Figure 5, indicating the successful training of the model. Two metrics, precision and recall, are used to evaluate the performance of a classifier when encountering new data that it was not presented with, during the training stage. Precision and recall refer to the ability of the model to correctly identify an item in the test set as belonging to a class. Precision is the ratio of true positives to the sum of true and false positives. Recall, on the other hand, is defined as the ratio of true positives to the sum of true positives and false negatives. Precision and recall can be combined into the F1 score, a metric that gives an overall assessment of the quality of the model. The F1 score of the best model was recorded on the test set at 0.91 ± 0.04 (97% confidence).

Table I. Class encodings.

		Wire Parallel		Wire Tilted		
Class	Parasitic	Defect	Perfect	Defect	Perfect	Null
Encoding	0	1	2	3	4	5

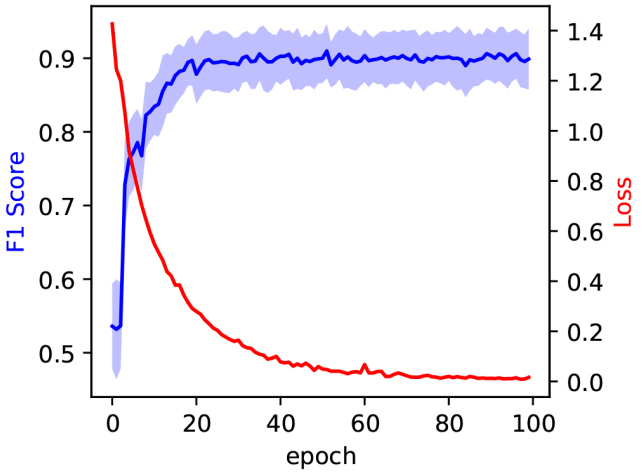

Figure 5. In blue, the evolution of the F1 score during model training, measured on the test set at each epoch. The blue shaded area corresponds to the 97% confidence interval. The evolution of the training loss is measured on the training set at each epoch and reported in red.

In some circumstances, such as when an imbalanced dataset is employed, a single number metric such as the F1 score can, however, give a misleading or incomplete "idea" of the model's performance. In such a situation, per-class metrics provide greater insight into a model's performance. The confusion matrix in Figure 6 summarizes the per-class performance of the model. The distribution of the predictions for each class is shown on each row. The data is presented as percentages: as such, the diagonal (top left to bottom right) also indicates the percentage recall of each class.

Results

The model shows outstanding performance in nanowire classification: achieving a total F1 score of 0.91 ± 0.04. This surpasses similar methods for nanowire classification by roughly 0.1[30] while using a more compact model with lower computational costs. The model shows excellent overall performance, exemplified by the high F1 score of 0.91 ± 0.04 obtained from training on an original dataset of only 240 images. The F1 Score saturates early in the training process, after around 30 epochs, as is evident by the blue curve in Figure 5.

The model's performance is different depending on the class it is trying to predict. The Recalls for each class are represented in the diagonal elements of the confusion matrix in Figure 6 and illustrate how the model performs when distinguishing between different classes. It can easily distinguish

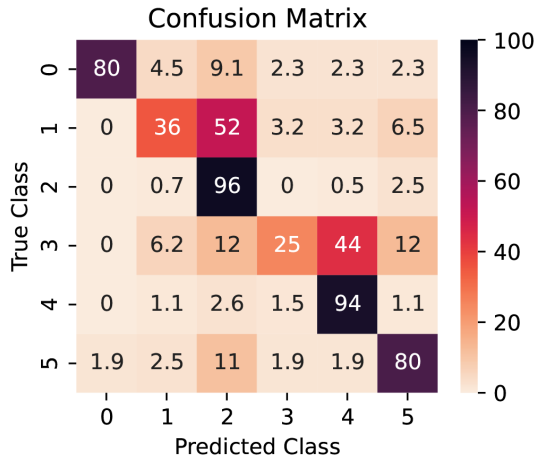

Figure 6. Confusion matrix for the model (from test set). The values are row-normalized and presented as percentages.

between non-defective parallel and tilted wires and reliably identify wrongly cut images containing partial III-V nanowires (non-defective class) or parasitic crystals. However, the model struggles to correctly classify defective wires in the test data set, with percentages of 36% and 5% of correctly identified parallel and tilted wires (classes 1 and 3). Conversely, defective wires are more likely to be classified as non-defective (52% and 44%). This is due to a combination of factors: there is a scarcity of defective wires in the data set, totaling less than 5% of the data, and growth failures can occur in more than one configuration, often with a small deviation from the desired shape creating the defect. Therefore, the preprocessing algorithm is not a contributing factor in this metric.

Conclusions

In this work, we have shown a novel algorithm to separate individual nanowires from nanowire arrays to create a general model to classify nanowires as defective and non-defective and differentiate between different growth configurations. We achieved an F1 score of 0.91 in the test set, and the recall and confusion matrix have shown a high competence in the distinction between parallel and tilted wires and parasitic growth.

Expanding the initial data set with more SEM images will likely help overcome the difficulties in classifying defective wires. We expect this expansion to not only aid in recognition of defective wires but also to be able to correctly classify tase wires grown with other crystalline orientations, given the current model's ability to distinguish between parallel and tilted wires. Furthermore, in an industrial application where the tilt of the sample and the contrast and brightness are more homogeneous than the ones in the present dataset, the prevalence of the Null class is expected to be reduced. A more complex machine learning model could achieve better performance; however, our preprocessing approach has proven capable of creating an input dataset well suited for a lightweight model.

Our manual segmentation approach is particularly powerful, as it relies on precise image gathering, easily achievable with SEM instrumentation, and can be further enhanced by a data acquisition algorithm. The preprocessing algorithm has proven to be a robust way to extract single nanowire images, reducing the complexity of the machine learning model's task. This produced a small, quick, and efficient model that has achieved a high degree of accuracy.

Ethics and consent

Ethical approval and consent were not required.

Data availability

The Dataset used in this study is available at https://doi.org/10.5281/zenodo.10204018[39].

This project contains the following data:

- SEM Images of Arrays of III-V Nanowires with Labelled Data.zip (.zip folder containing all SEM images used).

Data are available under the terms of the Creative Commons Attribution 4.0 International license (CC-BY 4.0).

Software availability

The software created in this project is available at: https://doi.org/10.5281/zenodo.10255657[32] under the terms of the Creative Commons Attribution 4.0 International license (CC-BY 4.0).

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Open Peer Review

Current Peer Review Status: ✗ ✓ ✓ ?

Version 2

Reviewer Report 08 July 2024

https://doi.org/10.21956/openreseurope.19539.r41761

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✓ **Chen Luo**
Fudan University, Shanghai, China

The authors responded to my questions and the article looks much better.

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: characterization, Semiconductor device, machine learning

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Reviewer Report 01 July 2024

https://doi.org/10.21956/openreseurope.19539.r41763

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✓ **Jin Chang**
Delft University of Technology, Delft, Netherlands Antilles

After revision, the current version is more suitable for acceptance.

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: quantum optics, superconducing nanowire single-photon detectors, integrated photonics, and optomechanics.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Version 1

Reviewer Report 25 May 2024

https://doi.org/10.21956/openreseurope.18032.r39757

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Ning Yu
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[2] UC Riverside, Riverside, California, USA
[3] Stanford University, Stanford, California, USA
[4] UC Riverside, Riverside, California, USA

In this article, the authors presented an innovative way to isolate and distinguish individual nanowires within nanowire arrays with machine learning. The ability to identify nanowires from SEM images, which usually contains high noise, could significantly improve the efficiency of characterization. This work is valuable if could be generalized to guide researchers in academia and industry.
In the meanwhile, I think there are aspects that this manuscript could improve. Some points the authors wished to make were vague. For example, “metal interconnects offer their own challenges at such small scales” could be more informative by listing a few of those challenges.
In array splitting, the authors stated the algorithm can work effectively with small degrees of tilt but may fail with larger tilts. Could the authors provide an estimation of the tilt range that could work?
I am also curious about if the performance of this methodology differs with different size of nanowires and if SEM images of different magnifications could be analyzed at the same time.

Is the work clearly and accurately presented and does it cite the current literature?
Yes

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
Yes

If applicable, is the statistical analysis and its interpretation appropriate?
Yes

Are all the source data underlying the results available to ensure full reproducibility?
Yes

Are the conclusions drawn adequately supported by the results?
Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: nanomaterials, catalysis, energy, optics

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 13 Jun 2024

Vihar Georgiev

Reply to 1: Added aspect ratio limit and cross talk as examples. The reference goes in greater detail about these.
Reply to 2: 5 degrees of tilt in either direction or more starts giving problems to the algorithm, as empirically observed.
Reply to 3: In theory yes. The main prerequisites for the splitting algorithm are that it assumes the geometry of the wire arrays, but if provided pictures of TASE nanowires the algorithm should be able to recognise them as such on the basis of the dataset. Unfortunately, as seen with the current dataset, it will likely not be able to recognise them ad defective if they are. Further development is necessary in this direction.

Competing Interests: No competing interests were disclosed.

Reviewer Report 25 May 2024

https://doi.org/10.21956/openreseurope.18032.r38958

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Jin Chang
[1] Delft University of Technology, Delft, Netherlands Antilles
[2] Delft University of Technology, Delft, Netherlands Antilles

Review Report

The authors Enrico et.al demonstrated a study and methodology for the classification of nanowires within scanning electron microscope (SEM) images. The study employs image

manipulation techniques and machine learning algorithms to accurately identify and categorize individual nanowires in SEM images depicting nanowire arrays. The methodology is demonstrated on a dataset comprising 240 III-V nanowire arrays grown on silicon substrates. Results indicate good precision and recall in distinguishing between different wire configurations and detecting parasitic crystals, with an average F1 score of 0.91. The paper emphasizes the importance of precise image gathering, robust preprocessing algorithms, and image processing paradigms to mitigate the influence of noise on nanowire classification. The findings highlight the viability of the proposed technique for academic research and potential practical commercial applications in the field of nanomaterials and microscopy imaging. Generally, the research topic is well-defined, supported by ample data, and analyzed appropriately. Below, I will outline several questions. If the authors address these questions and refine the manuscript accordingly, it will enhance the quality of the manuscript and render it suitable for acceptance.

Questions 1-4 are mainly about the background/motivation, and 5-9 focus on the methodology.

(1) In the introduction, the authors present the challenge of connecting transistors over short distances with III-V photonics components. This goal is ambitious; however, the references cited do not adequately represent the progress made in this area. Reference 6 primarily focuses on Photonic Integrated Circuits (PICs) rather than the interconnection of CMOS elements with photonics components, and reference 5 dates back to 2000. Are there any recent studies demonstrating advancements in connecting transistors with III-V elements? If so, they should be cited appropriately to strengthen the motivation behind this work.
(2) The author mentioned that "...selected growth conditions that stabilize a single {1 1 1} facet as a growth front perpendicular to the wafer surface18. From this knowledge, it is already possible to classify the wires as perfect from an SEM top-down view of the wire if the seed facet and the end facet are parallel along the growth direction and as defective otherwise." Understandably, opting for this choice simplifies the subsequent nanowire automatic classification process, as it relies solely on SEM pictures. However, the question arises: in real-world application scenarios, such as interconnecting transistors with III-V nanowires, is this nanowire growth configuration still appropriate for interconnection? If the answer is yes, proper citation would be beneficial. However, if the answer is no, it suggests that the mentioned classification method may not be versatile.
(3) What are the critical physical properties of the nanowires in this study in terms of future applications? For instance, are factors such as optical loss and emission wavelength significant? Given that the classification relies solely on SEM pictures, there may not be a rigorous connection between morphology and performance. Has the author measured any physical properties of the nanowires post-classification to confirm the relationship between SEM images and actual performance?
(4) What are the specific III-V materials utilized for the nanowires in this study? And could they be electrically pumped? Because this is important for interconnecting transistors with photonics.
(5) Regarding the software/code, although the code contains method names and some comments, it lacks comprehensive documentation that explains the purpose of each method, expected inputs, and return values. Adding proper notes to the code would be beneficial.
(6) It appears that there is no exception-handling function in the code. For instance, in SmartImage.py, there is no implementation of try-except blocks or other error-handling techniques. Consequently, if an error arises during image processing or manipulation, the code may crash without offering informative error messages.
(7) The dataset utilized for training the machine learning model comprises 240 SEM images of III-V

nanowire arrays. Is this quantity adequate, or is it somewhat constrained in terms of size? While the dataset might suffice for the initial development of the model, a larger and more varied dataset could enhance the model's resilience and its ability to generalize to unseen data. A limited dataset size could introduce bias into the model and might fail to capture the complete range of nanowire configurations.
(8) The code lacks explicit measures to prevent overfitting, such as regularization techniques or early stopping based on validation performance. This omission could result in the model memorizing the training data and subsequently performing poorly when faced with unseen data.
(9) The code overlooks the potential issue of class imbalance within the dataset. If certain classes are underrepresented, the model may face challenges in effectively learning from them, leading to biased predictions, especially considering that most nanowires are classified as "good."

If the aforementioned questions can be properly addressed, the manuscript may be considered for acceptance.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
Yes

If applicable, is the statistical analysis and its interpretation appropriate?
Partly

Are all the source data underlying the results available to ensure full reproducibility?
Partly

Are the conclusions drawn adequately supported by the results?
Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: quantum optics, superconducing nanowire single-photon detectors, integrated photonics, and optomechanics.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 13 Jun 2024

Enrico Brugnolotto

We thank the reviewer for the time taken to read the article and provide useful feedback.

1. Added a reference from 2017
2. Citations about TASE explain the advantages of this fabrication method in integration. The main one is the co-planar self-aligned integration of III-V active photonic elements with silicon waveguides.
3. The advantage of TASE is in it co-planar integration and self-alignment with silicon waveguides, on which ends active III-V photonic components can be grown. Optical loss and emission wavelength can be important, depending on the application, for example due to the use of wavelengths that can be guided losslesly in silicon. While it is possible that this growth approach would not make a large difference for some applications which do no require sophisticated hardware, it stands to reason that the ordered and reliable growth of III-V structure is preferrable to a disorganised growth. It is a simple fact that a greater variety of growth outcomes are directly correlated with a greater variery of performance outcomes. This situation is the one that is prevalent in growth in templates with methods like TASE and LART. While performance is important in industry, stardandization is crucial, and having different nanowire lengths and internal compositions (in the case of ternary materials) is not conductive to the type of automated processes in industry. Before the question of performance is asked, a simpler question is that of contacting. If the various material layers of a heterostructured p-i-n detectors all have different lengths in each wire contacting it requires a wire-by-wire adjustment of the lithography mask defining the metal contacts. This is obviously highly sub-optimal for large scale integration densities.
4. They are InP and InGaAs. A device based on these materials and created with TASE was tested with electrical pumping in reference 15.
5. Comments were added in the code to improve readability.
6. It will not be possible to revise the code substantially due to the project having ended.
7. While it is true that the dataset does not represent the entirety of the nanowire grown it is still a collection of 15k+ growth sites. The main issue with the dataset in terms of machine learning is that the fraction of defective wires is small compared to the total. This, coupled with the simple fact that the defective wires fail in different ways, makes those two classes have poor recalls. Unfortunately due to the project being already over, it will not be possible to supplement additional images to the existing dataset that, in our opinions, remains a large collection of nanowires imaged with SEM and is freely available for use even outside of the scope of the current publication.
8. It will not be possible to revise the code substantially due to the project having ended.
9. This is true and the bias towards “perfect” wires is seen in the recall, however the model has high performance distinguishing other classes, and not just markedly different ones such as “Parasitic” or Null” from perfect wires but also between tilted and perpendicular wires. It will not be possible to revise the code substantially due to

the project having ended. However, it is publicly available, and can be used and modified by anyone free of charge under the CC BY 4.0 licence. Both improvements to the existing code and new approach in the use of the dataset, maybe in conjunction with other datasets, by other researchers is something we are excited about.

Competing Interests: No competing interests were disclosed.

Author Response 13 Jun 2024

Vihar Georgiev

Repy to point 1: Added a reference from 2017, an exhaustive review
Reply to point 2: There are citations about TASE that explain the advantages of this fabrication method in integration. The main one is co-planar self-aligned integration of III-V active photonic elements with silicon waveguides.
Reply to point 3: The advantage of TASE is in it co-planar integration and self-alignment with silicon waveguides, on which ends active III-V photonic components can be grown. Optical loss and emission wavelength can be important, depending on the application, for example due to the use of wavelengths that can be guided losslesly in silicon. While it is possible that this growth approach would not make a large difference for some applications which do no require sophisticated hardware, it stands to reason that the ordered and reliable growth of III-V structure is preferrable to a disorganised growth. It is a simple fact that a greater variety of growth outcomes are directly correlated with a greater variery of performance outcomes. This situation is the one that is prevalent in growth in templates with methods like TASE and LART. While performance is important in industry, stardandization is crucial, and having different nanowire lengths and internal compositions (in the case of ternary materials) is not conductive to the type of automated processes in industry. Before the question of performance is asked, a simpler question is that of contacting. If the various material layers of a heterostructured p-i-n detectors all have different lengths in each wire contacting it requires a wire-by-wire adjustment of the lithography mask defining the metal contacts. This is obviously highly sub-optimal for large scale integration densities.
Reply to point 4: They are InP and InGaAs. A device based on these materials and created with TASE was tested with electrical pumping in reference 15.
Reply to point 5: Comments were added in the code to improve readability.
Reply to points 6 & 7: While it is true that the dataset does not represent the entirety of the nanowire grown it is still a collection of 15k+ growth sites. The main issue with the dataset in terms of machine learning is that the fraction of defective wires is small compared to the total. This, coupled with the simple fact that the defective wires fail in different ways, makes those two classes have poor recalls. Unfortunately due to the project being already over, it will not be possible to supplement additional images to the existing dataset that, in our opinions, remains a large collection of nanowires imaged with SEM and is freely available for use even outside of the scope of the current publication.
Reply to points 8 & 9: This is true and the bias towards “perfect” wires is seen in the recall, however the model has high performance distinguishing other classes, and not just

markedly different ones such as “Parasitic” or Null” from perfect wires but also between tilted and perpendicular wires. It will not be possible to revise the code substantially due to the project having ended. However, it is publicly available, and can be used and modified by anyone free of charge under the CC BY 4.0 licence. Both improvements to the existing code and new approach in the use of the dataset, maybe in conjunction with other datasets, by other researchers is something we are excited about.

Competing Interests: No competing interests were disclosed.

Reviewer Report 22 May 2024

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?

Chen Luo
[1] Fudan University, Shanghai, China
[2] Fudan University, Shanghai, China

The article introduces an innovative classification methodology to identify nanowires within SEM images. The topic is interesting but the article is not well organized. There are some problems that need to be solved.
1. Authors compared STEM and SEM methods in the introduction. The STEM method allows for the visualization of defects, while SEM determines whether they are parallel to the growth direction while stabilizing {1 1 1} facet as a growth front perpendicular to the wafer surface. Is there a possibility that even if the growth is parallel, there will still be defects? Or how to define “parallelism” from the perspective of SEM top down view? If the nanowires are not uniformly straight, how many degrees is considered parallel?
2. In Figure 3, each part in the SEM image needs to be labeled, such as which part is the nanowire and which part is the substrate. It is difficult to understand, for example, please show the difference in morphology between perfect nanowires and defective nanowires in the top down view.
3. Figure 4 mentioned first in the main text, followed by Figure 3.
4. All SEM images in the text should have a scale bar.
5. Figure 1 is too small, it would be best to show the images after each operation, such as splitting and after removing noise.

Is the work clearly and accurately presented and does it cite the current literature?
Yes

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?
Partly

Are all the source data underlying the results available to ensure full reproducibility?
Partly

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: characterization, Semiconductor device, machine learning

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 13 Jun 2024

Enrico Brugnolotto

We thank the reviewer for their time and precious feedback.

1. Yes, it is in theory possible, and it mostly depends on what defects are considered “acceptable” for the purpose of device fabrication. This is mainly a growth study, and the yields are mechanical, as in, we try to stabilise a certain growth type and achieve high yield of geometrically similar wires. As such no device characterisation was carried out. Further reading supporting the hypothesis that the internal composition is reproducible and can be inferred by the external shape of the wires is in reference 38. The nanowires are uniformly “straight” as in they are constrained to develop in the same direction by the template they grow in. I believe what you are asking is “how many degrees of difference can there be between the vector defining the plane of the seed and thant defining the plane of the end facet?” in reality small tilts of a handful of degrees (up to 5) can be seen as a stress relaxing avenue. This tilt originates in the III-V lattice in the very few first atomic bi-layers after nucleation. It is not indicative, however, of any defects in the wire and is very difficult to spot from a top down view of the wire. Real indicators of defects are end-interfaces that are composed of multiple crystalline facets, or are at high angles compared to the seed facet as shown later on in the class breakdown.
2. The differences between perfect and defective nanowires are shown in Figure 4.
3. It is mentioned first, but addressed second.
4. Figure 4 provides a scalebar which allows the reader to understand the scale of the nanowires. Of course, scale bars are present in all images in the freely available dataset allowing them to be reused in other project with the knowledge of the scale of the structures pictured.

5. Example of images after splitting are available in Figure 4(B), the denoised image does not visibly differ from those shown at this magnification level.

Competing Interests: No competing interests were disclosed.

Author Response 13 Jun 2024

Vihar Georgiev

Reply to Point 1: Yes, it is in theory possible, and it mostly depends on what defects are considered "acceptable" for the purpose of device fabrication. This is mainly a growth study, and the yields are mechanical, as in, we try to stabilise a certain growth type and achieve high yield of geometrically similar wires. As such no device characterisation was carried out. Further reading supporting the hypothesis that the internal composition is reproducible and can be inferred by the external shape of the wires is in reference 38. The nanowires are uniformly "straight" as in they are constrained to develop in the same direction by the template they grow in. I believe what you are asking is "how many degrees of difference can there be between the vector defining the plane of the seed and thant defining the plane of the end facet?" in reality small tilts of a handful of degrees (up to 5) can be seen as a stress relaxing avenue. This tilt originates in the III-V lattice in the very few first atomic bi-layers after nucleation. It is not indicative, however, of any defects in the wire and is very difficult to spot from a top down view of the wire. Real indicators of defects are end-interfaces that are composed of multiple crystalline facets, or are at high angles compared to the seed facet as shown later on in the class breakdown.
Reply to Point 2: The differences between perfect and defective nanowires are clearly shown in Figure 4.
Reply to Point 3: It is mentioned first, but addressed second.
Reply to Point 4: Figure 4 provides a scalebar which allows the reader to understand the scale of the nanowires. Of course, scale bars are present in all images in the freely available dataset allowing them to be reused in other project with the knowledge of the scale of the structures pictured.
Repy to Point 5: Example of images after splitting are available in Figure 4(B), the denoised image does not visibly differ from those shown at this magnification level.

Competing Interests: No competing interests were disclosed.

Reviewer Report 15 May 2024

https://doi.org/10.21956/openreseurope.18032.r38954

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Nasser Mohieddin Abukhdeir
[1] University of Waterloo, Waterloo, Ontario, Canada
[2] University of Waterloo, Waterloo, Ontario, Canada

The manuscript presents a computational method to classify SEM (or other microscopy) images of nanowire structures through the combination of a pre-processing image segmentation method followed by a convolutional neural network which has been trained for a sample qualitative classification. While the presented method is likely novel and both source data/code have been made available, the novelty and generality of the presented method is not well-supported in the manuscript. A significant literature of past image analysis and processing methods focused on nanowires has not been well-reviewed or cited, which does not provide the reader/reviewer with the basic context of this research within the current archival literature. Furthermore, apart from minimally showing that the method functions for a very limited set of experimental data, there are no results presented showing its application to other relevant experimental data sets and demonstration of its utility/impact to better understand these results. Unfortunately I do not think this manuscript meets the minimum standards for indexing.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Partly

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?
Yes

Are all the source data underlying the results available to ensure full reproducibility?
Yes

Are the conclusions drawn adequately supported by the results?
No

Competing Interests: No competing interests were disclosed.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to state that I do not consider it to be of an acceptable scientific standard, for reasons outlined above.

Author Response 13 Jun 2024

Vihar Georgiev

While it is true that the method has no aspiration to classify any nanowire grown with any technique, its application is in the context of TASE-grown nanowires. It is already sufficiently

accurate in distinguishing between two different TASE nanowire configurations and parasitic crystals. Further expansion of the dataset and code to include more

Competing Interests: No competing interests were disclosed.