

GRAFOS DE INTERCONEXIÓN DE REDES DE NANOHILOS A PARTIR DE SUS FOTOMICROGRAFÍAS

NANOWIRE NETWORKS' INTERCONNECTION GRAPHS FROM THEIR PHOTOMICROGRAPHS

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Los autoensamblados de unidades sintonizables son estudiados intensivamente como sistemas físicos con capacidades de procesamiento de señales. En particular, las redes de nanohilos de plata (AgNWNs) han demostrado acumulación, no-linealidad y retención de memoria en múltiples escalas temporales, características que permiten una amplia variedad de implementaciones neuromórficas. En este estudio, se extrae el esquema de interconexión para analizar la arquitectura experimental de la red y en un futuro poder usarla como entrada de una plataforma de simulación. Mediante el post-procesado de fotomicrografías de AgNWN, se presenta un procedimiento optimizado para extraer el diagrama de interconexión y determinar el grafo asociado a cada muestra física. Se estudian métricas de grafos como la distribución de grado, el tamaño de comunidades, el *coeficiente de aglomeración* y la *longitud de camino*, comparando los ensamblados experimentales con modelos topológicos de referencia denominados: **small-world**, **modular** y **scale-free**. Los ensambles experimentales revelan similitudes tanto con topologías **small-world** como **modulares**. Adicionalmente, se estudia el impacto en el grafo de eliminar artificialmente juntas mediante la cuantificación del *coeficiente de aglomeración* y de la *longitud de camino*.

Palabras Clave: redes de nanohilos, autoensamblados grafos, análisis topológico, neuromórfico, procesamiento de imágenes.

Self-assemblies of tunable units are being intensively studied as physical systems with signal processing abilities. Specifically, silver nanowire networks (AgNWNs) have demonstrated accumulation, non-linearity, and memory retention with multiple timescales, features that enable a wide variety of neuromorphic implementations. In this study, we aim to extract the interconnection scheme to analyze the experimentally obtained network architecture and, eventually, use it as the input of a previously developed simulation platform. By post-processing photomicrographs of AgNWN, we present a pipeline optimized to extract the interconnection diagram, recognizing the intersections formed among the nanowires, to determine the associated graph for each physical sample. Graph metrics such as degree distribution, community size, *clustering coefficient*, and *path-length* are studied to compare the experimental assemblies' attributes to topological models of reference. **Small-world**, **modular**, and **scale-free** are well-known structures in the field of mathematical graphs. The experimental assemblies reveal similarities to both **small-world** and **modular** topologies. This communication also studies the impact of artificially removing junctions from the resulting graphs on the previously calculated *clustering coefficient* and *path-length*.

Keywords: nanowire networks, self-assemblies, graphs, topological analysis, neuromorphic, image processing.

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I. INTRODUCTION

The computational strategies implemented by modern computers stem from concepts derived from the neurophysiology of biological brains[1]. The encoding of information as memory states or trapped charge in synthetic units is

one example (in hardware) of this[2]. The implementation of artificial neural networks composed of neuronal nodes and synaptic weights constitutes another example (this time in software) of the same original inspiration[3]. However, the course of technological progress has distanced synthetic implementations from their biological counterparts[4].

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The power consumption of current computing systems and the restrictions this may entail in the near future necessitate proposing an alternative: exploiting synthetic systems radically different from the CMOS gates that are presently at the heart of the hardware[2].

Self-assemblies of tunable units are being intensively studied as physical systems with signal-processing capabilities[2, 5-10]. Understood as complex networks of nanometric objects, these platforms (made of nanoparticles or nanowires, among others) resemble morphological, topological, and functional aspects of neural tissues[4]. In that regard, the extremely high number of units, the spontaneous interconnection scheme among them, and the non-trivial architecture[11] are desirable features for a new generation of neuromorphic hardware inspired by the collective attributes instead of the detailed fidelity of the individual constituents[12].

In this framework, self-assemblies are being studied either experimentally[2, 5-10, 13] or with simulation schemes[9, 14, 15]. Experimentally, synthesizing and measuring two or multi-electrode devices and subjecting them to a variety of incoming signals allows for the identification of desirable properties such as accumulation, non-linearity, short- and long-term memory, among others. Simulations performed on different platforms allow analysis of the impact of the properties of individual components (which are experimentally inaccessible) on the macroscopic collective response[16]. Except for a few cases[14, 17], the interconnection schemes fed into the simulation platforms are not usually consistent with the experimentally obtained geometry. As such, the obtained simulated responses are just qualitatively comparable to the physical assemblies. In this study, we aim to bridge the gap between the two approaches by interpreting photomicrographs of the real samples as graphs of interconnected nodes useful to configure the simulations. Additionally, the conversion of the experimental information (optical images) into mathematical objects makes the latter suitable for network analysis in terms of their topology and geometry-related metrics.

II. SYNTHESIS AND IMAGE ACQUISITION

The AgNWs assemblies were fabricated with a targeted geometry (~ 170 nm in diameter and ~ 70 μm in length), then dispersed in a solvent (containing polymeric residues coming from the NWs growth), and finally deposited onto a desired substrate to form the networks (AgNWNs)[18]. The desired areal density (~ 2500 mm^{-2}) is reached by sequential deposition steps[18]. As depicted in Fig. 1, two millimetric-sized Ag electrodes (1 mm apart) were sputtered to access the assembly electrically.

The resultant assemblies comprise metallic NWs, coated with a polymeric layer residual from the synthesis, which intersect with each other, forming capacitor-like junctions (Ag-polymer-Ag). The electrical connection between the two macroscopic electrodes is mediated by the conduction along the NWs themselves and across the tunable memristive junctions. The electrical conductivity requires geometrical percolation of the assembly, but is also conditioned by the state of the memristive intersections among the constituent NWs.

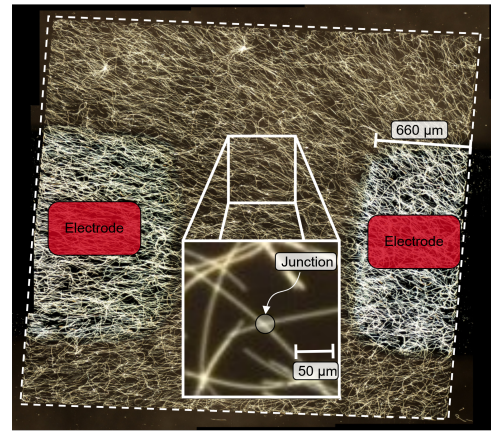


FIG. 1: Infograph of a typical nanowire network (NWN) depicting the constituent units. Each NWN comprises the network of nanowires (NWs) intersecting each other, enclosed by two macroscopic electrodes placed 1 mm apart. A zoomed-in area is included as an inset where individual NWs and their junctions can be spotted.

Dark-field optical images were taken with a Leica DM2700 M using a typical magnification of 10x. Samples of intermediate areal densities $\frac{N}{\text{mm}^2}$ (as reported in[9]) were characterized using this technique. While in-plane scanning the sample, multiple images are taken to completely cover the assembly. These partial images are primarily stitched to obtain an image of the full active area. The image produced from this collection will be the input to the pipeline designed for the following graph extraction.

III. PIPELINE FOR GRAPH GENERATION

The pipeline comprises a sequence of steps (schematically summarized in Fig. 2). First, the routine enables the identification of the macroscopic electrodes. This operation is of paramount importance since the graph objects contained within it will present a preferential hierarchy in the electrical percolation. In the following, the NWN itself needs to be interpreted.

Recognizing the nanowires and the intersections among them requires image processing strategies. Binarization of the image facilitates posterior identification of the constituents. Additionally, an image cleaning procedure is implemented, where spurious pixels are filtered, removing both small black holes and isolated white noise. Once cleaned, the image undergoes a *skeletonization*[19] process to reduce the NWs to a single-pixel-wide line. The image obtained from the previous step allows for the intersection identification as the cross-points between lines. Initially, the skeleton is converted into a graph by mapping junctions to nodes and NW segments to edges. Subsequently, this graph is transformed into its corresponding line graph, effectively reversing the roles of nodes and edges.

It is important to emphasize that a cross-point does not imply an intersection. From a zenithal view, it is not possible to determine whether two NWs occupying the same area and forming an angle between them are actually in contact or if there is some vertical space between them. After building the corresponding graphs, this will be accounted for by introducing a removal probability. This probability ran-

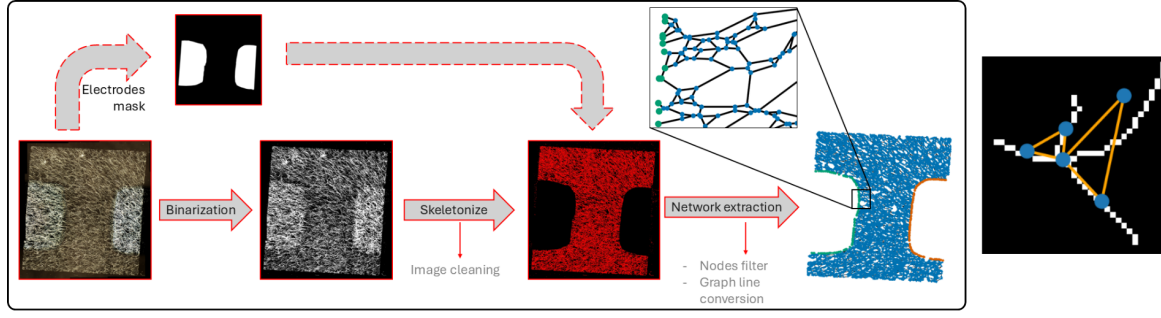


FIG. 2: Sketch of the pipeline flow. Starting from the stitched picture, the procedure identifies the electrodes and binarizes the RGB-format image to facilitate the skeletonization conversion. Once the network has been converted to a set of one-pixel-wide contours, network extraction is performed. The wires and their mutual intersections (zenithal view) are interpreted as a graph comprised of nodes and edges, respectively, depicted in the zoomed-in area. The right panel displays a section of the skeletonized image overlaid with the extracted graph.

ges from $p = 0$, where all cross-points are assumed to be physical junctions, to $p = 1$, where all cross-points are eliminated.

The result is a collection of segments and intersections. Since the segments are just portions of the original NWs (conductive and not tunable), while the intersections are the electrically active components, the segments will be coded as nodes and the junctions as edges. Together, the number of nodes, ‘N’ (formerly segments of NWs), and of edges, ‘e’ (the intersections among NWs from the zenithal point of view) and their interconnectivity map will determine the type of structure associated with each experimental assembly. The number of links each node possesses is referred to as its degree (k).

Three samples (A, B, and C) were optically imaged and translated into graphs using the developed pipeline, more details on the algorithms and their parameters can be consulted in the referenced GitHub repository [20]. The characteristics of the obtained graphs are summarized in Table 1. Samples A and B possess similar densities, while C is sparser.

TABLA 1: Graph features of the experimental samples.

Attribute ↓ / Sample →	A	B	C
Nodes (N)	66435	77477	26222
Edges (e)	121217	139293	41941
Degree (average)	3.65	3.60	3.20

IV. TOPOLOGICAL ANALYSIS

Graph generation from experimentally-acquired optical images enables geometrical considerations. Multiple metrics are defined as indicators of the network segregation and/or integration and are related to some archetypal interconnection schemes. Among them, we could mention: **small-world**, **modular**, and **scale-free** networks.

Small-world networks[21] are typically formed by clusters, within which the connectivity is high, and hubs linking nodes belonging to different clusters. Two metrics are defined: *clustering coefficient* (CC) and *path length* (PL).

The *clustering coefficient* defines the likelihood that a graph is formed by subgroups. Specifically, the local *clustering coefficient* of a node u is the fraction of possible trian-

gles through that node that exist[22, 23]:

$$CC = \frac{1}{N} \sum_u c_u = \frac{1}{N} \sum_u \frac{T(u)}{\deg(u)(\deg(u) - 1)} \quad (1)$$

where $T(u)$ is the number of triangles through node u and $\deg(u)$ is the degree of u . We evaluate the average *clustering coefficient*, defined as the mean of c_u over all N nodes in the graph.

The *path length* is defined as the mean of the minimum distance (in number of edges) between all pairs of nodes in the network:

$$PL = \frac{1}{N(N-1)} \sum_{u \neq v} d(u, v) \quad (2)$$

where $d(u, v)$ is the shortest distance between node u and v . A statistical approximation was implemented to handle the prohibitive computational cost for large-scale graphs: a representative subset of $m = 1000$ random seed nodes was sampled within the largest connected component, and the shortest paths from these seed nodes to all other nodes were evaluated.

Small-world networks, early proposed by Watts-Strogatz[21], possess a short average *path-length* and a high *clustering coefficient*. **Modular** networks[24] are characterized by presenting communities that determine a coexisting structure of sparse and dense connectivity zones. Finally, **scale-free** networks[25] have a highly heterogeneous connectivity distribution, with most nodes having very few links and a few nodes (hubs) linking to an exceptionally high number of nodes.

Fig. 3 represents some salient features of the three archetypal networks, quantified in artificially built networks generated with size $N = 70000$ and average degree $k = 4$, comparable to the experimental cases.

Fig. 4 depicts the degree distribution and adjacency matrix obtained from three different samples. Comparison of the obtained graph characteristics allows for identifying a moderate range of available connectivity degrees, compatible with **small-world**-like schemes. However, adjacency matrices show a **modular** arrangement as indicated by the presence and sustainable size of the squares forming around the matrices’ diagonals.

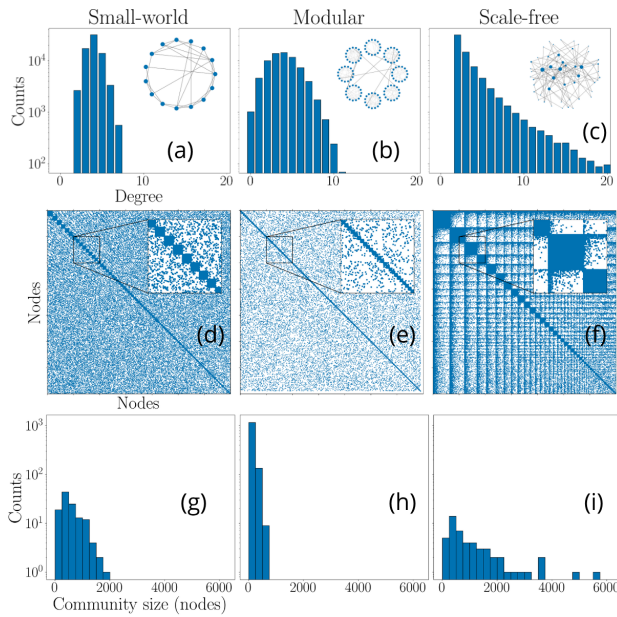


FIG. 3: Different network schemes used as a reference: small-world, modular, and scale-free. The top row, (a), (b), and (c), comprises a degree histogram including an inset with sketches. On the second row, (d), (e), and (f) show the adjacency matrix, while the bottom row, (g), (h), and (i), displays the distribution of community sizes for each case. Networks of size $N = 70000$ and average degree $k = 4$.

As mentioned in the Introduction, the experimentally available zenithal view does not enable distinguishing real junctions from concurrent NWs that may not be in physical contact. Here we explore the graph variability by quantifying some of the previous metrics as a function of an arbitrary edge-removal probability (p_{er}).

Clustering coefficient and path length are displayed as a function of p_{er} (Fig. 5). Starting from the clustering coefficient determined for the whole network, removing edges produces a reduction of the agglomeration capability. The same analysis was conducted with the three networks of reference, showing that despite the initial condition being different for each case, the overall evolution as a function of p_{er} is the same (inset of Fig. 5(d)).

The path length (Fig. 5(e)) has been calculated in three different ways, averaged over 20 independent runs. The **base graph** considers the interconnection scheme identified regardless of the electrodes. The **effective graph** considers that the nodes located within the electrodes' areas are equivalent to each other. The **effective electrode graph** redefines the path length considering only paths of electrical validity (origin nodes in V_{in} electrode and destination nodes in V_{out}). The topological analysis indicates that the experimental assemblies do not strictly correspond to just one type of archetypal network architecture, but hints of the three types could be found.

V. CONCLUSIONS

This work presents a pipeline developed to build a graph or network as a mathematical object associated with the optical images of experimental samples. Graphs' attributes, such as the number of obtained nodes and edges, reflecting NWs' segments and intersections, respectively, were

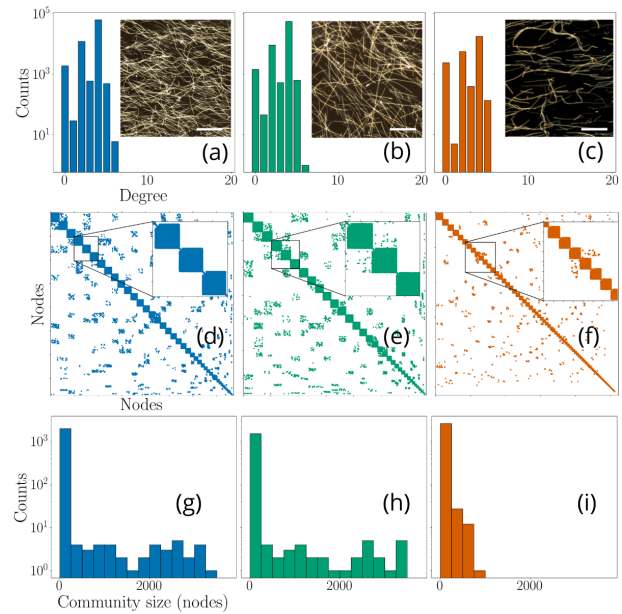


FIG. 4: Network metrics of graphs generated from experimental images. Degree distributions with optical images as insets with a scale bar of $100 \mu m$ ((a), (b), and (c)), adjacency matrices ((d), (e), and (f)), and community distributions ((g), (h), and (i)) for three experimental cases (samples A, B, and C, respectively).

compared among three experimental samples. Topological metrics and means of representation derived from three networks chosen as references were used to relate the obtained graphs to well-known structures. Considering that all the identified intersections reflect real junctions, all the resulting graphs displayed a degree distribution similar to a **small-world** distribution. Adjacency matrices showed the presence of communities of different sizes, which are not mutually isolated but interconnected.

Topological metrics such as the path length and clustering coefficient were calculated as a function of an artificially introduced edge-removal probability. This artificial insert, aimed at accounting for the realistic status of the NWN, allowed us to test the impact of the effective density on the metrics. Future work will be devoted to further exploring the impact of the electrodes' definition on the topology, and to testing multiple electrical protocols using previously developed simulation platforms.

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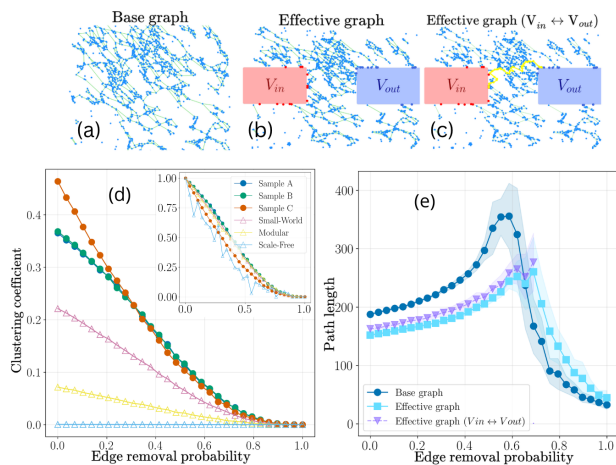


FIG. 5: Clustering coefficient and path length as a function of the edge-removal probability. (a), (b) and (c) depict schematics of the different graphs used to measure the path length. (d) shows the clustering coefficient as a function of p_{er} for the samples and the reference networks. (e) displays the path length as a function of p_{er} for Sample A in the three different cases shown above.

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