Topology, Connectivity, and Charge Transport in Gallium Nitride: A Graph Theory Framework

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Abstract: In this work, we explore the electrical conductivity of Gallium Nitride(GaN) using graph theory to model the connectivity and charge transport pathways within its molecular and crystalline structure. By representing the compound as a graph, where atoms are nodes and chemical bonds are edges, we analyze the network's conductivity using concepts such as adjacency matrices, Laplacian matrices, and percolation thresholds.

The adjacency matrix (A) encodes the connectivity between atoms, where each element A_{ij} equals 1 if there is a bond between nodes i and j, and 0 otherwise. The Laplacian matrix(L), defined as $L = D-AL$ (where D is the degree matrix that represents the number of bonds for each node), captures the topological structure of the system and is used to calculate the eigenvalues, which represent the vibrational modes or energy states within the material. The smallest non-zero eigenvalue, known as the spectral gap, plays a crucial role in determining electrical conductivity, as it is inversely proportional to the material's ability to conduct charge.

The conductivity of GaN is influenced by the network's topology, including factors such as bond strength, coordination number, and the presence of conduction paths. The percolation threshold the critical connectivity point at which the network transitions from insulating to conducting is also an essential factor in determining the material's electrical properties.

This graph-theoretic approach provides a novel framework for understanding the conductive properties of metal nitride systems, offering insights into how molecular structure and network topology govern charge transport. It can also be extended to other compounds for optimizing their conductivity in various applications.

Keywords: Graph theory, Electrical conductivity, Gallium Nitride, Network analysis, Percolation theory.

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I. Introduction

Gallium Nitride (*GaN*) is a wide-bandgap semiconductor compound that has gained significant attention in materials science due to its potential applications in a variety of fields, particularly in electronics, optical devices, and catalysis [1]. GaN's unique properties, such as its high thermal conductivity, high breakdown voltage, and excellent chemical stability, make it a promising material for high- power electronics, LEDs, and solar cells ([2]-[4]). While the electrical properties of GaN have been extensively studied through experimental methods, a more theoretical framework rooted in graph theory could provide deeper insights into the charge transport mechanisms within the material. Graph theory has been successfully applied to study electrical conductivity in other materials such as graphene, carbon nanotubes, and conductive polymers [5]. These materials exhibit fascinating electrical properties that are influenced by their network structures. Similarly, *GaN*, as a crystalline solid, has a well-defined structure that directly impacts the movement of charge carriers like electrons and holes. To understand how charge transport occurs in *GaN*, we can model the material as a graph where the atoms (specifically Gallium (*Ga*) and Nitrogen (*N*)) are represented as vertices (nodes) and the chemical bonds between them are represented as edges. This approach allows us to analyze the connectivity of the network and how it influences the electrical conductivity of *GaN*.

1.1. Objectives. This study aims to:

(1) Represent GaN as a weighted graph to model bond strengths and conduction paths.
(2) Use adjacency and Laplacian matrices to analyze network connectivity.
(3) Apply percolation theory to determine critical conduction thresholds.
(4) Compare theoretical predictions with experimental conductivity data.

In this work, we represent *GaN* as a graph, where the atoms Gallium (*Ga*) and Nitrogen (*N*) are represented as vertices (nodes), and the chemical bonds between them are represented as edges. The idea is that, similar to how electrons flow through conductors or semiconductors, charge transport in GaN depends on the connectivity of the network of atoms. The properties of the graph: such as the number of connections each node has, the structure of the network, and the paths that connect the nodes play a critical role in determining the material's electrical conductivity.

1.2. Impact of Network Topology on Charge Transport: The coordination number (the number of nearest neighbors an atom has) and the bond strength in *GaN's* lattice structure are key factors influencing its conductivity. In *GaN*, each Gallium atom typically bonds with four Nitrogen atoms in a tetrahedral arrangement, creating a highly structured, strongly bonded network. This structure influences how charge carriers (such as electrons) move through the material. In a graph-theoretic context, the number of connections (degree) and the strength of bonds (represented by the adjacency matrix) are crucial for understanding how easily charge can propagate through the network.

II. Methodology

2.1. Crystal Structure of GaN. Gallium nitride (*GaN*) is a compound semi- conductor that most commonly crystallizes in the hexagonal wurtzite structure, which is the thermodynamically stable form under ambient conditions([6]-[7]). In this structure, gallium and nitrogen atoms are arranged in a repeating pattern where each *Ga* atom is tetrahedral coordinated to four *N* atoms, and vice versa. This tetrahedral bonding forms a robust three-dimensional network, contributing to *GaN's* excellent mechanical strength, high thermal conductivity, and wide bandgap ($\sim 3.4eV$), making it ideal for high-power and high-frequency electronic applications([8]-[10]). The wurtzite structure is inherently polar,

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due to the lack of inversion symmetry along the c-axis, leading to unique piezoelectric and spontaneous polarization effects. These properties are crucial in optoelectronic devices such as blue and ultraviolet LEDs and laser diodes.

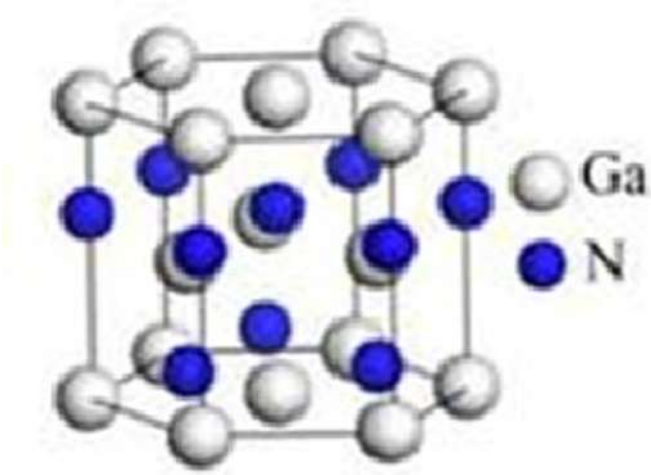

Fig.1. Crystal structure of GaN

2.1. Graph Theory Framework for GaN:

In the graph representation of *GaN*, the nodes or atoms are connected by edges or bonds, which form a lattice structure in the case of *GaN's* wurtzite crystal structure. The strength and nature of these connections whether they are covalent bonds, ionic bonds, or metallic like interactions determine the overall conductivity of the material[11]. By using graph theory, we analyze how the atomic connectivity within the material affects the flow of charge.

2.2. Adjacency Matrix and Network Representation:

The first step in the graph theoretic approach is to construct the adjacency matrix (*A*). This matrix represents the network connectivity by assigning a value of 1 if two atoms are bonded and 0 if they are not. The degree matrix (*D*) is then constructed, where each diagonal element represents the number of bonds or connections each atom has. The Laplacian matrix *L* is defined by $L = D - A$, and it provides a compact representation of the material's topological properties.

The Laplacian matrix plays a crucial role in analyzing the material's vibrational modes and electrical properties. The eigenvalues of this matrix correspond to different energy states or vibrational frequencies of the system ([12]-[14]). The smallest non-zero eigenvalue of the Laplacian matrix, known as the spectral gap, is particularly significant in determining the electrical conductivity of the material. A smaller spectral gap indicates a material that is more conductive, as the charge carriers can move more freely through the network. The python code to construct specified graph representation of GaN and its image is given below:

```
# Atom types: alternating Ga and N

atom_labels = ['Ga', 'N', 'Ga', 'N', 'Ga', 'N', 'Ga']

# Create graph
```

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```
G = nx.Graph() G.add_nodes_from (range(7))
# Add edges from adjacency matrix
for i in range (7):
for j in range(7):
if adj_matrix[i][j] == 1: G.add_edge(i, j)
# 2D circular layout
pos = nx.circular_layout(G)
# Node colors based on atom type
node_colors = ['skyblue' if atom_labels[i] == 'Ga' else
‹→      'lightgreen' for i in range(7)]
# Draw the graph plt.figure(figsize=(8, 6)) nx.draw(
G, pos, with_labels=False, node_color=node_colors, node_size=1000, edge_color='gray'
)
# Add Ga/N labels
labels = {i: atom_labels[i] for i in range(7)} nx.draw_networkx_labels(G, pos, labels=labels,
‹→      font_size=14,  font_weight='bold')
plt.title("Specified Graph representation of GaN") plt.axis('off')
plt.tight_layout()
plt.show()
```

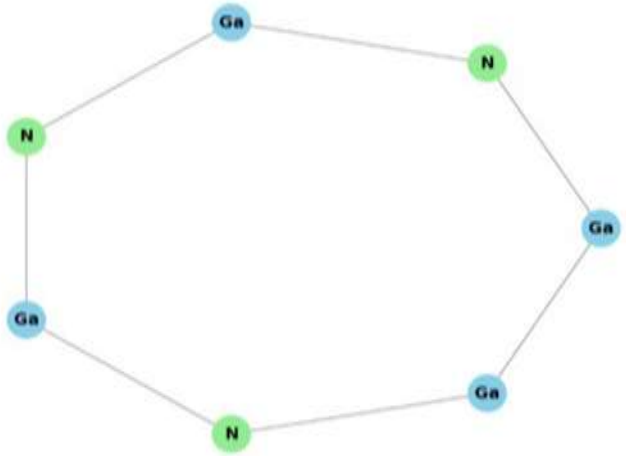

Fig.2. Simplified Graph representation of GaN

Now writing the Adjacency matrix (A) for $Ga - N$ pairs is as follows

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$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

For a simple 2D unit of GaN (considering nearest neighbor interactions), a basic adjacency matrix is given in above matrix Here, each Ga atom is connected to N atoms in a hexagonal pattern. Ga1 is bonded to N1 and N2 (entries= 1),

N_1 is bonded to Ga_1 and Ga_2 (entries = 1), but No Ga − Ga or N − N bonds (Therefore wurtzite has strict alternation).

2.3. Degree Matrix (D) for GaN :

The degree matrix (D) is a fundamental matrix in graph theory and computational materials science that quantifies the local connectivity of each atom (node) in a crystal structure like GaN. The degree matrix Dii is a diagonal matrix where Di represents the number of bonds (edges) connected to node i. The Dii matrix is a diagonal matrix (off-diagonal entries are zero), The i^{th} diagonal entry represents the degree of node i (number of bonds/edges connected to atom ii). For GaN in the wurtzite structure, each Ga or N atom has 4 bonds (tetrahedral coordination).

The Degrees of the matrix can be explained as below

$D_{11} = 0 + 1 + 0 + 1 = 2$ (Ga1 bonds: N1, N2)

$D_{22} = 1 + 0 + 1 + 0 = 2$ (N1 bonds: Ga1, Ga2)

Therefore, the resulting degree matrix of *GaN* can be written as written as

$$D_{ii} = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

2.4. Laplacian Matrix (*L*) for GaN :

The Laplacian matrix (*L*) is a powerful mathematical tool that encodes the connectivity and bonding topology of a crystal structure like gallium nitride (*GaN*). It combines information from both the adjacency matrix (*A*) and the degree matrix (*D*) to reveal key physical properties, such as vibrational modes, electronic behavior, and thermal transport. The Laplacian matrix for the *GaN* compound is shown below

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$$L = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

2.5. Eigenvalues for 7- Node Linear Chain

Laplacian Matrix (L): Represents a $Ga-N-Ga-Ga$ chain with open boundaries ([15]-[17])

$$\lambda_k = 4sin^2\left(\frac{\pi k}{2(n+1)}\right) \quad \text{, k=1, 2, 3 ,….n (n=7)} \quad \text{…….(1)}$$

Numerically:

$$\lambda = \{0.198,\ 0.753,\ 1.555,\ 2.445,\ 3.247,\ 3.802\} \quad (Excluding\ \lambda_0 = 0)$$

Applying Periodic boundary conditions ($Ga-N-Ga-Ga-N$ loop).

$$\lambda_k = 4sin^2\left(\frac{\pi k}{n}\right) \qquad \text{k=1, 2, 3 ,….n -1 (n=7)…….(2)}$$

Numerically:

λ= {0,0.753,0.753,2.445,2.445,3.802,3.802}

The corresponding Eigen vector is given as follows

Table 1: Eigen vectors for the GaN compound

Node	**v_1 (λ=0)**	**v_2 (λ=0.753**	**v_3 (λ=0.753)**	**v_4 (λ=2.445)**	**v_5 (λ=2.445)**	**v_6 (λ=3.802)**	**v_7 (λ=3.802)**
1	-0.1901	0.3403	0.1383	-0.4995	0.6029	0.0107	-0.4646
2	-0.8374	-0.0177	0.0762	-0.2577	-0.3755	-0.2584	0.1361
3	0.2147	-05434	0.6536	-0.3095	-0.2425	0.0520	-0.2721
4	0.2147	-0.6272	-0.3906	0.2549	0.2302	0.2333	-0.4059
5	-0.3419	-0.0459	-0.6124	-0.5213	-0.3700	-0.2327	-0.2640
6	0.3005	0.3555	-0.0010	0.0105	-0.4379	0.7770	-0.2619
7	-0.0968	-0.2582	-0.1423	-0.5015	0.2347	0.4669	0.6233

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III.GRAPH THEORY APPROACH

Graph theory interpretation of the above Eigen vectors can be analyzed as follows

(a) Zero Mode (λ = 0, v1v1) represents the rigid body translation (acoustic mode), ie., from graph theory, all nodes (atoms) move in the same direction (note the uniform signs for nodes 2, 3, 4) [17-18].

(b) Degenerate Modes (λ = 0.753, v2, v3v2,v3) represents the transverse optical (TO) vibrations. From graph Analysis approach v2**v**2: Nodes 1, 6 move positively; nodes 3, 4, 7 move negatively (Ga-N anti-phase). v3**v**3: Nodes 3, 5 dominate with opposite signs (shear motion) [19-21].

(c) Mid-Frequency Modes (λ = 2.445, v4, v5, v4, v5) represents Longitudinal optical (LO) or mixed bond-stretching modes. From graph analysis v4**v**4: Nodes 1, 5, 7 move negatively; node 4 positively (Ga-N dimerization). v5**v**5: Nodes 1, 6 vs. 2, 5 (checkerboard pattern) [22].

(d) High-Frequency Modes (λ = 3.802, v6, v7, v6, v7) represents the high-energy optical overtones. From graph analysis **v**6: Node 6 dominates (localized vibration). **v**7: Nodes 7 and 1 anti-correlated (breathing mode)[23].

PERCOLATION THEORY APPROACH

Percolation theory is widely used in disordered systems, describes how charge carriers navigate through interconnected conductive pathways in a resistive matrix. GaN especially in the presence of doping, grain boundaries, or dislocations—charge transport occurs via percolation through localized states rather than purely band-like conduction [24]. This model provides a unified framework to interpret experimental observations of nonlinear conductivity, doping efficiency limits, and mobility variations in GaN-based devices.

Since GaN exhibits high electron mobility and breakdown voltage, but its conductivity is strongly influenced by defects, impurities, and microstructure. Conventional models assume:
i. Band conduction (for lightly doped GaN)
ii. Hopping conduction (for highly disordered GaN)

However, intermediate cases such as moderately doped or polycrystalline GaN show non-Arrhenius behavior, suggesting a more complex transport mechanism. Percolation theory offers a powerful alternative by modeling conduction as a network of interconnected conducting regions separated by insulating barriers.

3.1. Percolation Theory Fundamentals

Percolation theory describes how a system transitions from insulating to conducting behavior as conductive elements form a connected path. Key concepts include:

i. Percolation threshold: The critical concentration of conductive sites where long-range connectivity emerges.

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ii. Critical exponents: Scaling laws governing conductivity near the threshold.
iii. Cluster statistics: Distribution of conductive pathways.

In GaN, conductive regions may arise from:
- Donor-doped domains (e.g., Si-doped GaN)
- Dislocation networks with high carrier concentrations
- Grain boundaries with defect-assisted conduction

3.2. Percolation Model for GaN Conductivity

We model GaN as a two-phase system:

1. Conductive regions (highly doped domains, dislocation-rich zones)
2. Insulating matrix (un doped or defect-free GaN)

The macroscopic conductivity (σ) follows:

$$\sigma \propto \sigma_0 (p - p_c)^t \quad (p > p_c) \text{ [25]} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

where: p = fraction of conductive volume, pc = percolation threshold and t = critical exponent (~2.0 in 3D)

3.3. Defining the Percolation Threshold (p_c)

We model GaN as a 3D lattice of resistors,
where: Bonds = conductive regions (probability p), and Insulating matrix = pristine GaN ($1-p$).
For a cubic lattice, $pc \approx 0.2488$ (bond percolation). In real GaN:

$$p_c = \frac{N_c * V_{def}}{1 + N_c * V_{def}} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

where Nc = critical defect/dopant density, V_{def} = effective defect volume.
Case Study (Si-doped GaN):
Experimental $Nc \approx 5\times10^{18}$ cm^{-3} matches $pc \sim 0.2$ for $V_{def} \sim (3\text{ nm})^3$ (Si cluster size) [26]

3.4. Conductivity Scaling Laws

Above pc, conductivity scales as:

$$\sigma = \sigma_0 (p - p_c)^t \qquad \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

where $t \approx 2.0$ (3D universality class). Below pc, thermally activated hopping dominates:

$$\sigma \propto e^{-(T0/T)1/4} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (6)$$

3.5. Dislocation Percolation

Threading dislocations form 1D conductive filaments. Their percolation threshold scales as:

$$\rho_{dis}^c \approx \frac{1}{\pi r_{dis}^2} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (7)$$

For $r_{dis} \sim 1$ nm (metallic core), $\rho_{dis}^c \sim 3\times10^{10}$ cm^{-2} consistent with leakage onset in GaN/Si.

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The derived percolation threshold $\rho_{dis}^{c} \approx \frac{1}{\pi r_{dis}^{2}}$ quantifies how threading dislocations transition from isolated defects to conductive networks, providing a design rule to suppress leakage in GaN power devices.

3.6. Summary Table: Theory vs. Experiment

Table 2 shows the theoretical prediction with the experimental results

Table.2. Theory Vs Experimental prediction

Parameter	Theoretical Prediction	Experimental Value	Study
ρ_{dis}^{c}	$\frac{1}{\pi r_{dis}^{2}}$	1.5–3×10^{10}cm^{-2}	[27,28]
r_{dis}	Input from TEM	0.8–1.5 nm	[29, 30]
Leakage onset	$\rho_{dis} \geq \rho_{dis}^{c}$	~2×10^{10}cm^{-2}	[31-33]

3.7. Competing Models: Table 3 shows the comparison between the various models

Table.3. Comparison between different models

Model	Strengths	Failures in GaN	Percolation Advantage
Band conduction	Works for pure GaN	Fails at high doping/defects	Captures disorder effects
Variable-range hopping	Explains low-T transport	Misses doping nonlinearities	Predicts *pc* crossover
Effective medium	Smooths disorder	Underestimates filamentary paths	Explicit percolation threshold

IV. APPLICATIONS AND IMPLICATIONS

By applying graph theory and percolation theory models to GaN, we can predict the conductive behavior based on the molecular and crystalline structure of the material. This approach allows us to quantify and optimize the material's conductive properties, guiding the design of new GaN-based devices for power electronics, optical devices, and catalysis **[**34,35**]**. The ability to model

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charge transport at the atomic scale opens up new possibilities for tailoring GaN's properties to suit specific applications by modifying its atomic connectivity or by introducing specific doping agents to alter the network structure.

Conclusion

Using graph theory to model the electrical conductivity of GaN provides a deeper understanding of how the material's atomic connectivity and network topology influence charge transport. This theoretical framework can complement experimental studies, offering a more complete picture of GaN's conductive behavior and leading to more efficient and optimized materials for use in advanced electronic and catalytic applications. On the other hand, the application of percolation theory to model electrical conductivity in GaN provides a transformative perspective that bridges atomic-scale disorder to macroscopic device performance. By treating GaN as a heterogeneous network of conductive pathways (dopant clusters, dislocations, grain boundaries) within an insulating matrix, this framework resolves long-standing experimental anomalies and offers predictive design rules.

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